

Appendix G




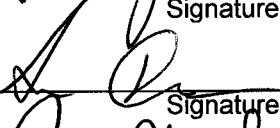
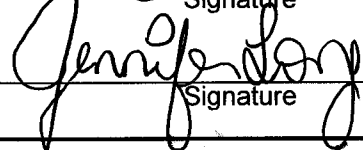
<p style="text-align: center;">NUCLEAR WASTE MANAGEMENT PROCEDURE</p> <p>Sandia National Laboratories</p>	<h2 style="margin: 0;">User's Manual Criteria</h2>	<p>Form Number: NP 19-1-6</p> <p>Page 1 of 1</p>
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Does the user's manual contain as appropriate:

- 1. **Software Name:** BRAGFLO
- 2. **Software Version:** 6.02
- 3. **Document Version:** 6.02
- 4. **ERMS #:** 558663

Prior to sign-off of the User's Manual, all items shall be appropriately addressed by the code sponsor so that "Yes" or "N/A" may be checked. Include this form as part of the User's Manual.

- 5. A statement(s) of functional requirements (consistent with those in the RD) and system limitations? Yes
- 6. An explanation of the mathematical model and numerical models, where applicable as based on code functionality? Yes N/A
- 7. Physical and mathematical assumptions, where applicable as based on code functionality? Yes N/A
- 8. The capabilities and limitations inherent in the software? Yes
- 9. Instructions that describe the user's interaction with the software? Yes
- 10. The identification of input parameters, formats, and valid ranges? Yes
- 11. Messages initiated as a result of improper input and how the user can respond? Yes
- 12. The identification and description of output specifications and formats? Yes
- 13. A description of any required training necessary to use the software? Yes
- 14. The identification of components of the code that were not tested? Yes N/A

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Information Only

User's Manual

for

BRAGFLO, Version 6.02

Document Version 6.02

ERMS# 558663

Information Only

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Acronyms

BRAGFLO	BRine And Gas FLOW code
CCA	Compliance Certification Application
CDB	CAMDAT Database
CRA	Compliance Recertification Application
DEC	Digital Electronic Corporation
DOE	U.S. Department of Energy
DRZ	Disturbed Rock Zone
EOS	Equation of State
PA	Performance Assessment
PAVT	Performance Assessment Verification Tests
PDE	Partial Differential Equation
PREBRAG	Preprocessor for BRAGFLO
POSTBRAG	Postprocessor for BRAGFLO
RKS	Redlich-Kwong-Suave
QA	Quality Assurance
QAP	Quality Assurance Procedure
RKS	Redlich-Kwong-Soave (gas equation of state)
VMS	Virtual Memory System (a DEC operating system)
WIPP	Waste Isolation Pilot Plant

1.0 INTRODUCTION

This document serves as a User's Manual for BRAGFLO Version 6.02. As such, it describes the purpose and function of the code, the user's interaction with the code, and the models and methods employed by the code. Examples of user-accessible input and output files are included for the user's convenience.

1.1 Software Identifier

Code Name: BRAGFLO
WIPP Prefix: BF2
Version: 6.02
Platform: Compaq FORTRAN 7.5 for OpenVMS AXP, version 8.2, on DEC Alpha.
The previous version of BRAGFLO was Version 6.0.
The previous version of the RD/VVP was Version 6.0, ERMS# 545014.

1.2 Points of Contact

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2.0 Functional Requirements

The functional requirements for BRAGFLO version 6.02 include all of those specified for BRAGFLO version 6.0 (Nemer 2006), with one change to requirement R.20, and are listed below.

- R.1 Input defining the problem to be run is read in, including mesh size, simulation time specifications, and output files to be used.
- R.2 The time and/or frequency of output to each output file and the variables whose values will be output are specified in the input.
- R.3 The code reads input defining the finite difference grid for the problem to be run, including values of Δx , Δy , and Δz , and elevations of grid block centers, or input parameters that allow BRAGFLO to calculate the elevations. These input parameters may also specify how the mesh is rotated or dipped relative to a reference right hand coordinate system.
- R.4 The default boundary conditions are no-flow conditions. BRAGFLO also allows constant pressure (Dirichlet) boundary conditions to be applied at specified grid blocks. The Dirichlet conditions fix the brine pressure and gas saturation at their initial values.
- R.5 The following initial conditions are specified on input at each grid block: brine pressure, brine saturation, iron concentration, the concentration of biodegradables and the MgO concentration.
- R.6 Parameters are input that controls the numerical behavior of BRAGFLO. These include specifications of convergence tolerances, iteration limits, upstream weighting control parameters, dependent variable increments used to calculate Jacobian element derivatives numerically, and the solver to be used. Two solvers are currently available, the original LU decomposition solver and the point successive over-relaxation (SOR) solver, and only the original LU decomposition solver is qualified for use in WIPP compliance calculations.
- R.7 Material maps at specified times are input. For each material, material properties are input, including two-phase flow parameters, intrinsic permeability's, reference condition porosities, and compressibility's. Also specified are the relative permeability and capillary pressure model to be used for each material. Furthermore, BRAGFLO allows for the change of pressure and saturation values, as well as the capability to turn off the chemistry reactions when materials change as specified by the .INP input file.
- R.8 Relative permeabilities and capillary pressure are calculated for each material using one of several available models. The compliance calculations will use both a modified Brooks-Corey model and a van Genuchten/Parker model. Some of the QA verification and validation tests use relative permeability models that are included in BRAGFLO specifically for those tests.

- R.9 A simplified rock fracture model allows the porosity and permeability to increase as pore pressure increases above a threshold value, simulating a fracture network. In the absence of fracturing, porosity may vary slightly with pressure due to rock compressibility effects.
- R.10 The Klinkenberg effect is included, allowing the gas-phase permeability to become elevated over the intrinsic brine-phase permeability at low pressures in low-permeability materials.
- R.11 Brine salinity, density at reference conditions, and compressibility are specified by input values, and the density of brine varies as a function of pressure.
- R.12 Gas properties are given by the Redlich-Kwong-Soave (RKS) equation of state (EOS). WIPP compliance calculations will use a single pure gas, H₂.
- R.13 Two chemical reactions are modeled in BRAGFLO: anoxic corrosion of iron and microbial degradation of cellulose. Both of these reactions produce gas (H₂) and consume brine according to specified stoichiometry. Reaction rates and stoichiometry are specified for brine-inundated conditions and for humid conditions. BRAGFLO reads the necessary parameters from the .INP input file.
- R.14 The effects of salt creep, whereby the surrounding halite closes in on the waste or other excavated regions, compressing them, may be simulated in BRAGFLO. Using this model, the porosity of the waste changes with time and brine pressure. The input file, containing the closure surface data (.CSD), is an ASCII input file that is read by BRAGFLO if creep closure is to be simulated as specified by a parameter in the ASCII input file (.INP). If creep closure is not to be simulated a dummy file must be included even though this dummy file will not be read. The information in the .CSD file, that is used in the validation of BRAGFLO, will be the same information that was incorporated into the BRAGFLO 4.10 executable file. BRAGFLO reads the necessary information from the .INP and .CSD input files.
- R.15 BRAGFLO numerically calculates the flow of two phases, brine and gas, in porous media as a function of time and space, using an implicit finite difference method with variable time step control.
- R.16 Well models in BRAGFLO allow simulation of wells with a single completion within the formations or porous media being modeled. The types of wells that can be modeled are constant injection or production rate wells and constant down-hole pressure wells. Well data are assigned values in the input control file.
- R.17 BRAGFLO simulates flow through heterogeneous as well as homogeneous porous media.
- R.18 BRAGFLO writes binary and ASCII output files. These files regurgitate much of the input file information as well as primary and secondary dependent variables at user specified frequencies or at specific times. Many output variables are user selected and defined.

- R.19 BRAGFLO provides the user with an error check on the consistency with how waste regions are specified.
- R.20 Six additional chemical reactions are modeled in BRAGFLO: sulfidation of iron hydroxide; sulfidation of iron; hydration of MgO; carbonation of MgO; carbonation of Mg(OH)₂; and conversion of hydromagnesite. Stoichiometry is specified for each reaction. BRAGFLO reads the necessary parameters from the .INP input file.
- R.21 Chemical rates of all seven reactions are zero below a specified cutoff value in brine saturation, which is set in the .INP input file.
- R.22 Chemical rates of all seven reactions are multiplied by their respective initial concentrations if specified by a flag in the .INP input file.
- R.23 BRAGFLO calculates the change in solid volume from the chemical reactions.
- R.24 BRAGFLO allows for the smooth change in permeability of materials with time, as specified by the .INP input file.
- R.25 Software: For input, this code reads the output file generated by the code PREBRAG.
- R.26 Software: For input, BRAGFLO reads an external file that contains the creep closure look-up table data.
- R.27 Software: The output of this code is read as input by the code POSTBRAG.

3.0 REQUIRED USER TRAINING AND/OR BACKGROUND

In order to run the BRAGFLO code successfully, the user will need a basic knowledge of

- OpenVMS
- Digital Command Language
- Sandia's CAMDAT database, (Gilkey, 2006a).

In addition, users should also have access to the WIPP cluster of Alpha microcomputers. To interpret the input to and results from BRAGFLO, users should have:

- knowledge of basic mathematics through calculus and computational linear algebra
- an understanding of two-phase flow in porous media.

4.0 Description of the Models and Methods

Quantification of the effects of gas and brine flow on radionuclide transport for undisturbed and disturbed conditions requires use of a two-phase flow code. For performance assessment at the WIPP repository, the U.S. Department of Energy (DOE) uses the two-phase flow code BRAGFLO to simulate brine and gas flow. The BRAGFLO code incorporates the effects of disposal room consolidation and closure, gas generation from corrosion and biodegradation reactions, brine consumption from corrosion, and inter-bed fracturing in response to gas pressure. This section develops the governing equations for BRAGFLO, its initial and boundary conditions, and the submodels incorporated in BRAGFLO that were developed specifically for performance assessment of the WIPP.

4.1 One-Dimensional Fluid Flow in Porous Media

Historically, BRAGFLO was developed as a two-phase flow model for petroleum production applications. For this reason, BRAGFLO uses terminology common to the petroleum industry. Further details of the concepts necessary for the finite difference solution of reservoir simulation problems are available in Peaceman (1977), Aziz and Settari (1979), and Thomas (1982).

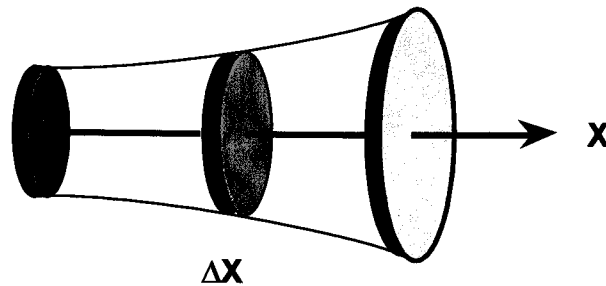


Figure 1. One dimensional reservoir with area-normal-to-flow as a function of x .

Consider now the material balance equation governing the flow of a fluid in a one-dimensional porous media. Figure 1 shows a one-dimensional reservoir with area-normal-to-flow as a function of x ; area = $A(x)$. The flow streamlines will actually flare in or out due to the variable area. However, we make the assumption that density and velocity are representative of average properties over the area normal to flow. From the reservoir, select an element of volume of incremental length Δx . Let

- Q = volume flow rate [l^3/t]
- ρ = fluid density [m/l^3]
- q = mass flow rate [m/t]
- v = flow velocity [l/t]
- ϕ = porosity [pore volume/bulk volume]
- A = normal cross-section area [l^2]

where the generic units are:

- m = mass
- l = length

t = time.

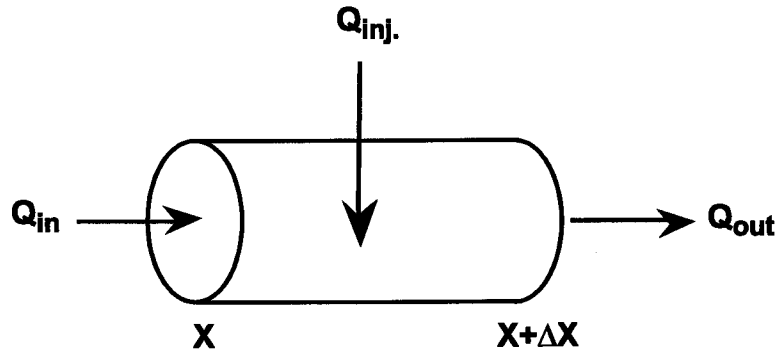


Figure 2. Element of volume of length Δx .

The mass rate and volume rate of flow are related by $q = \rho Q$. The sign convention on Q_{inj} is

$$Q_{inj} > 0, \text{ injection,} \quad (1)$$

$$Q_{inj} < 0, \text{ production.} \quad (2)$$

Also, Q_{inj} = volume rate/injected volume, which implies fluid injection is uniformly distributed over control volume $A\Delta x$. Mass balance requires that

$$q_{in} - q_{out} + q_{inj} A\Delta x = \text{change in fluid mass/time} \quad (3)$$

where

$$q_{inj} = \text{mass injection rate/unit volume.} \quad (4)$$

Now

$$q_{in} = (vA\rho)_x \quad (5)$$

$$q_{out} = (vA\rho)_{x+\Delta x} \quad (6)$$

and

$$\text{rate of change of fluid mass} = \frac{\partial}{\partial t}(\phi A\Delta x\rho) \quad (7)$$

The mass balance is then

$$(vA\rho)_x - (vA\rho)_{x+\Delta x} + q_{inj} A\Delta x = \frac{\partial}{\partial t}(\phi A\Delta x\rho) \quad (8)$$

Express the area as $A = \alpha(x)$, then dividing by Δx yields

$$\frac{(\alpha v\rho)_x - (\alpha v\rho)_{x+\Delta x}}{\Delta x} + \alpha q_{inj} = \frac{\partial}{\partial t}(\alpha\phi\rho). \quad (9)$$

In the limit as $\Delta x \rightarrow 0$, we get the material balance equation for one-dimensional single phase flow

$$-\frac{\partial}{\partial x}(\alpha v\rho) + \alpha q_{inj} = \frac{\partial}{\partial t}(\alpha\phi\rho). \quad (10)$$

4.2 Darcy's Law

For the viscous flow of a fluid through a porous medium the flow velocity is related to the fluid potential by Darcy's Law (Darcy, 1856) a mathematical model developed from empirical data gathered in experiments using a device similar to the one illustrated in Figure 3.

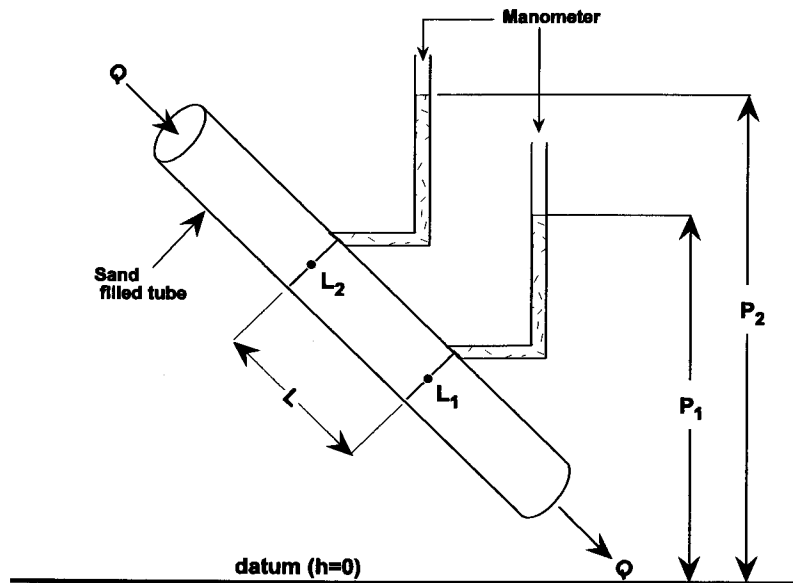


Figure 3. Experiment for illustration of Darcy's Law.

In Figure 3, Q is volumetric flow rate, and distance is measured in the positive x -direction, from L_2 to L_1 , where the fluid pressure is P_2 and P_1 , respectively. The height above a reference datum is h . The cross-sectional area is A , and the fluid has viscosity, μ , and density, ρ . The permeability of the porous medium is k . The differential form of Darcy's Law is:

$$Q = \frac{-kA}{\mu} \left(\frac{dP}{dx} + \rho g \frac{dh}{dx} \right). \quad (11)$$

The negative sign in Darcy's Law indicates that flow is in the direction of decreasing pressure or height above the datum.

The units used in BRAGFLO are

$$\begin{aligned} Q &= \text{m}^3/\text{s} \\ k &= \text{m}^2 \\ A &= \text{m}^2 \\ \frac{dP}{dx} &= \text{Pa}/\text{m} \\ \mu &= \text{Pa} \cdot \text{s} \\ \rho &= \text{kg}/\text{m}^3 \\ \frac{dh}{dx} &= \text{m}/\text{m} \\ g &= \text{m}/\text{s}^2. \end{aligned}$$

Velocity is given by

$$v = \frac{Q}{A} = -\frac{k}{\mu} \left(\frac{dP}{dx} + \rho g \frac{dh}{dx} \right), \quad (12)$$

where v is called the Darcy velocity or superficial flow velocity. The quantity

$$V = \frac{Q}{A\phi} = \frac{v}{\phi} = \frac{\text{bulk volume}}{\text{normal area}} / \text{time} \quad (13)$$

is called the interstitial or average linear velocity, where ϕ is the formation porosity.

The distinction between the Darcy velocity and the interstitial velocity is demonstrated in Figure 4. Assume fluid in the unit bulk volume at the left end of the reservoir is displaced by a piston over unit time into a media with porosity $\phi = 0.20$. The cubic meter of fluid will occupy 5 m³ of the porous material and the fluid will advance to a position 5 meters from the interface. The velocity of the fluid in the bulk volume is Q/A , or the Darcy velocity, while the fluid velocity in the porous material is $Q/(A\phi)$, or the interstitial velocity. For example, if a tracer element were introduced into the porous material, it would travel at the interstitial velocity. The Darcy velocity is the rate at which the bulk volume is transported.

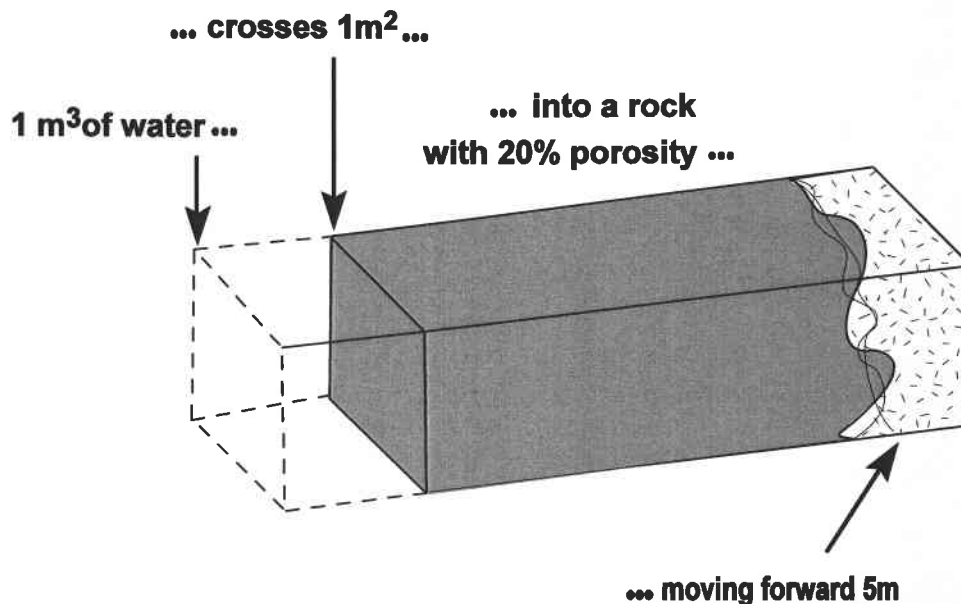


Figure 4. Volume versus porous media displacement.

4.3 Permeability Tensor, Darcy's Law, and Material Balance in Higher Dimension

The permeability of a geological formation can be direction dependent (anisotropic). For example, a sedimentary formation may consist of uniform sand or lime laminae of high permeability alternating with thin, uniform layers of silty, shaley laminae of low permeability. The large scale permeability characteristics can be approximated as uniformly anisotropic. That is, the layered system is replaced by a homogeneous system having permeability k_1 parallel to the

plane of the laminae and k_2 normal to this plane. Further, the direction of the laminae may not be parallel or normal to the formation boundary as evident in a cross-bedded structure.

Figure 5 shows two Cartesian coordinate systems (ξ, η) and (x, y) . Suppose the principal permeabilities are given with respect to (ξ, η) system with k_1 the permeability in the ξ direction and k_2 the permeability in the η direction. Further, assume the reservoir geometry is aligned with respect to the (x, y) system, which implies that the fluid flow equations are to be formulated with respect to the (x, y) -axes.

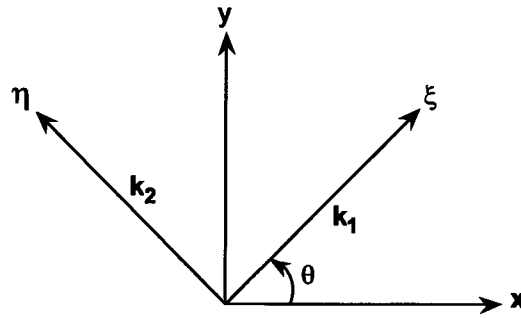


Figure 5. Permeability with anisotropic values k_1 and k_2 in direction ξ and η

The coordinate transformation from the (ξ, η) system to the (x, y) system is

$$\begin{aligned} x &= \xi \cos \theta - \eta \sin \theta \\ y &= \xi \sin \theta + \eta \cos \theta \end{aligned} \tag{14}a,b$$

If $\hat{\mathbf{i}}_\xi$ and $\hat{\mathbf{i}}_\eta$ represent the unit vectors in the ξ, η -directions, respectively, then the Darcy velocity vector (ignoring gravitational effects for now) is

$$\hat{\mathbf{v}} = -\frac{k_1}{\mu} \frac{\partial P}{\partial \xi} \hat{\mathbf{i}}_\xi - \frac{k_2}{\mu} \frac{\partial P}{\partial \eta} \hat{\mathbf{i}}_\eta. \tag{15}$$

The coordinate transformation maps the unit vectors into

$$\hat{\mathbf{i}}_\xi \rightarrow \cos \theta \hat{\mathbf{i}}_x + \sin \theta \hat{\mathbf{i}}_y \tag{16}$$

and

$$\hat{\mathbf{i}}_\eta \rightarrow -\sin \theta \hat{\mathbf{i}}_x + \cos \theta \hat{\mathbf{i}}_y. \tag{17}$$

The chain rule gives

$$\frac{\partial P}{\partial \xi} = \cos \theta \frac{\partial P}{\partial x} + \sin \theta \frac{\partial P}{\partial y} \tag{18}$$

and

$$\frac{\partial P}{\partial \eta} = -\sin \theta \frac{\partial P}{\partial x} + \cos \theta \frac{\partial P}{\partial y}. \tag{19}$$

Then the Darcy velocity is

$$\begin{aligned} \hat{v} = & \frac{-k_1}{\mu} \left(\cos \theta \frac{\partial P}{\partial x} + \sin \theta \frac{\partial P}{\partial y} \right) (\cos \theta \hat{\mathbf{i}}_x + \sin \theta \hat{\mathbf{i}}_y) \\ & - \frac{k_2}{\mu} \left(-\sin \theta \frac{\partial P}{\partial x} + \cos \theta \frac{\partial P}{\partial y} \right) (-\sin \theta \hat{\mathbf{i}}_x + \cos \theta \hat{\mathbf{i}}_y) \end{aligned} \quad (20)$$

The vector components of the Darcy velocity are

$$v_x = \frac{-k_1}{\mu} \left(\cos^2 \theta \frac{\partial P}{\partial x} + \sin \theta \cos \theta \frac{\partial P}{\partial y} \right) - \frac{k_2}{\mu} \left(\sin^2 \theta \frac{\partial P}{\partial x} - \sin \theta \cos \theta \frac{\partial P}{\partial y} \right), \quad (21)$$

$$v_y = \frac{-k_1}{\mu} \left(\sin \theta \cos \theta \frac{\partial P}{\partial x} + \sin^2 \theta \frac{\partial P}{\partial y} \right) - \frac{k_2}{\mu} \left(-\sin \theta \cos \theta \frac{\partial P}{\partial x} + \cos^2 \theta \frac{\partial P}{\partial y} \right). \quad (22)$$

The dependence of the Darcy velocity components on pressure gradients in both x - and y -directions will add significantly to the complexity of the material balance equation in 2-dimensions. A similar analysis with more complexity could be performed in 3-dimensions.

A significant simplification occurs if the directions of the permeability tensor are aligned with the reservoir coordinate axis; that is, $\theta = 0$. If $\theta = 0$, then

$$v_x = \frac{-k_1}{\mu} \frac{\partial P}{\partial x} \quad \text{and} \quad v_y = \frac{-k_2}{\mu} \frac{\partial P}{\partial y}. \quad (23)$$

BRAGFLO makes this assumption. Thus, in three dimensions with anisotropic permeability, the components of the Darcy velocity are

$$v_x = \frac{-k_x}{\mu} \frac{\partial P}{\partial x}, \quad v_y = \frac{-k_y}{\mu} \frac{\partial P}{\partial y}, \quad v_z = \frac{-k_z}{\mu} \frac{\partial P}{\partial z} \quad (24)$$

where k_x , k_y , k_z are input permeabilities in the direction of the corresponding coordinate axes.

When the effect of gravity is included, the components of the Darcy velocity become

$$v_x = \frac{-k_x}{\mu} \left(\frac{\partial P}{\partial x} + \rho g \frac{\partial h}{\partial x} \right), \quad v_y = \frac{-k_y}{\mu} \left(\frac{\partial P}{\partial y} + \rho g \frac{\partial h}{\partial y} \right), \quad v_z = \frac{-k_z}{\mu} \left(\frac{\partial P}{\partial z} + \rho g \frac{\partial h}{\partial z} \right) \quad (25)$$

To generalize the flow equation to higher dimension, we replace the flux term with (Peaceman, 1977)

$$\begin{aligned} & \nabla \cdot \left[\frac{\alpha \rho [k]}{\mu} (\nabla P + \rho g \nabla h) \right] \\ & = \left(\frac{\partial}{\partial x} \hat{\mathbf{i}} + \frac{\partial}{\partial y} \hat{\mathbf{j}} + \frac{\partial}{\partial z} \hat{\mathbf{k}} \right) \cdot \left[\frac{\alpha \rho k_x}{\mu} \left(\frac{\partial P}{\partial x} + \rho g \frac{\partial h}{\partial x} \right) \hat{\mathbf{i}} + \frac{\alpha \rho k_y}{\mu} \left(\frac{\partial P}{\partial y} + \rho g \frac{\partial h}{\partial y} \right) \hat{\mathbf{j}} + \frac{\alpha \rho k_z}{\mu} \left(\frac{\partial P}{\partial z} + \rho g \frac{\partial h}{\partial z} \right) \hat{\mathbf{k}} \right] \end{aligned}$$

$$= \frac{\partial}{\partial x} \left[\frac{\alpha \rho k_x}{\mu} \left(\frac{\partial P}{\partial x} + \rho g \frac{\partial h}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[\frac{\alpha \rho k_y}{\mu} \left(\frac{\partial P}{\partial y} + \rho g \frac{\partial h}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[\frac{\alpha \rho k_z}{\mu} \left(\frac{\partial P}{\partial z} + \rho g \frac{\partial h}{\partial z} \right) \right] \quad (26)$$

where

- [k] = permeability tensor,
- α = area normal to flow direction in one dimension (x), or
- = thickness normal to flow plane in two-dimensions (x, y), or
- = 1 in three-dimensions (x, y, z).

The three-dimensional flow of a single fluid incorporating Darcy's law is

$$\frac{\partial}{\partial x} \left[\frac{\alpha \rho k_x}{\mu} \left(\frac{\partial P}{\partial x} + \rho g \frac{\partial h}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[\frac{\alpha \rho k_y}{\mu} \left(\frac{\partial P}{\partial y} + \rho g \frac{\partial h}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[\frac{\alpha \rho k_z}{\mu} \left(\frac{\partial P}{\partial z} + \rho g \frac{\partial h}{\partial z} \right) \right] + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \phi \rho) \quad (27)$$

4.4 Equation of State

From the previous section the three dimensional flow of a single phase fluid is governed by the equation

$$\frac{\partial}{\partial x} \left[\frac{\alpha \rho k_x}{\mu} \left(\frac{\partial P}{\partial x} + \rho g \frac{\partial h}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[\frac{\alpha \rho k_y}{\mu} \left(\frac{\partial P}{\partial y} + \rho g \frac{\partial h}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[\frac{\alpha \rho k_z}{\mu} \left(\frac{\partial P}{\partial z} + \rho g \frac{\partial h}{\partial z} \right) \right] + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \phi \rho) \quad (28)$$

This equation has two dependent variables, pressure, P , and density, ρ . Independent variables are space (x, y, z) and time (t). We must relate ρ and P and hence eliminate one of the dependent variables. This problem is generally treated over three fluid regimes:

- incompressible fluid ($\rho = \text{constant}$)
- slightly compressible fluid (water, oil)
- highly compressible fluid (gas)

The incompressible fluid assumption is not valid for most applications and will not be considered.

Slightly compressible fluid assumes:

$$\left(\frac{\partial \rho}{\partial P} \right)_T = c \rho, \quad (29)$$

where c is fluid compressibility. For ideal fluid $c = \text{constant}$. Then the differential equation can be solved as

$$\rho = \rho_o \exp[c(P - P_o)] \quad (30)$$

where ρ_o is density at reference pressure P_o . This is the equation BRAGFLO uses to evaluate brine density.

Recall the series for the exponential function

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots \quad (31)$$

and if x is close to zero

$$e^x \cong 1 + x. \quad (32)$$

Therefore, if $c(P-P_o)$ is relatively small, then

$$\rho \cong \rho_o [1 + c(P - P_o)]. \quad (33)$$

This linearization is sometimes used as an approximation to the exponential density function.

A highly compressible fluid such as gas requires a real gas equation of state

$$\rho = \rho(P, T) \quad (34)$$

which, for isothermal flow, gives density as a function of pressure. BRAGFLO uses the Redlich-Kwong-Soave equation of state to relate gas density to pressure (Walas, 1985).

The formation rock behaves as a slightly compressible material, which yields an expression for porosity analogous to the expression for brine density. In BRAGFLO the formation porosity is evaluated as

$$\phi = \phi_o \exp[c_r(P - P_o)] \quad (35)$$

where ϕ_o is the porosity at reference pressure P_o and c_r denotes rock compressibility.

With the equation of state the material balance equation is formulated and solved in terms of a single dependent variable, namely pressure. Note that the partial differential equation (PDE) is nonlinear. Non-linearity occurs from several sources:

- nonlinear dependence of density on pressure
- product of density and pressure gradient
- product of porosity and density in accumulation term since porosity is pressure dependent due to rock compressibility
- viscosity could be pressure dependent for gases, however, BRAGFLO treats viscosity constant for both water and gas.

For the one-dimensional case of the equation presented at the end of Section 4.3,

$$\frac{\partial}{\partial x} \left[\frac{\alpha \rho k_x}{\mu} \left(\frac{\partial P}{\partial x} + \rho g \frac{\partial h}{\partial x} \right) \right] + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \phi \rho), \quad (36)$$

The material balance equation (PDE) requires:

Initial conditions:

$$P(x, 0) = f(x), \quad 0 \leq x \leq L \quad (37)$$

and

Boundary conditions:

$$P(0, t) = g_o(t), \quad P(L, t) = g_L(t), \quad t \geq 0 \quad (38)$$

or

$$\frac{\partial P}{\partial x}(0,t) = g_o(t), \quad \frac{\partial P}{\partial x}(L,t) = g_L(t) \quad t \geq 0. \quad (39)$$

The first type of boundary condition in which the solution is specified at the boundary is called a Dirichlet boundary condition. The condition in which the pressure gradient is specified is called a Neumann boundary condition. Generally, most reservoir simulations assume $\partial P/\partial x = 0$ on the boundary (no-flow boundary condition). The boundary condition may be of mixed type. BRAGFLO assumes a no-flow Neumann type boundary condition at all exterior grid boundaries.

BRAGFLO has the capability of maintaining (Dirichlet condition) pressure and/or saturation at specified grid blocks. This allows the maintenance of initial conditions at far field locations in the upper formations such as the Culebra.

4.5 Finite Difference and Discretization of Material Balance Equation

Recall Taylor's formula with remainder for a function f expanded about x_o :

$$\begin{aligned} f(x) = & f(x_o) + f'(x_o)(x - x_o) + \frac{f^{(2)}(x_o)}{2!}(x - x_o)^2 \\ & + \dots + \frac{f^{(n)}(x_o)}{n!}(x - x_o)^n + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_o)^{n+1} \end{aligned} \quad (40)$$

where ξ is the interval between x and x_o . Thus

$$f(x) = p(x) + R_n(x, x_o) \quad (41)$$

or

$$f(x) - p(x) = R_n(x, x_o), \quad (42)$$

where $p(x)$ is a polynomial approximation to f and the remainder term is the error.

If $f^{(n+1)}$ is continuous on some interval $[a,b]$ containing (x, x_o) , then $f^{(n+1)}$ is bounded,

$$|f^{(n+1)}(x)| \leq M, \quad (43)$$

and

$$|f(x) - p(x)| \leq C|x - x_o|^{n+1} \quad (44)$$

Therefore, as $x \rightarrow x_o$, the error goes to zero like $(x - x_o)^{n+1}$. Consider the following derivative approximations. First order forward difference requires the Taylor formula:

$$f(x) = f(x_o) + f'(x_o)(x - x_o) + R_2(x, x_o) \quad (45)$$

Let $x = x_o + h$, then

$$\left| \frac{f(x_o + h) - f(x_o)}{h} - f'(x_o) \right| = \left| \frac{R_2(x, x_o)}{h} \right| \leq \frac{Ch^2}{h} = Ch. \quad (46)$$

The difference approximation

$$f'(x_o) \cong \frac{f(x_o + h) - f(x_o)}{h} \tag{47}$$

is said to be first order in h . This type of approximation is used for the time derivative.

Second order central approximation:

$$f(x_o + h) = f(x_o) + f'(x_o)h + \frac{f^{(2)}(x_o)}{2!}h^2 + R_3(x_o, x_o + h) \tag{48}$$

$$f(x_o - h) = f(x_o) - f'(x_o)h + \frac{f^{(2)}(x_o)}{2!}h^2 + R_3(x_o, x_o - h) \tag{49}$$

where subtraction yields

$$f(x_o + h) - f(x_o - h) = 2hf'(x_o) + R_3(x_o, x_o + h) - R_3(x_o, x_o - h). \tag{50}$$

This is rearranged to give:

$$\frac{f(x_o + h) - f(x_o - h)}{2h} - f'(x_o) = \frac{R_3(x_o, x_o + h) - R_3(x_o, x_o - h)}{2h} \tag{51}$$

which produces the estimate

$$\left| \frac{f(x_o + h) - f(x_o - h)}{2h} - f'(x_o) \right| \leq \frac{Ch^3}{h} = Ch^2. \tag{52}$$

Therefore, the difference approximation $\frac{f(x_o + h) - f(x_o - h)}{h}$ is a second order approximation to $f'(x_o)$.

Consider discretization of the one-dimensional material balance equation:

$$\frac{\partial}{\partial x} \left[\frac{\alpha \rho k_x}{\mu} \left(\frac{\partial P}{\partial x} \right) \right] + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \phi \rho) \tag{53}$$

where we assume the gradient of the depth, dh/dx is zero.

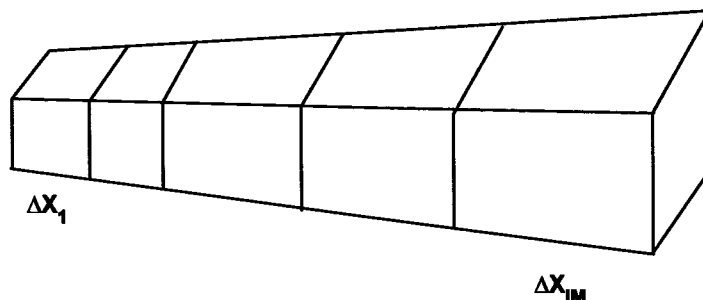


Figure 6. Partition interval $[0,L]$ into IM subintervals.

Space discretization requires the partition of the interval $[0,L]$ into IM subintervals with length $\Delta x_i, i=1, 2, \dots, IM$, as shown in Figure 6. Consider an arbitrary grid block i and its neighbors $i-1, i+1$ as shown in Figure 7.

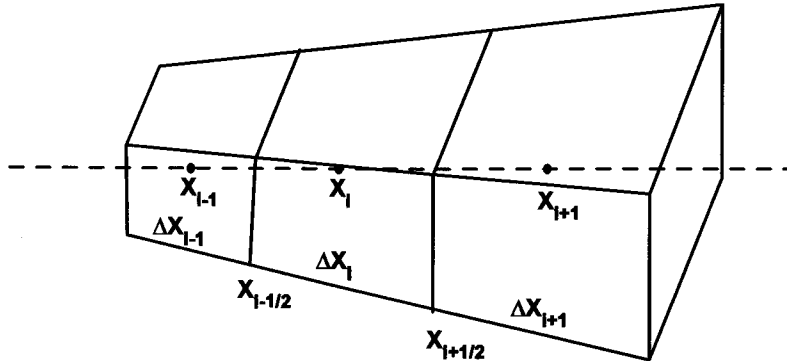


Figure 7. Depiction of arbitrary grid block.

We reference the location of the grid block interfaces as

$x_{i-1/2}$ = location of interface between $i-1$ and i ,

$x_{i+1/2}$ = location of interface between i and $i+1$.

For example,

$$x_{i-1/2} = x_{i-1} + \Delta x_{i-1/2}. \quad (54)$$

On the i^{th} grid block the partial derivative in the flux term is approximated by the 2nd order correct finite difference

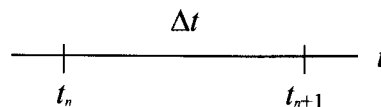
$$\frac{\partial}{\partial x} \left(\frac{\alpha k \rho}{\mu} \frac{\partial P}{\partial x} \right) \cong \frac{\left(\frac{\alpha k \rho}{\mu} \frac{\partial P}{\partial x} \right)_{i+1/2} - \left(\frac{\alpha k \rho}{\mu} \frac{\partial P}{\partial x} \right)_{i-1/2}}{\Delta x_i} \quad (55)$$

The partials are approximated at the interface by the 2nd order correct finite difference

$$\left(\frac{\alpha k \rho}{\mu} \frac{\partial P}{\partial x} \right)_{i-1/2} = \left(\frac{\alpha k \rho}{\mu} \right)_{i-1/2} \frac{P_i - P_{i-1}}{x_i - x_{i-1}}. \quad (56)$$

A similar expression exists at $i + 1/2$. If the gridding is non-uniform then the above approximations are no longer 2nd order correct.

Time discretization is as shown below.



Assume the solution is known at time t_n , and we wish to compute a solution at time t_{n+1} with time step size $\Delta t = t_{n+1} - t_n$. The time discretization of the accumulation term in the i^{th} grid block uses the first order correct finite difference

$$\frac{\partial}{\partial t} (\alpha\phi\rho) \cong \frac{(\alpha\phi\rho)_i^{n+1} - (\alpha\phi\rho)_i^n}{\Delta t}, \quad (57)$$

where the superscript references the time index. The fully discretized system of equations can be written as

$$\begin{aligned} & \frac{(\alpha\phi\rho)_i^{n+1} - (\alpha\phi\rho)_i^n}{\Delta t} - \frac{1}{\Delta x_i} \left(\frac{\alpha k \rho}{\mu} \right)_{i+1/2} \frac{P_{i+1} - P_i}{x_{i+1} - x_i} \\ & + \frac{1}{\Delta x_i} \left(\frac{\alpha k \rho}{\mu} \right)_{i-1/2} \frac{P_i - P_{i-1}}{x_i - x_{i-1}} - \alpha_i (q_{inj})_i = 0, \quad i = 1, 2, \dots, IM \end{aligned} \quad (58)$$

In this equation, the time level is not indicated on the pressure and pressure dependent variables in the flux and injection terms.

If all the pressures and pressure dependent variables in the flux and source/sink terms are evaluated at the beginning of the time step, $t = t_n$, then the formulation is called explicit. If these quantities are evaluated at the end of the time step, $t = t_{n+1}$ the formulation is called implicit.

The numerical solution of the material balance equation starts at initial time with specified initial pressures. The evaluation of the pressure solution in time requires at each time step the solution of a system of nonlinear algebraic equations for the grid block pressures. The error introduced by the discretization of the continuum equation is called truncation error. Errors will also be introduced in the nonlinear equation solver since it will not solve the system exactly (see Subsection 4.6, Newton-Raphson Method). Another source of error involves the choice of discretization. A numerical artifact of the solution of evolution equations is that small errors introduced at early time can either be damped with time (stable) or grow with time (unstable). The errors in an unstable solution will usually grow large enough to dominate the solution with numerical noise. The numerical stability of a discretization can sometimes depend of the size of the space discretization (Δx) relative to the time discretization (Δt). In this case, the method is said to be conditionally stable.

In the above formulations (explicit, implicit) we observe that

Formulation Advantages:

- * Explicit is simplistic computationally.
- * Implicit is unconditionally stable.

Formulation Disadvantages:

- * Implicit is complex computationally.
- * Explicit is conditionally stable.

The stability question dictates that the BRAGFLO formulation be fully implicit. The evaluation of the inter-block flux coefficients at $x \pm 1/2$ will be discussed in Subsection 4.8, Two Phase Flow.

4.6 Newton-Raphson Method for Solution of Nonlinear Algebraic Equations

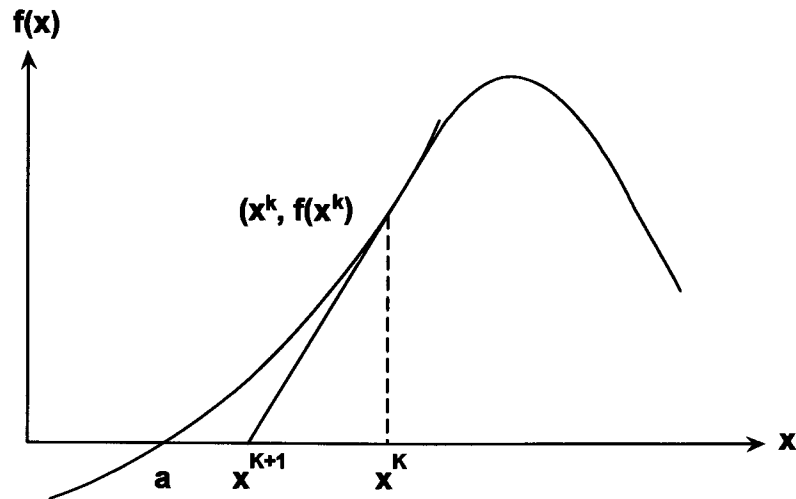


Figure 8. Newton-Raphson method.

Consider a real valued function of a real variable (scalar case). A root of f is a value $x = a$ such that $f(a) = 0$. Let x^k be an approximation to the root of f (k^{th} iterate approximation). Expand $f(x)$ in a Taylor series about x^k :

$$f(x) = f(x^k) + f'(x^k)(x - x^k) + \frac{f^{(2)}(x^k)}{2!} (x - x^k)^2 + \dots = 0. \quad (59)$$

Replace the nonlinear root problem with the linear approximation:

$$f(x^k) + f'(x^k)(x - x^k) = 0 \quad (60)$$

with solution $x = x^{k+1}$. Define

$$\delta x^k = x^{k+1} - x^k \quad (61)$$

Then

$$\delta x^k = -\frac{f(x^k)}{f'(x^k)}, \quad (62)$$

and

$$x^{k+1} = x^k + \delta x^k. \quad (63)$$

The Newton-Raphson iteration requires an initial guess to the root. In Figure 8 it appears from the geometry that the iteration would proceed to the root of f . If the initial guess was not close to the solution, such as to the right of the maximum in Figure 8, then the iteration may not converge, or it could converge to another solution. When solving the system of nonlinear material balance equations over a time step, the solution at the beginning of the time step is used as an initial guess for the Newton-Raphson iteration.

In general, consider a system of n nonlinear equations (64) in n unknowns:

$$\begin{aligned}
 f_1(x_1, \dots, x_n) &= 0 \\
 f_2(x_1, \dots, x_n) &= 0 \\
 &\vdots \\
 f_n(x_1, \dots, x_n) &= 0
 \end{aligned} \tag{64}$$

In vector notation, the system is written

$$\mathbf{F}(x_1, \dots, x_n) = \begin{pmatrix} f_1(x_1, \dots, x_n) \\ \vdots \\ f_n(x_1, \dots, x_n) \end{pmatrix} = \mathbf{0}, \tag{65}$$

and further, if $\hat{\mathbf{x}} = (x_1, \dots, x_n)$, then $\mathbf{F}(\hat{\mathbf{x}}) = \mathbf{0}$ is equivalent to (64).

Consider Newton-Raphson for $n = 2$. Let (x_1^k, x_2^k) be an approximation to the root of

$$\begin{aligned}
 f_1(x_1, x_2) &= 0 \\
 f_2(x_1, x_2) &= 0.
 \end{aligned} \tag{66)a,b$$

The Taylor series through linear terms expanded about $(x_1^k, x_2^k) = \hat{\mathbf{x}}^k$ are

$$\begin{aligned}
 f_1(x_1, x_2) &= f_1(x_1^k, x_2^k) + \frac{\partial f_1}{\partial x_1}(x_1^k, x_2^k)(x_1 - x_1^k) + \frac{\partial f_1}{\partial x_2}(x_1^k, x_2^k)(x_2 - x_2^k) \\
 f_2(x_1, x_2) &= f_2(x_1^k, x_2^k) + \frac{\partial f_2}{\partial x_1}(x_1^k, x_2^k)(x_1 - x_1^k) + \frac{\partial f_2}{\partial x_2}(x_1^k, x_2^k)(x_2 - x_2^k).
 \end{aligned} \tag{67)a,b$$

Replace the system of nonlinear equations in equation (66)a,b by the linear system

$$\begin{aligned}
 \frac{\partial f_1}{\partial x_1}(\hat{\mathbf{x}}^k)(x_1^{k+1} - x_1^k) + \frac{\partial f_1}{\partial x_2}(\hat{\mathbf{x}}^k)(x_2^{k+1} - x_2^k) &= -f_1(\hat{\mathbf{x}}^k) \\
 \frac{\partial f_2}{\partial x_1}(\hat{\mathbf{x}}^k)(x_1^{k+1} - x_1^k) + \frac{\partial f_2}{\partial x_2}(\hat{\mathbf{x}}^k)(x_2^{k+1} - x_2^k) &= -f_2(\hat{\mathbf{x}}^k).
 \end{aligned} \tag{68)a,b$$

Define the change in iterate values

$$\begin{aligned}
 \delta x_1 &= x_1^{k+1} - x_1^k \\
 \delta x_2 &= x_2^{k+1} - x_2^k.
 \end{aligned} \tag{69)a,b$$

Then the above linear system is written

$$\frac{\partial f_1}{\partial x_1}(\hat{\mathbf{x}}^k)\delta x_1 + \frac{\partial f_1}{\partial x_2}(\hat{\mathbf{x}}^k)\delta x_2 = -f_1(\hat{\mathbf{x}}^k)$$

$$\frac{\partial f_2}{\partial x_1}(\hat{\mathbf{x}}^k)\delta x_1 + \frac{\partial f_2}{\partial x_2}(\hat{\mathbf{x}}^k)\delta x_2 = -f_2(\hat{\mathbf{x}}^k). \quad (70)\text{a,b}$$

The coefficient matrix

$$\mathbf{J}(\hat{\mathbf{x}}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\hat{\mathbf{x}}) & \frac{\partial f_1}{\partial x_2}(\hat{\mathbf{x}}) \\ \frac{\partial f_2}{\partial x_1}(\hat{\mathbf{x}}) & \frac{\partial f_2}{\partial x_2}(\hat{\mathbf{x}}) \end{pmatrix} \quad (71)$$

is called the Jacobian matrix for the nonlinear system.

Then the $(k+1)^{\text{th}}$ iterative step of the Newton-Raphson method is

$$\mathbf{J}(\hat{\mathbf{x}}^k)\delta\hat{\mathbf{x}} = -\mathbf{F}(\hat{\mathbf{x}}^k) \quad (72)$$

or

$$\delta\hat{\mathbf{x}} = -\mathbf{J}^{-1}(\hat{\mathbf{x}}^k)\mathbf{F}(\hat{\mathbf{x}}^k) \quad (73)$$

and

$$\hat{\mathbf{x}}^{k+1} = \hat{\mathbf{x}}^k + \delta\hat{\mathbf{x}}. \quad (74)$$

For a system of n equations in n unknowns the Jacobian matrix generalizes to

$$\mathbf{J}(\hat{\mathbf{x}}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\hat{\mathbf{x}}) \cdots \frac{\partial f_1}{\partial x_n}(\hat{\mathbf{x}}) \\ \vdots \\ \frac{\partial f_n}{\partial x_1}(\hat{\mathbf{x}}) \cdots \frac{\partial f_n}{\partial x_n}(\hat{\mathbf{x}}) \end{pmatrix} \quad (75)$$

or

$$J(\hat{\mathbf{x}})_{i,j} = \frac{\partial f_i}{\partial x_j}(\hat{\mathbf{x}}). \quad (76)$$

The computation procedure in Newton-Raphson method computes the Jacobian matrix, $\mathbf{J}(\hat{\mathbf{x}}^k)$, and the function vector, $\mathbf{F}(\hat{\mathbf{x}}^k)$. The matrix inversion is equivalent to the solution of a system of linear equations which returns the changes in iterate values. The iterates are then updated.

When analytical derivatives are not tractable, Newton-Raphson uses difference quotient approximation for partials

$$\frac{\partial f_i}{\partial x_j}(\hat{\mathbf{x}}) = \frac{f_i(x_1, \dots, x_j + \Delta x_j, \dots, x_n) - f_i(x_1, \dots, x_n)}{\Delta x_j} \quad (77)$$

The major computational effort involves the function evaluations. The above numerical approach to the Jacobian requires n^2+n evaluations of the function f .

If the Jacobian is evaluated by an analytic derivative then any change in the formulation of properties would require significant code changes. Also, some properties, see Characteristic Curves (Subsection 4.9), use different model descriptions with user input control. In this case it would be difficult to implement the analytic derivative treatment. For these reasons BRAGFLO uses the difference approximation for the Jacobian evaluation.

The modified Newton-Raphson algorithm is

$$\mathbf{J}(\hat{\mathbf{x}}^1)\delta\hat{\mathbf{x}} = -\mathbf{F}(\hat{\mathbf{x}}^k), \quad k = 1, 2, \dots, \quad (78)$$

that is, the Jacobian is not updated each iteration. In BRAGFLO the user can specify from input directives the iteration frequency for the Jacobian evaluation.

Consider now the solution of the nonlinear flow equation. The i^{th} equation represents material balance in i^{th} grid block. Newton-Raphson iteration requires solution of the linear system

$$\begin{bmatrix} J_{11} & J_{12}\cdots & J_{1IM} \\ J_{21} & J_{22}\cdots & J_{2IM} \\ \vdots & & \\ J_{IM1} & J_{IM2}\cdots & J_{IMIM} \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta p_2 \\ \vdots \\ \delta p_{IM} \end{bmatrix} = - \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_{IM} \end{bmatrix} \quad (79)$$

and $p_i^{(k+1)} = p_i^{(k)} + \delta p_i$ where Jacobian and right hand side are evaluated at k^{th} iteration pressures. If the Newton-Raphson iteration converges then

$$\lim_{k \rightarrow \infty} p_i^{(k)} = p_i^{n+1}. \quad (80)$$

When testing for convergence during the Newton-Raphson iteration, the following test criteria are applied uniformly over all grid blocks:

- Test gas saturation and brine pressure for physically real values.
- Test if the change in gas saturation over an iteration is sufficiently small.
- Test if the gas material balance equation is satisfied.
- Test if the change in brine pressure over an iteration is sufficiently small.
- Test if the brine material balance equation is satisfied.
- Test if the changes in gas saturation and brine pressure over the time step are sufficiently small.

See Subsection 7.2.7 for input parameters that specify when convergence has been obtained or that affect the rate of convergence.

From the one-dimensional flow equations we note the Jacobian matrix has a tridiagonal structure

$$\begin{bmatrix} J_{11} & J_{12} & 0 & \dots & \dots & \dots & 0 \\ J_{21} & J_{22} & J_{23} & & & & \\ \vdots & \vdots & \vdots & \ddots & & & \\ 0 & \dots & J_{i,i-1} & J_{ii} & J_{i,i+1} & \dots & 0 \\ \vdots & & \vdots & \vdots & \vdots & & \\ 0 & \dots & & & J_{IM,IM-1} & J_{IM,IM} & \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta p_2 \\ \vdots \\ \delta p_i \\ \vdots \\ \delta p_{IM} \end{bmatrix} = - \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_i \\ \vdots \\ F_{IM} \end{bmatrix} \quad (81)$$

For both storage and computational considerations the linear equation solver should take advantage of the banded structure. This is true for the BRAGFLO direct solvers.

4.7 Discretization in Two-Dimensions

Consider the two-dimensional flow equation with gravitational effects neglected:

$$\frac{\partial}{\partial x} \left(\frac{\alpha k_x \rho}{\mu} \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\alpha k_y \rho}{\mu} \frac{\partial p}{\partial y} \right) + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \phi \rho) \quad (82)$$

Discretized equation in 2-dimensions with implicit treatment of the well and flux terms is

$$\begin{aligned}
 & - \frac{(\alpha \phi \rho)_{i,j}^{n+1} - (\alpha \phi \rho)_{i,j}^n}{\Delta t} + \frac{1}{\Delta x_i} \left(\frac{\alpha k_x \rho}{\mu} \right)_{i+1/2,j}^{n+1} \frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{x_{i+1} - x_i} \\
 & - \frac{1}{\Delta x_i} \left(\frac{\alpha k_x \rho}{\mu} \right)_{i-1/2,j}^{n+1} \frac{p_{i,j}^{n+1} - p_{i-1,j}^{n+1}}{x_i - x_{i-1}} + \frac{1}{\Delta y_j} \left(\frac{\alpha k_y \rho}{\mu} \right)_{i,j+1/2}^{n+1} \frac{p_{i,j+1}^{n+1} - p_{i,j}^{n+1}}{y_{j+1} - y_j} \\
 & - \frac{1}{\Delta y_j} \left(\frac{\alpha k_y \rho}{\mu} \right)_{i,j-1/2}^{n+1} \frac{p_{i,j}^{n+1} - p_{i,j-1}^{n+1}}{y_j - y_{j-1}} + \alpha_{i,j} (q_{inj})_{i,j} = 0. \quad (83)
 \end{aligned}$$

A typical two-dimensional grid is shown in Figure 9.

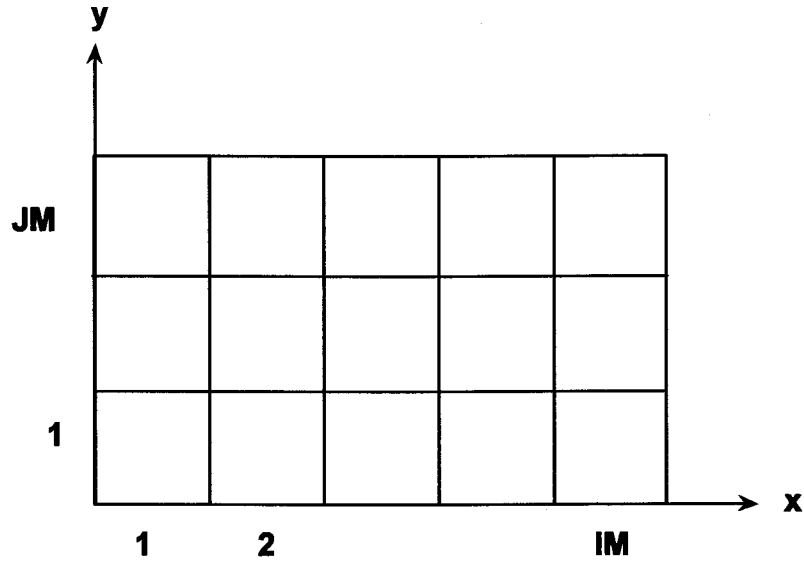


Figure 9. 2-dimensional grid.

A computational molecule or stencil is shown in Figure 10 and the stencil shows the indices of the pressures which appear in the material balance equation for the (i,j) grid block.

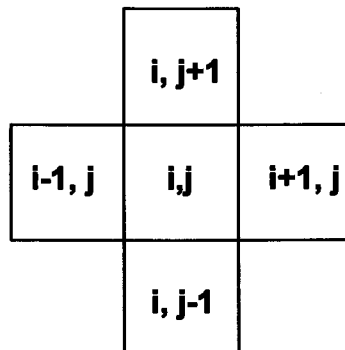


Figure 10. Computational molecule (or stencil).

With $IM=5$ and $JM=3$ in Figure 9, the number of equations is $NEQ = IM \times JM = 5 \times 3 = 15$. Suppose the equations or grid blocks are sequentially indexed as in Figure 11.

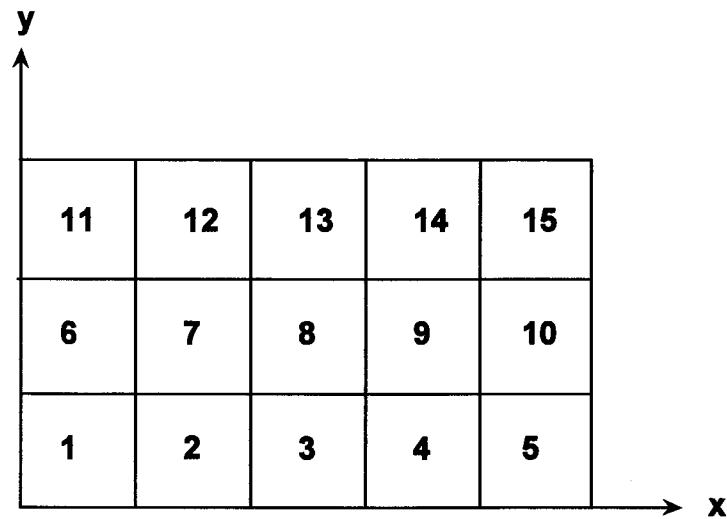


Figure 11. Sequential indexing of equations.

Then the Jacobian matrix has the structure shown in Figure 12 where * entries are the only nonzero values. This is said to have pentadiagonal band structure, with bandwidth = $IBW = 2 \times IM + 1$ (for the example, $IBW=11$).

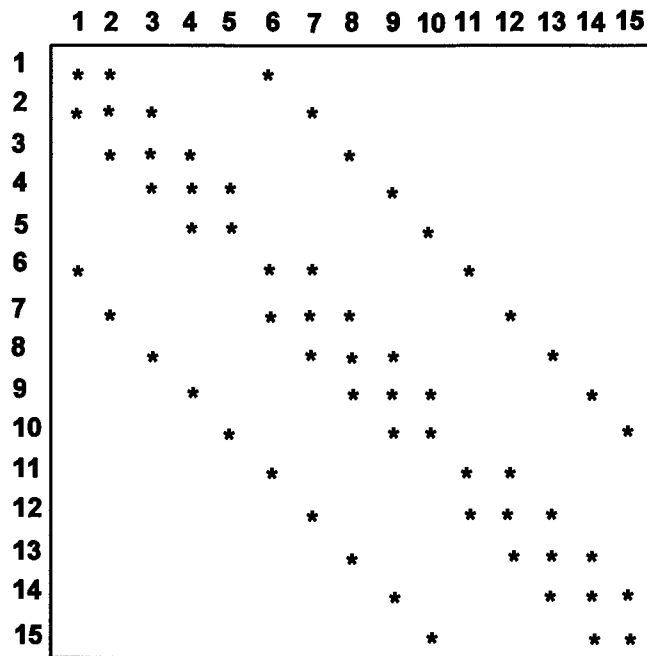


Figure 12. Jacobian matrix.

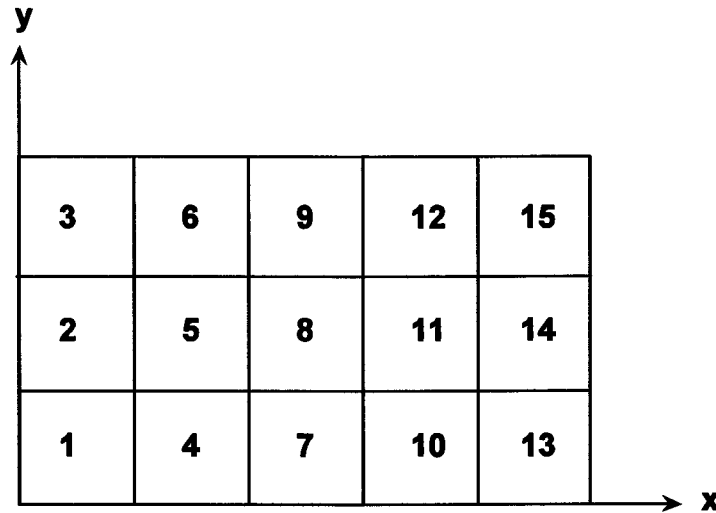


Figure 13. A different sequential indexing.

Suppose the grid is indexed as in Figure 13. Then $IBW = 2 \times JM + 1$ (for the example, $IBW=7$). Therefore, to minimize the bandwidth, BRAGFLO orders the grid blocks so that sequential indexing proceeds first in the shortest grid direction, then in the longest grid direction. In this case

$$IBW = 2 \times \min(IM, JM) + 1.$$

Storage requirements are as follows:

$$\text{Full matrix storage} = (IM \times JM)^2 \text{ words of memory}$$

$$\text{Band matrix storage} = IM \times JM \times IBW \text{ words of memory}$$

If $IM \leq JM$ then

$$\frac{\text{Band storage}}{\text{Full matrix storage}} = \frac{(2 \times IM + 1) \times IM \times JM}{(IM \times JM)^2} = \frac{2 \times IM + 1}{IM \times JM} \approx \frac{2}{JM}$$

For various values of JM, storage ratios are given by:

JM	Storage ratio
5	0.4 (40%)
10	0.2 (20%)
50	0.04 (4%)
100	0.02 (2%)

To determine the required computational effort, assume the major effort is the multiplication/division.

Banded structure:

multiplication/division \cong NEQ \times IB \times IB, where IB is the half bandwidth,
 IB = min (IM,JM).

Full matrix:

multiplication/division \cong 1/3 NEQ³

A typical performance assessment grid is

IM	=	33
JM	=	31
NEQ	=	31(33) = 1023
IBW	=	2(31) + 1 = 63
IB	=	31

Computational effort

banded matrix structure	=	1023 (31 \times 31)	= 983,103
full matrix structure	=	1/3 (1023) ³	\cong 3.57 \times 10 ⁸ .

The disparity in storage and computation between a band matrix solver and a full matrix solver is greater in two-dimensions than in one dimension. Of course, when solving 3-dimensional problems this disparity becomes even greater.

Although the equation solver is a major part of the time step calculation, other calculations involve evaluation of pressure dependent functions, coefficient generation, reporting and other overhead. However, the equation solver is a good indication of the computational effort for the time step solution. If the multiplication/division count of NEQ \times IB \times IB is used as a measure of equation solver speed, then a grid refinement for which the number of grid blocks is doubled in both the *x*- and *y*-direction (2-dimensional) would result in an increase in the number of equations by a factor of 4 and an increase in the half bandwidth by a factor of 2. Therefore, the computational effort would increase by a factor of 16. This estimate should warn the user that when attempting a grid refinement the computation (and also storage) does not depend linearly on the grid size.

4.8 Two-Phase Flow

BRAGFLO assumes a water/gas system. For miscible flow, the fluids will diffuse within each other, and there is not a defined interface between the fluids. Specifically, there is no capillary pressure effect. Immiscible fluids are not capable of mixing and have interfaces across which pressure discontinuities exist. This interfacial tension effect produces a capillary pressure between phases. In BRAGFLO fluids are assumed to be immiscible.

Phase saturation is the fraction of the pore space occupied by the fluids in a given phase. The notation is

S_w = water saturation,
 S_g = gas saturation.

For example, the volume occupied by water within a bulk volume *V* with porosity ϕ is $V\phi S_w$.

The saturation constraint for fully saturated media is

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$$S_w + S_g = 1. \quad (84)$$

Capillary pressure is defined by

$$P_c = P_g - P_w = P_c(S_w). \quad (85)$$

For a water wetting phase, $P_c \geq 0$.

The ability of a fluid to flow is affected by the presence of another fluid. The relative permeability is the ratio of the effective permeability of a given fluid phase to the permeability at 100% saturation. This is written as

$$k_{r1} = \frac{k_1}{k} \quad (86)$$

where k is the formation or absolute permeability, k_1 is the effective permeability of phase 1, and k_{r1} is the relative permeability of phase 1. We observe that $0 \leq k_{r1} \leq 1$ and k_{r1} will be dependent on the phase saturation.

Typical relative permeability curves are shown in Figure 14, where S_{wr} is the residual water saturation. For water saturation at or below S_{wr} , water will not flow.

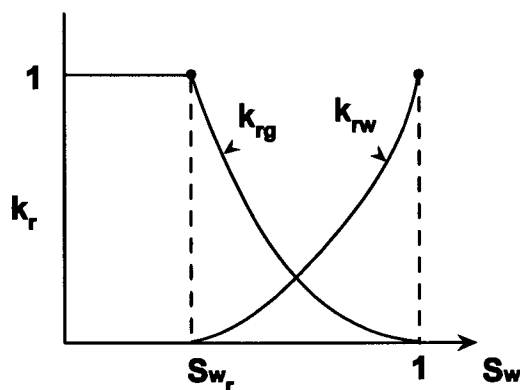


Figure 14. Typical relative permeability curve.

Darcy's Law extended to multiphase flow replaces absolute permeability with an effective permeability

$$\hat{q}_1 = -\frac{kk_{r1}\rho}{\mu}(\nabla P + \rho g \nabla h). \quad (87)$$

The following system of two mass balance equations and two constraint equations is the BRAGFLO description of the two-phase flow within a repository site:

Gas Mass Balance:

$$\nabla \cdot \left[\frac{\alpha \rho_g [k] k_{rg}}{\mu_g} (\nabla P_g + \rho_g g \nabla h) \right] + \alpha q_g + \alpha q_{rg} = \alpha \frac{\partial (\phi \rho_g S_g)}{\partial t} \quad (88)$$

Brine Mass Balance:

$$\nabla \cdot \left[\frac{\alpha \rho_w [k] k_{rw}}{\mu_w} (\nabla P_w + \rho_w g \nabla h) \right] + \alpha q_w + \alpha q_{rw} = \alpha \frac{\partial (\phi \rho_w S_w)}{\partial t} \quad (89)$$

Saturation Constraint:

$$S_g + S_w = 1. \quad (90)$$

Capillary Pressure Constraint:

$$P_c = P_g - P_w. \quad (91)$$

Additional terms include:

q_g = rate of gas production (or consumption, if negative) due to chemical reaction.

q_{rw} = rate of water production (or consumption, if negative) due to chemical reaction.

The above system of four equations describes the time and space behavior of the four variables S_g , S_w , P_g , P_w . The finite difference method requires the introduction of a grid in one, two, or three dimensions and then a discretization of the gas and brine mass balance equations with respect to this grid and with respect to time. The resulting system of nonlinear algebraic equations is solved over a time step by the Newton-Raphson method.

The discretization of the gas mass balance equation in two dimensions (x,y) is given by

$$\begin{aligned} & \frac{1}{\Delta x_i} \left\{ (k_{rg})_{i+1/2,j}^{n+1} \left[\frac{\alpha \rho_g k_x}{\mu_g} \right]_{i+1/2,j}^{n+1} (\Phi_{g_{i+1,j}}^{x-} - \Phi_{g_{i,j}}^{x+})^{n+1} - (k_{rg})_{i-1/2,j}^{n+1} \left[\frac{\alpha \rho_g k_x}{\mu_g} \right]_{i-1/2,j}^{n+1} (\Phi_{g_{i,j}}^{x-} - \Phi_{g_{i-1,j}}^{x+})^{n+1} \right\} \\ & + \frac{1}{\Delta y_j} \left\{ (k_{rg})_{i,j+1/2}^{n+1} \left[\frac{\alpha \rho_g k_y}{\mu_g} \right]_{i,j+1/2}^{n+1} (\Phi_{g_{i,j+1}}^{y-} - \Phi_{g_{i,j}}^{y+})^{n+1} - (k_{rg})_{i,j-1/2}^{n+1} \left[\frac{\alpha \rho_g k_y}{\mu_g} \right]_{i,j-1/2}^{n+1} (\Phi_{g_{i,j}}^{y-} - \Phi_{g_{i,j-1}}^{y+})^{n+1} \right\} \\ & + \alpha_{i,j} q_{wg_{i,j}}^{n+1} + \alpha_{i,j} q_{rg_{i,j}}^{n+1} - \frac{(\alpha \phi \rho_g S_g)_{i,j}^{n+1} - (\alpha \phi \rho_g S_g)_{i,j}^n}{\Delta t} = 0, \end{aligned} \quad (92)$$

where Φ represents the phase potentials:

$$\Phi_{g_{i,j}}^{x+} = P_{g_{i,j}} + \rho_{g_{i+1/2,j}} g h_{i,j} \quad (93)$$

$$\Phi_{g_{i,j}}^{x-} = P_{g_{i,j}} + \rho_{g_{i-1/2,j}} g h_{i,j}$$

and

$$\Phi_{g_{i,j}}^{y+} = P_{g_{i,j}} + \rho_{g_{i,j+1/2}} g h_{i,j} \quad (94)$$

$$\Phi_{g_{i,j}}^{y-} = P_{g_{i,j}} + \rho_{g_{i,j-1/2}} g h_{i,j}.$$

Subscripts denote:

- i = x -direction grid index,
- j = y -direction grid index,
- $i\pm 1/2$ = x -direction grid block interface,
- $j\pm 1/2$ = y -direction grid block interface,

and superscripts denote:

- n = index in the time discretization, known solution time level,
- $n+1$ = index in the time discretization, unknown solution time level.

The inter-block densities are defined by:

$$\begin{aligned} \rho_{g_{i+1/2,j}} &= \frac{\Delta x_{i+1,j}}{\Delta x_{i,j} + \Delta x_{i+1,j}} \rho_{g_{i,j}} + \frac{\Delta x_{i,j}}{\Delta x_{i,j} + \Delta x_{i+1,j}} \rho_{g_{i+1,j}} \\ \rho_{g_{i-1/2,j}} &= \frac{\Delta x_{i,j}}{\Delta x_{i-1,j} + \Delta x_{i,j}} \rho_{g_{i-1,j}} + \frac{\Delta x_{i-1,j}}{\Delta x_{i-1,j} + \Delta x_{i,j}} \rho_{g_{i,j}} \end{aligned} \quad (95)$$

and

$$\begin{aligned} \rho_{g_{i,j+1/2}} &= \frac{\Delta y_{i,j+1}}{\Delta y_{i,j} + \Delta y_{i,j+1}} \rho_{g_{i,j}} + \frac{\Delta y_{i,j}}{\Delta y_{i,j} + \Delta y_{i,j+1}} \rho_{g_{i,j+1}} \\ \rho_{g_{i,j-1/2}} &= \frac{\Delta y_{i,j}}{\Delta y_{i,j-1} + \Delta y_{i,j}} \rho_{g_{i,j-1}} + \frac{\Delta y_{i,j-1}}{\Delta y_{i,j-1} + \Delta y_{i,j}} \rho_{g_{i,j}}. \end{aligned} \quad (96)$$

Similar equations for the brine mass balance are obtained by replacing the subscript for gas (g) with the subscript for brine (w). Note that the flux and rate terms are evaluated at time level $n+1$, where the solution is not yet known. Therefore, the formulation is fully implicit.

Evaluation at grid block interfaces (*i. e.*, at $i\pm 1/2$ and $j\pm 1/2$) of mobility $\left[\frac{\alpha \rho_g k_{x \text{ or } y}}{\mu_g} \right]$, using

harmonic averaging, and relative permeabilities (k_{rg}), using upstream weighting, will be discussed later.

For each grid block there are two material balance equations. The saturation constraint is used to eliminate brine saturation and the capillary pressure equation is used to eliminate the gas pressure. The remaining unknowns for each grid block are gas saturation, S_g , and brine pressure, P_w . Consequently, at each time step it is necessary to solve $2 \times NX \times NY$ equations for $2 \times NX \times NY$ unknowns, where NX and NY are the number of grid blocks in the x - and y -directions, respectively.

In order to investigate the Jacobian matrix structure, assume for sake of argument that $NY < NX$. In this case the grid indexing moves most rapid in the y -direction and then in the x -direction. If the number of grid blocks is denoted NGB , then $NGB = NX \times NY$. In BRAGFLO the equation

indexing is first with respect to the gas equation, then the brine equation and outer most indexing with respect to the grid block. For example, the equation ordering is as follows:

equation index	equation
1	gas equation in grid block 1
2	brine equation in grid block 1
3	gas equation in grid block 2
4	brine equation in grid block 2
•	
•	
•	
$2 \times \text{NGB}-1$	gas equation in grid block NGB
$2 \times \text{NGB}$	brine equation in grid block NGB

The unknowns are gas saturation and brine pressure. The unknowns are ordered by gas saturation, then brine pressure and then with respect to grid block. The unknown indexing is:

unknown index	unknown
1	gas saturation in grid block 1
2	brine pressure in grid block 1
3	gas saturation in grid block 2
4	brine pressure in grid block 2
•	
•	
•	
$2 \times \text{NGB}-1$	gas saturation in grid block NGB
$2 \times \text{NGB}$	brine pressure in grid block NGB

Information at the i,j grid block and its neighboring grid blocks will use the compass notation:

- P** corresponds to information with respect to grid block i,j
- E** corresponds to information with respect to grid block $i+1,j$
- W** corresponds to information with respect to grid block $i-1,j$
- N** corresponds to information with respect to grid block $i,j+1$
- S** corresponds to information with respect to grid block $i,j-1$.

Assume that the i,j grid block has sequential index ℓ . Then the Jacobian matrix has a 2×2 block pentadiagonal structure and the resulting linear system in the Newton-Raphson iteration step can be represented as follows

In the above, F_1 denotes the left-hand side of the gas mass balance equation, and F_2 denotes the left-hand side of the brine mass balance equation.

An inspection of the above discretized gas mass balance equation shows that the flux between neighboring grid blocks involves inter-block flow terms evaluated at grid block interfaces, such as $i+1/2$, $i-1/2$, $j+1/2$ and $j-1/2$. It is necessary to discuss how BRAGFLO evaluates these inter-block flow terms.

Consider the following term in the brine equation for flow in the x -direction between grid blocks i and $i+1$, with gravitational effects neglected to simplify the discussion:

$$\frac{(k_{rw})_{i+1/2}}{\Delta x_i(x_{i+1} - x_i)} \left(\frac{\alpha \rho_w k_x}{\mu_w} \right)_{i+1/2} (P_{w_{i+1}} - P_{w_i}). \quad (103)$$

Since pressure and saturation are determined at grid block centers x_i and x_{i+1} , the question remains as to how to evaluate the interface term at $x_{i+1/2}$.

First, we define the harmonic average, H , of a_1 , a_2 , as

$$\frac{1}{H} = \frac{1}{2} \left(\frac{1}{a_1} + \frac{1}{a_2} \right) \quad (104)$$

or

$$H = \frac{2a_1a_2}{a_1 + a_2}. \quad (105)$$

Further, the harmonic weighted-average of a_1 , a_2 is

$$\frac{1}{H} = \frac{w_1}{a_1} + \frac{w_2}{a_2} \quad (106)$$

or

$$H = \frac{a_1a_2}{w_2a_1 + w_1a_2}, \quad (107)$$

where the weights satisfy $w_1 + w_2 = 1$. Now introduce the shorthand notation

$$\tau_{i+1/2} = \left(\frac{\alpha \rho_w k_x}{\mu_w} \right)_{i+1/2}. \quad (108)$$

At the $i+1/2$ interface, assume the mass flux is continuous

$$\bar{q}_{i+1/2} = q_{i+1/2}^- = q_{i+1/2}^+ \quad (109)$$

where

$\bar{q}_{i+1/2}$ is average flow between x_i and x_{i+1} ,

$q_{i+1/2}^-$ is flow to the left of interface,

$q_{i+1/2}^+$ is flow to the right of interface.

From Darcy's Law, neglecting gravitational effects,

$$\bar{q}_{i+1/2} = \tau_{i+1/2} (k_{rw})_{i+1/2} \frac{P_{i+1} - P_i}{x_{i+1} - x_i} \quad (110)$$

or

$$\bar{q}_{i+1/2} = \tau_{i+1/2} (k_{rw})_{i+1/2} \frac{P_{i+1} - P_i}{1/2(\Delta x_i + \Delta x_{i+1})} \quad (111)$$

This yields

$$P_{i+1} - P_i = \frac{\bar{q}_{i+1/2} \frac{1}{2} (\Delta x_i + \Delta x_{i+1})}{\tau_{i+1/2} (k_{rw})_{i+1/2}} \quad (112)$$

Similarly,

$$q_{i+1/2}^- = \tau_i (k_{rw})_{i+1/2} \frac{(P_{i+1/2} - P_i)}{\frac{1}{2} \Delta x_i} \quad (113)$$

$$q_{i+1/2}^+ = \tau_{i+1} (k_{rw})_{i+1/2} \frac{(P_{i+1} - P_{i+1/2})}{\frac{1}{2} \Delta x_{i+1}} \quad (114)$$

Pressure drop is then written as

$$P_{i+1} - P_i = P_{i+1} - P_{i+1/2} + (P_{i+1/2} - P_i). \quad (115)$$

Then

$$\bar{q}_{i+1/2} \frac{1}{2} (\Delta x_i + \Delta x_{i+1}) = q_{i+1/2}^+ \frac{1}{2} \Delta x_{i+1} + q_{i+1/2}^- \frac{1}{2} \Delta x_i. \quad (116)$$

Solving for $\tau_{i+1/2}$ yields

$$\tau_{i+1/2} = \frac{\tau_i \tau_{i+1}}{\frac{\Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}} \tau_i + \frac{\Delta x_i}{\Delta x_i + \Delta x_{i+1}} \tau_{i+1}}. \quad (117)$$

This is the harmonic mean of τ_i , τ_{i+1} , weighted with respect to the distance to the interface.

The inter-block relative permeability is evaluated by upstream weighting:

$$(k_{rw})_{i+1/2} = \begin{cases} k_{rw_{i+1}}, & P_{w_i} < P_{w_{i+1}} \\ k_{rw_i}, & \text{otherwise.} \end{cases} \quad (118)$$

The following process typical in performance assessment analysis justifies this treatment of the interblock flow term. Assume gas is generated and is displacing water from the left to the right as in Figure 15. At the gas front, the gas pressure, P_g , is highest in the i^{th} grid block. Therefore, gas wants to flow from i to $i+1$ grid block. Although the gas is mobile ($k_{rg} > 0$) in the i^{th} block, it is immobile ($k_{rg} = 0$) in the $i+1^{\text{th}}$ block. If the relative permeability is included in the inter-block harmonic averaging, then $\tau_{i+1/2}$ is zero and no gas is transported. By upstream weighting the gas relative permeability we allow the mobile gas to flow from i to $i+1$ block.

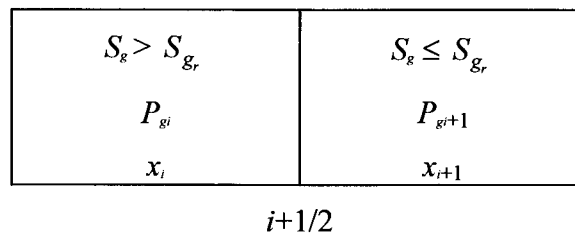


Figure 15. Gas displacement front.

Another treatment of relative permeability is to evaluate it as an arithmetic average of the two adjacent relative permeabilities.

$$(k_{rw})_{i+1/2} = w_i k_{rw_i} + w_{i+1} k_{rw_{i+1}} \tag{119}$$

where the weights sum to 1. The arithmetic average of inter-block relative permeability does not correctly treat the following case. Suppose water is displaced from left to right in Figure 16:

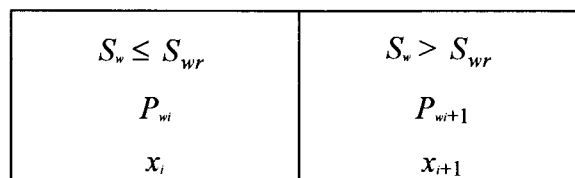


Figure 16. Displacement of immobile water.

with pressure satisfying $P_{wi} > P_{wi+1}$. The pressure tries to move water from i to $i+1$ block. Since $k_{rw_i} = 0$ and $k_{rw_{i+1}} > 0$, the inter-block relative permeability by arithmetic averaging is greater than zero and the immobile water would be transported from the i^{th} block. Upstream weighting would yield inter-block relative permeability of zero with no water transported. Thus the upstream weighting prevents immobile fluid from being transported. The upstream weighting of relative permeability is controlled by input parameters.

4.9 Characteristic Curves

Relative permeability and capillary pressure are computed from several different empirical relations (Brooks, 1964; van Genuchten, 1978; WIPP PA, 1992a). Input directives control choice of the characteristic curves.

The van Genuchten-Parker model determines

Capillary Pressure:

$$P_c = P_o \left(S_{e_2}^{-1/m} - 1 \right)^{1-m} \quad (120)$$

where P_o is a constant determined by equating the van Genuchten-Parker capillary pressure with the Brooks-Corey capillary pressure (discussed below) at $S_{e_1} = 0.5$.

Relative Permeabilities:

$$k_{rw} = S_{e_1}^{1/2} \left[1 - \left(1 - S_{e_1}^{1/m} \right)^m \right]^2 \quad (121)$$

$$k_{rg} = \left(1 - S_{e_2} \right)^{1/2} \left(1 - S_{e_2}^{1/m} \right)^{2m} \quad (122)$$

where the effective saturations are

$$S_{e_1} = \frac{S_w - S_{wr}}{1 - S_{wr}} \quad (123)$$

and

$$S_{e_2} = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}. \quad (124)$$

In the original van Genuchten-Parker model the residual gas saturation S_{gr} was zero. BRAGFLO has the capability of using nonzero residual gas saturation in the calculation of S_{e_2} .

The parameter m is related to the input parameter, λ , by

$$m = \frac{\lambda}{1 + \lambda}. \quad (125)$$

Typical characteristic curves using the van Genuchten-Parker model are shown in Figure 17 with parameters

$$\lambda = 0.7 \quad (m = 0.41)$$

$$S_{wr} = 0.2.$$

The original Brooks-Corey model determines

Capillary Pressure:

$$P_c = P_t / S_{e_1}^{1/\lambda} \quad (126)$$

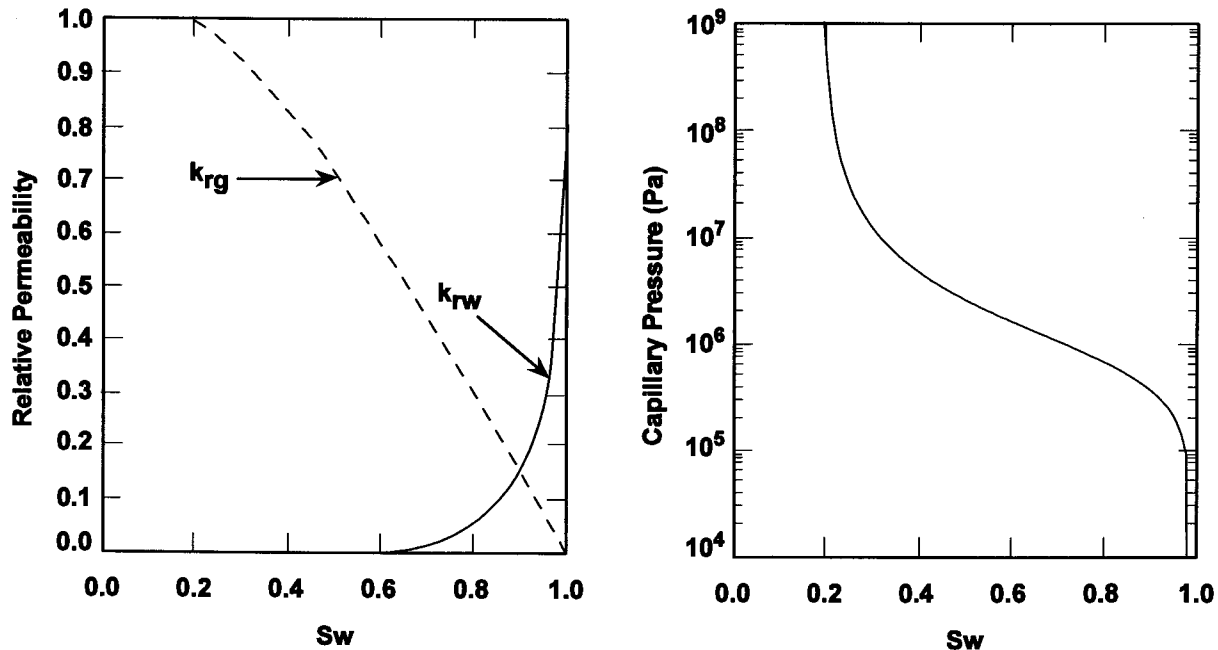


Figure 17. Relative permeabilities for van Genuchten-Parker model (left plot) and capillary pressure for van Genuchten-Parker model (right plot).

Relative Permeabilities:

$$k_{rw} = S_{e_1}^{(2+3\lambda)/\lambda} \tag{127}$$

$$k_{rg} = (1 - S_{e_1})^2 (1 - S_{e_1}^{(2+\lambda)/\lambda}) \tag{128}$$

where P_t is threshold pressure and λ is pore size distribution parameter. Note that if this option is used with $P_t = 0$, then P_c is identically zero.

Typical characteristic curves using the original Brooks-Corey model are shown in Figure 18 with parameters

$$\begin{aligned} \lambda &= 0.7 \\ S_{wr} &= 0.2 \\ P_t &= 1.0 \times 10^6 \text{ Pa.} \end{aligned}$$

Two modifications of the Brooks-Corey model are available which differ in the treatment of the effective saturation, S_e .

The first modified Brooks-Corey model computes both phase relative permeabilities using an effective saturation

$$S_{e_2} = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}} \tag{129}$$

where S_{gr} is residual gas saturation.

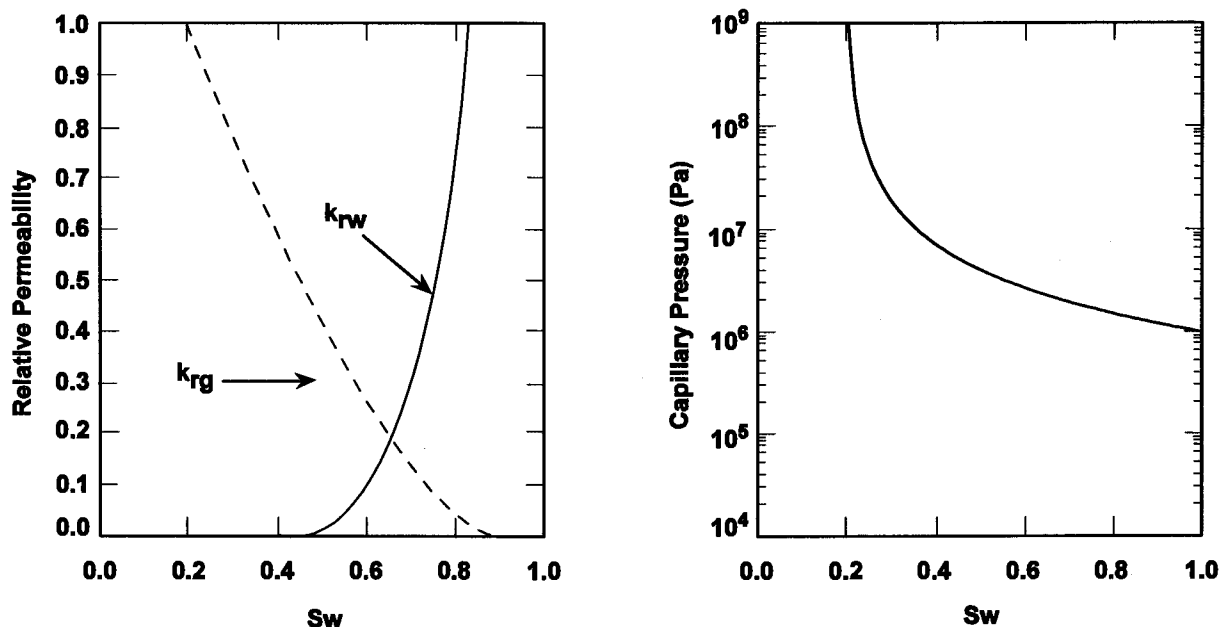


Figure 18. Relative permeabilities for original Brooks-Corey model (left plot) and capillary pressure for original Brooks-Corey model (right plot).

Characteristic curves for this option are shown in Figure 19 with input parameters

$$\begin{aligned} \lambda &= 0.7 \\ S_{wr} &= 0.2 \\ S_{gr} &= 0.2 \\ P_i &= 1.0 \times 10^6 \text{ Pa.} \end{aligned}$$

Note that for $S_w \geq 1 - S_{gr}$, gas is immobile and water has 100% mobility. Also, note that the capillary pressure curve assumes the threshold capillary pressure at $S_w = 1 - S_{gr}$.

The second modified Brooks-Corey model includes residual gas saturation in the calculation of effective saturation (S_{e2}) only for the gas phase. This treatment results in the characteristic curves shown in Figure 20.

Finally, a linear model is available with relative permeability and capillary pressure shown in Figure 21. The only input parameters honored are $S_{wr} = 0.2$ and $P_c = P_i$.

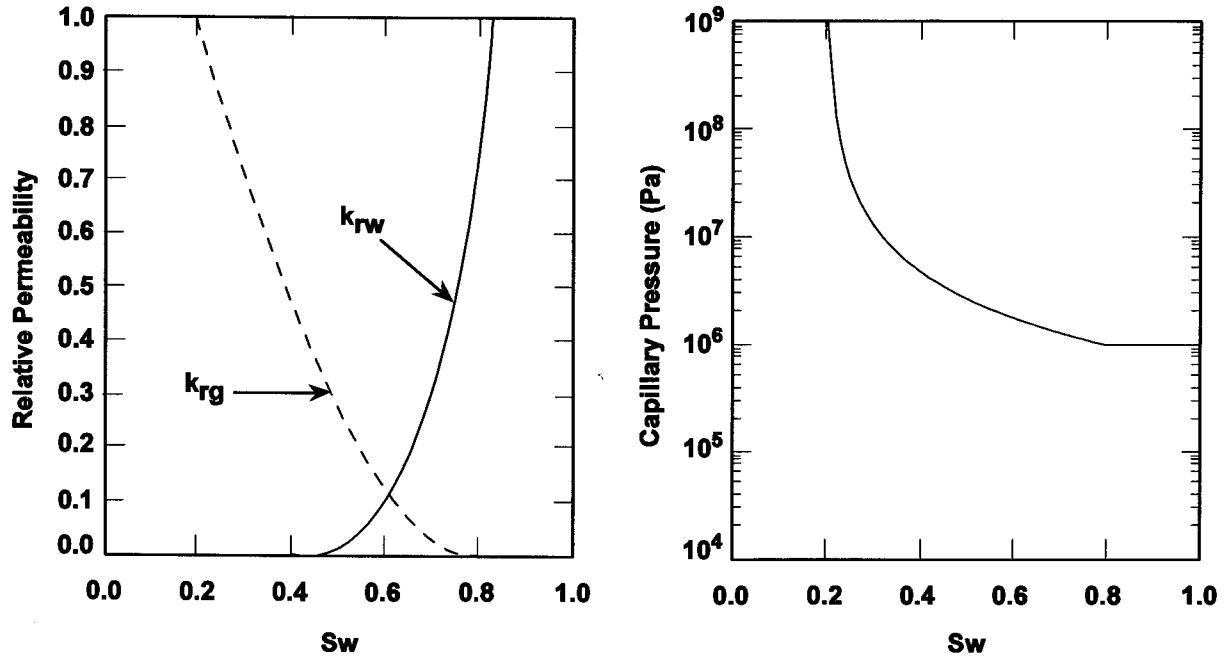


Figure 19. Relative permeabilities for modified Brooks-Corey model (left plot) and capillary pressure for modified Brooks-Corey model (right plot).

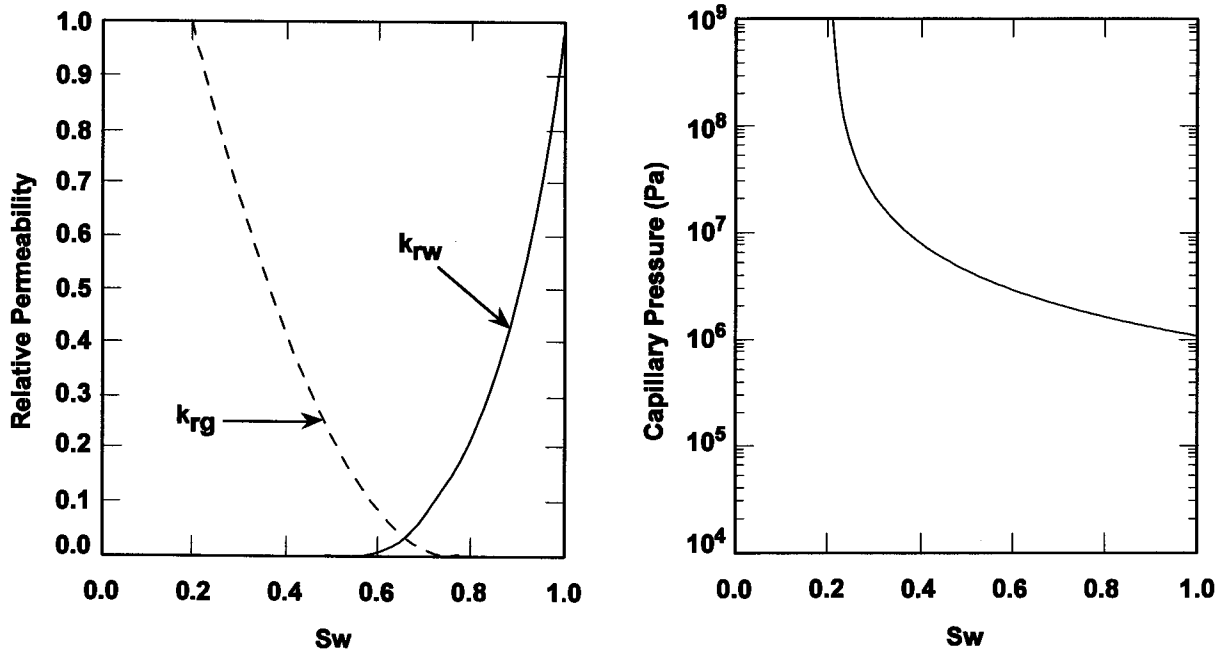


Figure 20. Relative permeabilities for second modified Brooks-Corey model (left plot) and capillary pressure for second modified Brooks-Corey model (right plot).

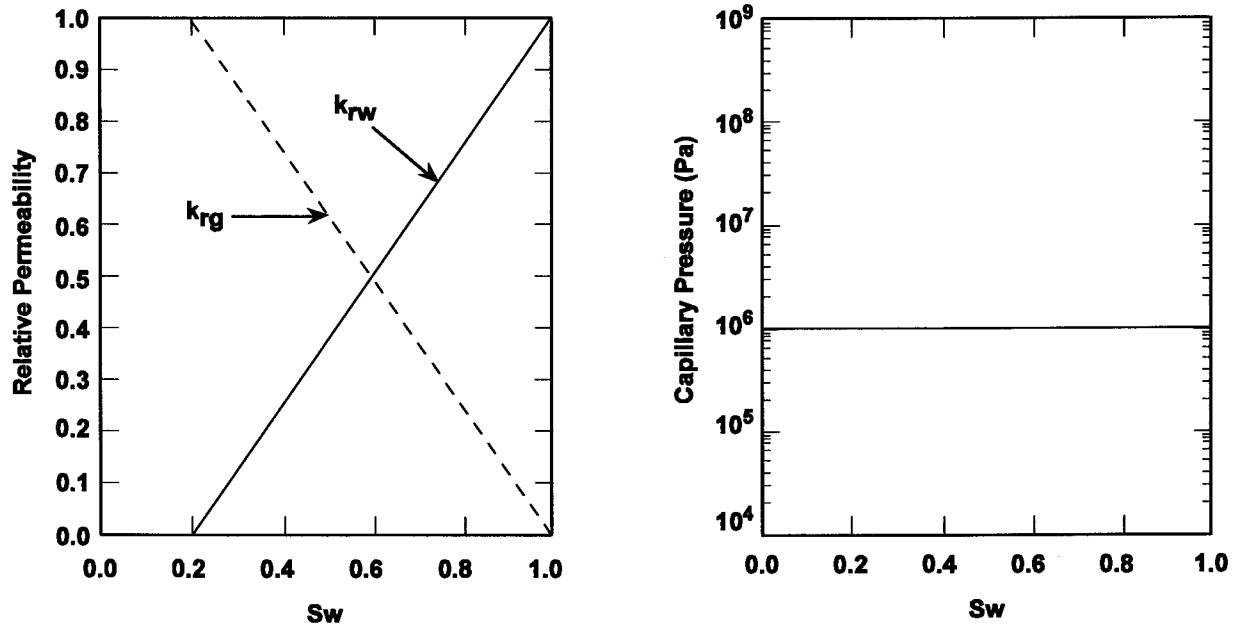


Figure 21. Relative permeabilities for linear model (left plot) and capillary pressure for linear model (right plot).

For both the van Genuchten-Parker and the Brooks-Corey model, the capillary pressure function is unbounded from the right ($S_w = S_w^+$). An option is available which truncates the capillary pressure function at the PCMAX value. The capillary pressure curve with this option and $PCMAX = 1.0 \times 10^8$ Pa is shown in Figure 22 (left plot) for the van Genuchten-Parker model and in Figure 22 (right plot) for the original Brooks-Corey model.

The dependence of the characteristic curves for both van Genuchten-Parker and Brooks-Corey on the pore size distribution parameter λ is shown in Figure 23 and Figure 24.

When the Jacobian is calculated, derivatives with respect to saturation are taken so as not to cross residual brine saturation, where the capillary pressure is either discontinuous or has discontinuous derivatives, depending on which option is chosen to model capillary pressure.

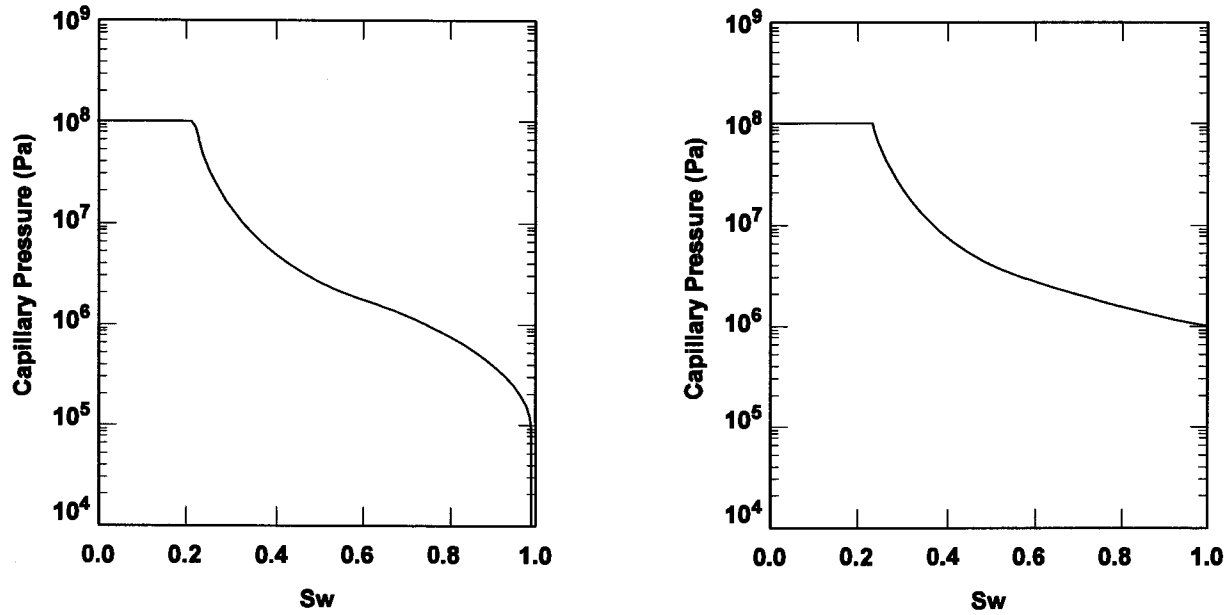


Figure 22. Capillary pressure for van Genuchten-Parker model PCMAX = 10^8 Pa (left plot) and capillary pressure for original Brooks-Corey model PCMAX = 10^8 Pa (right plot).

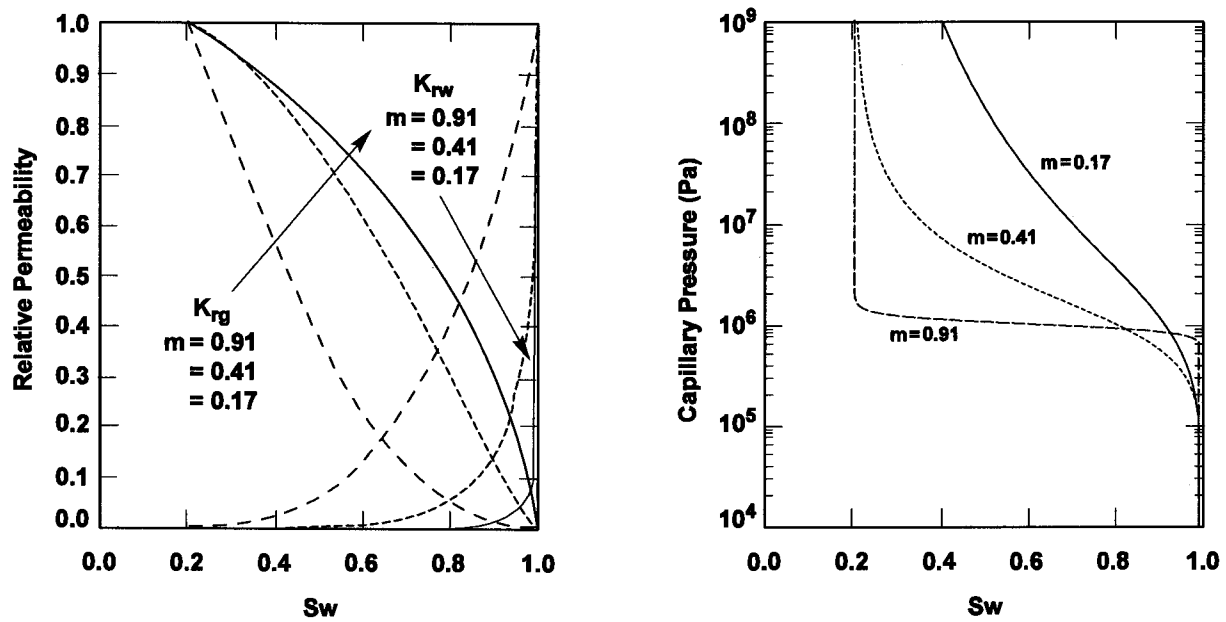


Figure 23. Relative permeabilities for van Genuchten-Parker model, effect of parameter m (left plot) and capillary pressure for van Genuchten-Parker model, effect of parameter m (right plot).

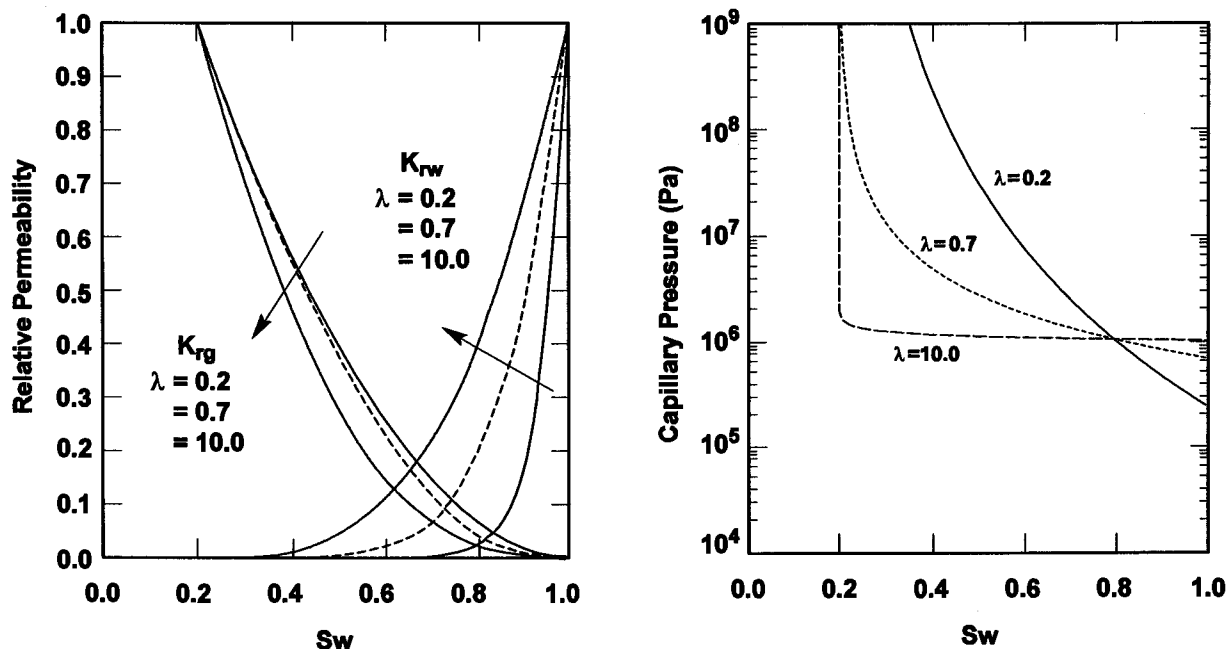


Figure 24. Relative permeabilities for Brooks-Corey model effect of pore size distribution parameter (left plot) and capillary pressure for Brooks-Corey model effect of pore size distribution parameter (right plot).

In running BRAGFLO, the capillary pressure-saturation relationships were typically turned off in waste-filled regions because they caused the solver to take very small time steps around $S_w \sim S_{wr}$. When the Jacobian is calculated, derivatives with respect to saturation are taken so as not to cross residual brine saturation. Nonetheless the Newton-Raphson solver can have difficulty finding a solution around the discontinuous derivative in capillary pressure when capillary pressure is capped at PCMAX. In past calculations this problem occurred when iron corrosion (which consumes water) reduced the saturation below residual saturation in the waste-filled regions.

To remedy the numerical problem due to the discontinuity in capillary-pressure, a new modified Brooks-Corey model was implemented in BRAGFLO. This model is in the subroutine RELPERM, and is activated by setting $KRP = 12$. In this model, the relative permeabilities are unchanged from the modified Brooks-Corey model but the capillary pressure is now calculated using equation (126) with a modified saturation

$$S_{e21} = \frac{S_w - S_{min} - S_{eff\ min}}{1 - S_{min} - S_{eff\ min}}, \quad (130)$$

where S_{min} is a new cut off in saturation that we consider numerically dry (see Subsection 4.13.1) and $S_{eff\ min}$ is a small tolerance which pushes the singularity in equation (126) to a saturation slightly below S_{min} .

Previously, in BRAGFLO, an inconsistency occurred during the -5 to 0 year operational period during which BRAGFLO is run. During this period the operational areas were modeled as open-completely-saturated cavities with porosity equal to 1. If capillary pressure were turned on during this period, the model would predict significant capillary-pressure effects on the relative permeabilities. It's clear that the now-open WIPP repository is not completely saturated and

does not have significant capillary pressure effects on pressure or permeability. A new model for the relative permeabilities has been added with $KRP = 11$ to remove capillary-pressure effects from the relative permeabilities for open cavities. In this model the relative permeabilities decrease from 1 to zero linearly between the residual saturations (brine and gas) and the residual saturation plus a tolerance,

$$k_{rel} = 0 \quad \text{for} \quad S < S_r, \quad (131)$$

$$k_{rel} = \frac{(S - S_r)}{tol} \quad \text{for} \quad S_r \leq S \leq S_r + tol, \quad (132)$$

$$k_{rel} = 1 \quad \text{for} \quad S > S_r + tol, \quad (133)$$

where k_{rel} is the relative permeability, S is saturation (brine or gas), S_r is the residual saturation (brine or gas) and tol is a tolerance over which the relative permeability changes linearly from zero to 1.

4.10 Pressure-Induced Fracture Treatment

Most fluid flow models for porous media, such as BRAGFLO, allow for coupling to the mechanical system (rock matrix) through the introduction of rock compressibility, which is defined as the relative rate of change of porosity with respect to pressure

$$C = \frac{1}{\phi} \frac{d\phi}{dP} \quad (134)$$

where

$$\begin{aligned} C &= \text{rock compressibility,} \\ \phi &= \text{porosity,} \\ P &= \text{pore pressure.} \end{aligned}$$

For constant compressibility, porosity can be expressed as a function of pressure

$$\phi = \phi_o \exp[C(P - P_o)] \quad (135)$$

where ϕ_o is the porosity at reference pressure, P_o .

The fracture treatment in BRAGFLO (Key, 1994) allows for pressure induced alterations to the porosity by introducing a pressure-dependent porosity. Figure 25 shows the piecewise linear rock compressibility function. Below an initiating pressure, P_i , compressibility is a constant intact value, C_i . For pressures above P_i , the compressibility increases linearly to a fully altered compressibility, C_a , at the fully altered pressure, P_a . For pressures above P_a no further alteration occurs, which implies that $C = 0$.

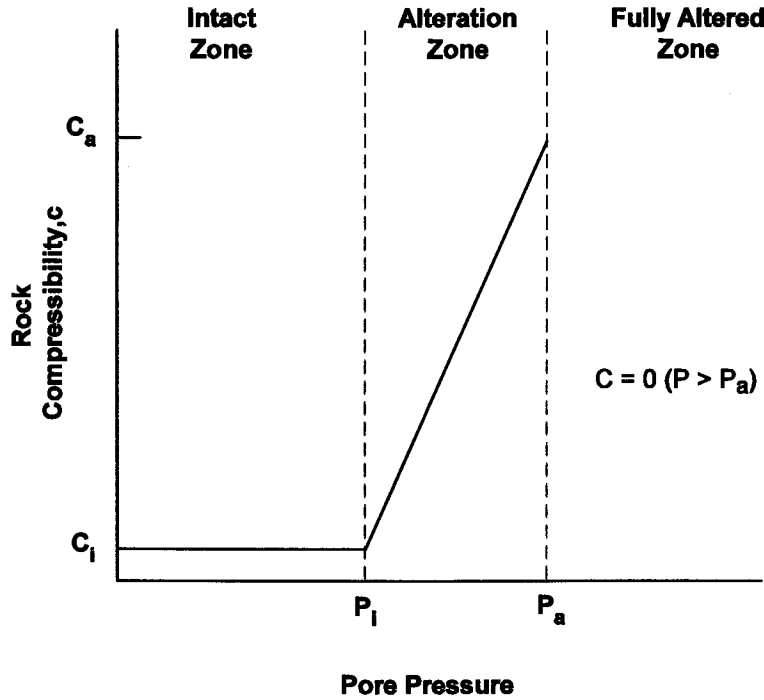


Figure 25. Pressure dependent compressibility.

The porosity can now be computed from the compressibility definition giving

$$\phi = \begin{cases} \phi_0 \exp[C_i(P - P_0)] & P \leq P_i \\ \phi_0 \exp\left\{C_i(P - P_0) + \frac{(C_a - C_i)(P - P_i)^2}{(P_a - P_i)^2}\right\} & P_i < P < P_a \\ \phi_a & P_a \leq P \end{cases} \quad (136)$$

BRAGFLO input requires the pressures P_i and P_a and the porosity at the fully altered conditions, ϕ_a be specified. From this information, the fully altered compressibility, C_a , is determined as

$$C_a = C_i \left[1 - 2 \frac{(P_a - P_0)}{P_a - P_i} \right] + \frac{2}{(P_a - P_i)} \ln \left(\frac{\phi_a}{\phi_0} \right). \quad (137)$$

The BRAGFLO fracture treatment further allows for change in the fracture material permeability. The often-used parallel plate analogy for flow in fractured rock suggests the form

$$\frac{k}{k_i} = \left[\frac{\phi}{\phi_i} \right]^n \quad (138)$$

where

- k = permeability of altered material,
- k_i = permeability of intact material,
- ϕ = porosity of altered material,
- ϕ_i = porosity of intact material,
- n = an empirical parameter.

The altered permeability model requires as input n . Also, the anisotropic nature of permeability is specified for the fracture materials.

A geometric realization of the pressure-dependent porosity and permeability within a fracture material is shown in Figure 26.

In a system where gas is displacing water, the fracture treatment can influence the gas migration distance. At elevated pressure, the increased porosity will produce more storage with corresponding shorter gas migration distance, while the increase in permeability will enhance the fluid mobility with resulting longer gas migration. The net effect will depend on the relative magnitudes of the storage and permeability effects.

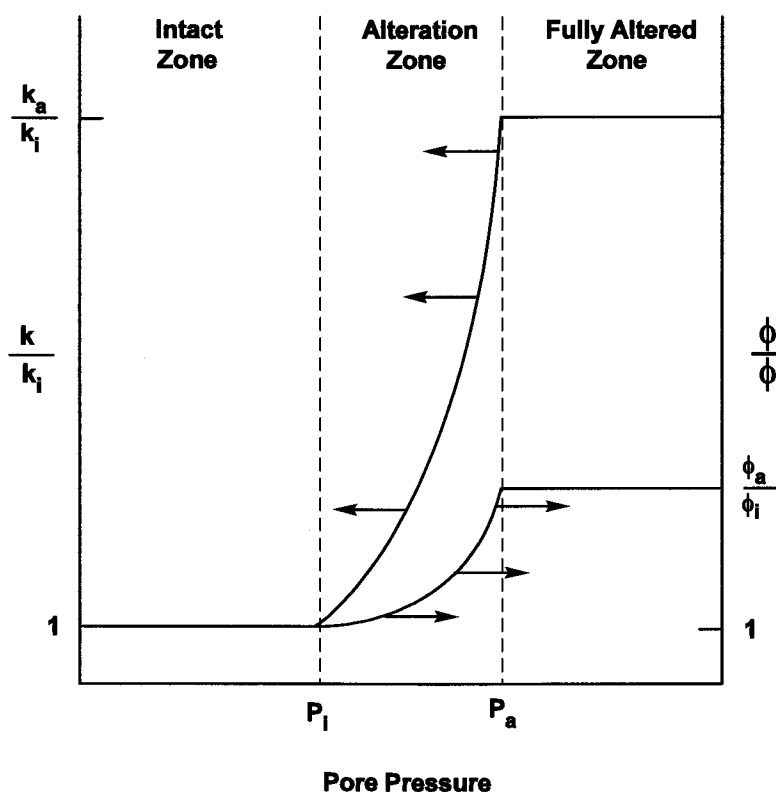


Figure 26. Pressure dependent porosity and permeability.

4.11 Creep Closure

The excavation of the WIPP will result in the plastic deformation of the salt material (creep) and resultant closure (creep closure) of excavated areas. The principal effect of this closure for performance assessment is its effect on repository pressure due to the reduction in void volume accompanying creep closure. Accordingly, creep closure is represented in BRAGFLO by changing the porosity of the waste disposal area in a manner consistent with expectations developed from detailed modeling studies. Detailed modeling studies used the code SANCHO (Butcher et al., 1995), and more recently, SANTOS (Park and Hansen, 2003), to develop time- and pressure-dependent predictions of waste disposal area void volume. Pressure variation was consistent with variation in the gas generation rates possible in the waste disposal areas. The

results were used to develop a look-up table of porosity as a function of time and waste disposal area pressure that is used in BRAGFLO to vary waste disposal area porosity. Essential features of the look-up table (porosity surface) are shown in Figure 27.

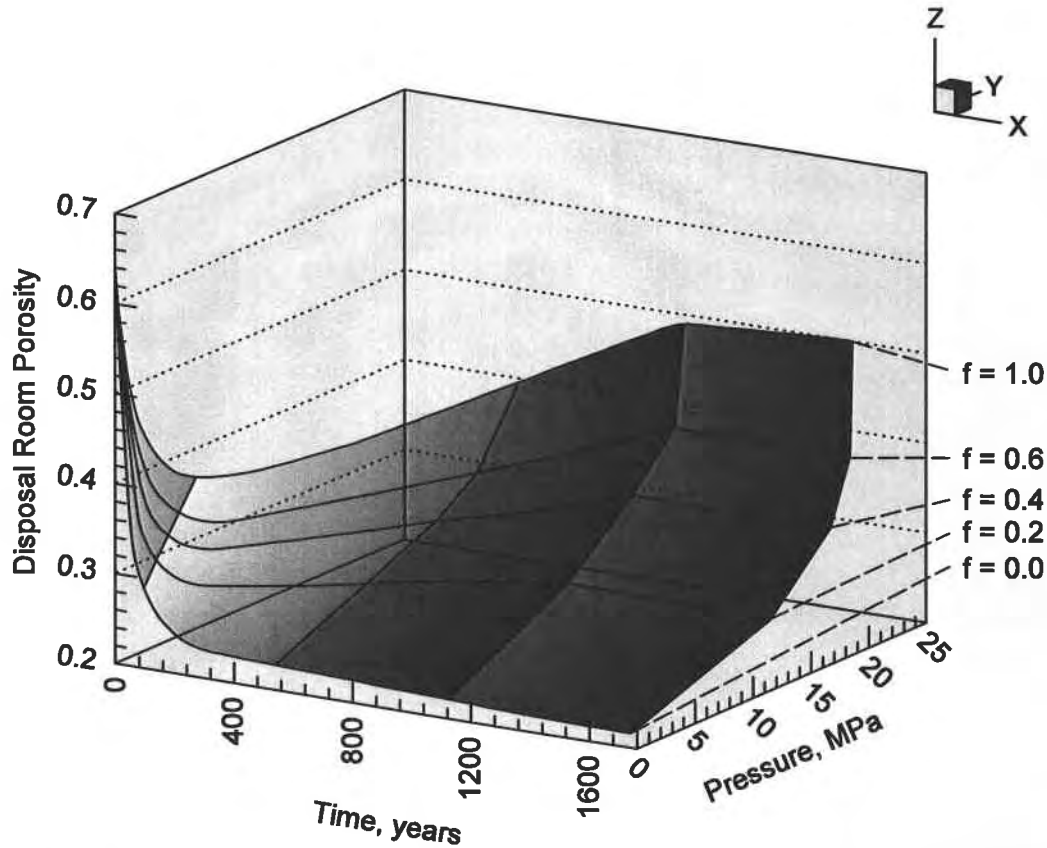


Figure 27. Pressure driven porosity function generated from SANTOS structural mechanics code.

The surface is generated by a family of f factors which is representative of the level of gas generation. The value of $f = 1.0$ corresponds to 2 moles of gas per drum per year for 550 years, 1 mole per drum per year from 550 to 1050 years, and zero gas generation after 1050 years. For each f factor the above rates are scaled by f . Four porosity surfaces or “look-up” tables are available as discussed in the Subsection 7.2.11. For compliance calculations the porosity “look-up” is done on a grid block scale and uses grid block pressure.

4.12 Klinkenberg Effect

For gases in a tight porous material at low pressures the boundary condition of zero gas velocity at the solid surface is not satisfied (Klinkenberg, 1941; Corey, 1990; WIPP PA, 1992a). This phenomenon has been called gas slippage and results in a larger gas velocity. This slipping of the gas flow contributes to an apparent pressure-dependent increase in permeability, which was originally observed by Klinkenberg. A correction to the formation permeability to the gas phase is related to pressure by

$$k_g = k_w \left(1 + b k_w^{-a} / P \right) \quad (139)$$

where

- k_g = formation permeability to gas [m^2],
- k_w = formation permeability to water [m^2],
- a, b = formation dependent constants,
- P = pressure [Pa].

The constants a, b are input. The recommended values found in the BRAGFLO User's Manual are from a tight gas/sand correlation. Figure 28 shows the gas phase permeability as a function of pressure for a family of k_w with $a = 0.33$ and $b = 0.98$.

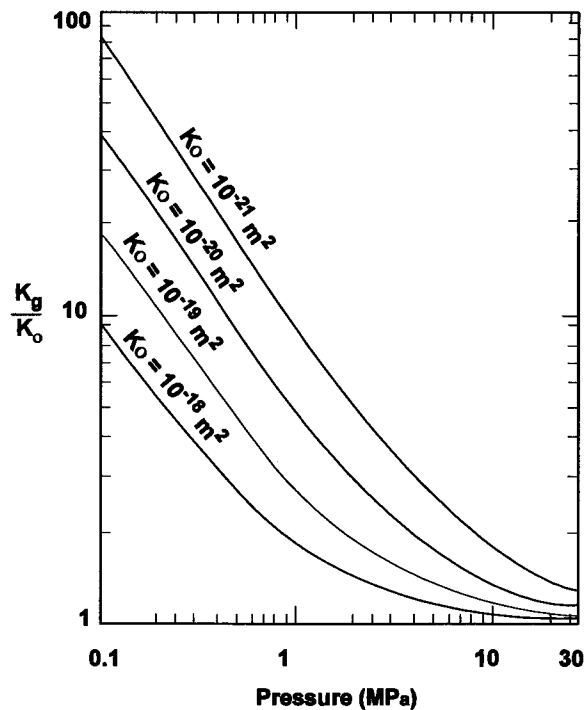


Figure 28. Increase in gas phase permeability due to Klinkenberg effect.

4.13 Chemistry Model

Within BRAGFLO there are chemical reactions with the effect of consuming/producing brine and gas. In BRAGFLO, the kinetics of most chemical reactions are assumed to be zero'th order.

Several new routines and changes have been made to accommodate MgO hydration and carbonation, and steel sulfidation. These changes include subroutines to calculate the rates of chemical reactions, changes to the way in which all of the chemical reactions are calculated, and changes to the input file and output files to handle these changes.

4.13.1 Wicking and the Effective Saturation

Brine-consuming reactions such as anoxic iron corrosion and MgO hydration tend to dry out the waste-filled regions of the repository. MgO hydration tends to dry out the repository quickly because the rate of hydration far exceeds the rate of brine inflow. The BRAGFLO code and the

underlying models (being a two-phase porous media flow code) cannot simulate completely dry ($S_w = 0$) cells. Furthermore there is no reason to believe that MgO hydration will stop at the residual brine saturation, since MgO hydrates under humid and inundated conditions. Thus to accommodate MgO hydration and allow the code to run, in BRAGFLO Version 6.0 we have introduced a lower cut off in saturation S_{min} in the waste filled areas that we consider numerically dry. This cut off is to be chosen small enough such that the amount of water in the waste filled areas at the cut off is small, but large enough to prevent numerical difficulties. Below this saturation MgO hydration, biodegradation, and iron corrosion ceases. The parameter S_{min} shows up in the subroutines PROPS and PROPS1, which calculate the properties of the grid or a single cell, respectively. In these routines an effective saturation S_{eff} is calculated and sent to each of the chemistry routines which calculate the rates of reactions, based on the effective saturation (not the actual saturation). In BRAGFLO Version 5.0 (in the subroutines PROPS and PROPS1) the effective saturation is calculated from

$$S_{eff} = S_w + S_{wick} (1 - e^{-\alpha S_w}), \tag{140}$$

where factor α is ALPHARXN, and S_{wick} is SATWICK. In BRAGFLO Version 6.0 and above, equation (140) has been replaced with,

$$S_{eff} = S_w - S_{min} + S_{wick} \left(1 - \text{Exp} \left[200\alpha (\text{Max}(S_w - S_{min}, 0))^2 \right] \right). \tag{141}$$

Equation (141) mimics equation (140) except that S_{eff} now goes to zero as S_w approaches S_{min} . The factor of 200 in the exponential function was chosen to make the difference between equation (140) and equation (141) small away from $S_{eff} = 0$. The term $(S_w - S_{min})^2$ insures that the value and first derivative of S_{eff} are continuous around $S_{eff} = 0$. The parameter S_{min} is also used in determining the capillary pressure in the waste filled areas, as described above in Subsection 4.9. The parameter S_{min} enters BRAGFLO through the input file.

4.13.2 Stoichiometry Matrix

In BRAGFLO Version 6.0 and above the stoichiometric coefficients for the chemical reactions have been reorganized into a single matrix S(I,J); stoichiometric coefficients are dimensionless. This matrix is organized as follows: I represents the reaction and J represents the individual compound, which are given below in Table 1 and Table 2. A positive value of S(I,J) represents production, and negative represents consumption.

Table 1. Stoichiometric matrix S(I,J) row number I and corresponding reaction

Index (I)	Reaction
1	Anoxic corrosion of iron
2	Microbial gas generation
3	Iron hydroxide sulfidation
4	Metallic iron sulfidation
5	MgO hydration

6	Magnesium hydroxide (brucite) carbonation
7	MgO carbonation
8	Hydromagnesite conversion

Table 2. Stoichiometric matrix S(I,J) column number J and corresponding compound

Index (J)	Compound
1	H ₂
2	H ₂ O
3	Fe
4	Cellulosics
5	Fe(OH) ₂
6	FeS
7	MgO
8	Mg(OH) ₂
9	Hydromagnesite
10	MgCO ₃

The individual reactions are described below.

4.13.3 Iron Corrosion

In WIPP PA, the anoxic iron corrosion reaction is modeled as:



In order to account for the material balance of brine and gas, the rate of reaction must be specified. BRAGFLO assumes iron corrosion reaction rates are zero order (constant). However, BRAGFLO recognizes a different reaction rate if the steel is in contact with liquid brine (inundated condition) or if the steel reacts with brine in the gas phase (humid condition). The input directives describing the two reaction rates are

RK(1) = brine inundated corrosion reaction rate [gm-mol Fe/m³/s],
 HF(1) = factor multiplying RK(1) to get humid corrosion reaction rate.

We introduce the notation

K_{ci} = RK(1), inundated reaction rate,
 K_{ch} = HF(1) × RK(1), humid reaction rate.

The portion of steel in contact with brine is assumed to react at the inundated rate, while the portion of steel in contact with gas reacts at the humid rate as long as some liquid phase brine is present to be in equilibrium with the brine in the gas phase. The fraction of steel in contact with brine in a grid block is assumed equal to the volume fraction of brine in the pore space, S_w . Similarly, the fraction of steel in contact with gas is equal to the volume fraction of gas, $(1-S_w)$. Thus the effective corrosion reaction rate becomes

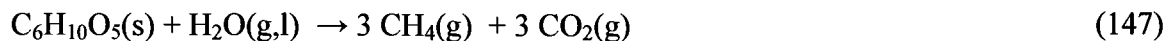
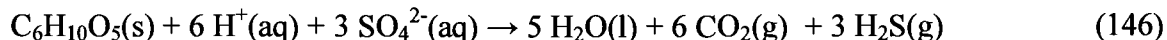
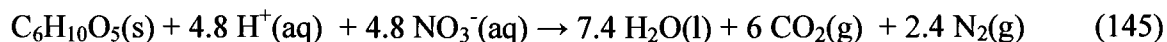
$$K_C = K_{CI} S_w + K_{CH} (1 - S_w). \quad (143)$$

4.13.4 Microbial Gas Generation

In BRAGFLO, the biodegradation reaction assumes microbial consumption of cellulose, $C_6H_{10}O_5$, with hydrogen gas as a product



The major pathways for biodegradation include the following reactions:



These reactions are assumed to proceed sequentially, consuming the limited amount of nitrate (NO_3^-) and sulfate (SO_4^{2-}) in the repository. Currently, it is assumed that there is sufficient sulfate in the surrounding rock to consume all the cellulose, and hence reaction (147) is not used.

Reaction rates for biodegradation are analogous to the iron corrosion reaction rates; that is, rates are specified for both inundated and humid conditions. The input directives describing the two reaction rates are

RK(2) = brine inundated biodegradation rate [gm-mol [$C_6H_{10}O_5$]/6 /m³/s]

HF(2) = factor multiplying RK(2) to get humid biodegradation rate

and are used to determine the overall biodegradation rate K_B in the same way RK(1) and HF(1) are used to determine the overall corrosion rate,

$$K_B = K_{BI} S_w + K_{BH} (1 - S_w), \quad (148)$$

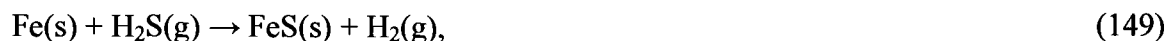
where

K_{BI} = RK(2), inundated reaction rate,

K_{BH} = HF(2) × RK(2), humid reaction rate,

and S_{eff} from equation (141) is sent to the subroutines BIOSAT and BIOHUM as S_w .

When cellulose is degraded by sulfate reduction, hydrogen sulfide (H_2S) is produced. The reactions of iron and its corrosion products with H_2S are modeled as,



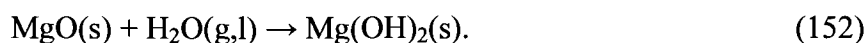
A new subroutine BIOFES has been added to calculate the effective rates of iron sulfidation. It is assumed that these reactions are much faster than the biodegradation and so effectively happen instantaneously and hence the rate is calculated as the biodegradation rate multiplied by a factor,

$$K_{FeS} = RXH2S K_B, \quad (151)$$

where the factor *RXH2S* is the ratio of moles of H₂S produced per mole of carbon generated by the biodegradation. For example, with no nitrate in the repository, only reaction (146) would be used and *RXH2S* would be calculated as 0.5. We assume that reaction (150) kinetically dominates reaction (149) if iron hydroxide is available. If iron hydroxide is not available we assume that equation (150) occurs. This is rarely used since iron corrosion is generally faster than biodegradation, but is included for completeness.

4.13.5 MgO Hydration and Carbonation

In BRAGFLO the subroutine CORMGO has been added to calculate the effective rate of MgO hydration to form brucite, Mg(OH)₂, under inundated and humid conditions

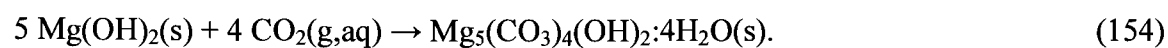


This routine takes as input the base rates of hydration of MgO under humid (*BRUCITEH*) and inundated (*BRUCITEI*) conditions, which enter BRAGFLO through the input file. We assume that if water is present, the humidity of WIPP is constant at 70% relative humidity (see Subsection 1.10.3 of Brush, 1990). The rate of MgO hydration is calculated analogously to the previously discussed chemistry rates under inundated and humid conditions,

$$K_{Mg(OH)_2} = BRUCITEI S_w + BRUCITEH (1 - S_w), \quad (153)$$

where S_{eff} from equation (141) is sent to the subroutine CORMGO as S_w .

The subroutine BIOMGO has been added to calculate the rate of brucite carbonation to hydromagnesite, Mg₅(CO₃)₄(OH)₂:4H₂O,

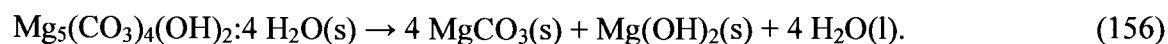


It is assumed that this reaction is much faster than the biodegradation and so effectively happen instantaneously and hence the rate is calculated as the biodegradation rate multiplied by a factor,

$$K_{HYDRO} = RXCO2 K_B, \quad (155)$$

where the factor *RXCO2* is the ratio of moles of CO₂ produced per mole of carbon generated by the biodegradation. For example, using reactions (145) and (146) gives a *RXCO2* of 1.0. In the event that there is production of CO₂, but no brucite available, the BIOMGO subroutine will convert MgO directly to magnesite. This is rarely used since MgO hydration is generally faster than biodegradation, but is included for completeness.

Since hydromagnesite is not thermodynamically stable under repository conditions, it is expected to dehydrate to form magnesite. The subroutine HYDROCONV has been added to calculate the rate of hydromagnesite conversion to magnesite, MgCO₃,



This routine takes as input the intrinsic rate of hydromagnesite conversion (*HYMAGCON*), which enters BRAGFLO through the input file. The rate of hydromagnesite conversion is calculated as the product of the intrinsic rate and the hydromagnesite concentration, C_{HYDRO} ,

$$K_{MgCO_3} = HYMAGCON C_{HYDRO}, \quad (157)$$

4.13.6 Rate Smoothing and Tapering

In BRAGFLO, an additional smoothing is performed on the total (inundated+hydrated) rates of all chemical reactions,

$$K_{smoothed} = K \text{Exp}(\alpha C / C_i), \quad (158)$$

where K is the unsmoothed rate of a reaction described in Subsections 4.13.3-4.13.5, C is the concentration of the species being produced (or destroyed) by the reactions described in Subsections 4.13.3-4.13.5, C_i is a initial concentration of a relevant compound, and α is described in Subsection 4.13.1. For all MgO reactions (hydration and carbonation) the initial concentration of MgO is used for C_i . For all iron reactions the initial concentration of iron is used for C_i . For all biodegradation reactions the initial concentration of cellulose is used for C_i . This smoothing prevents a discontinuity in the first derivative of the rates when a reaction runs out of a reactant (other than water which is handled by equation (141)). This is necessary because most of the reactions in BRAGFLO are assumed to be zero'th order and some reactions will continuously have and run out of reactants, such as brucite carbonation, and sulfidation of iron hydroxide.

In BRAGFLO, the initial concentrations of cellulose, iron, and MgO, are stored on a cell by cell basis in the arrays CONCBIOL, CONCFEI, and CONCMGI respectively. This is accomplished in the subroutine STOREINT. The initial concentrations enter BRAGFLO through the input file.

In BRAGFLO all of the chemistry rates (including the new rates) are tapered in the event that a reaction will run out of a reactant (other than water) in the middle of a time step. If given the current time step and current concentrations, a reactant will be used up in the current time step, the rate is adjusted so that the reactant will have zero concentration at the end of the time step.

4.13.7 Solids Production

In BRAGFLO the volume of solids produced (or consumed) from the chemical reactions discussed in Subsection 4.13 are calculated.

The total volume of solids produced (or consumed) normalized by cell volume is calculated from the concentrations of species 3 through 10 in Table 2, and the concentration of salt produced by dehydrating brine minus the initial concentrations

$$\Delta V = \sum_{i=1}^9 \Delta V_i, \quad (159)$$

where

$$\Delta V_i = (C_{i,t} - C_{0,i}) / DEN(i), \tag{160}$$

$C_{i,t}$ is the concentration of species i at time t (in kg/m^3), $C_{0,i}$ is the initial concentration of species i , and $DEN(i)$ the density of species i , which is part of the RXN common block. The index and identity of the species in this subroutine is given in Table 3.

Table 3. Index and corresponding compound in density array DEN

Index	Compound
1	Fe
2	Fe(OH) ₂
3	FeS
4	cellulosics
5	MgO
6	Mg(OH) ₂
7	Hydromagnesite
8	MgCO ₃
9	Salts

4.13.8 Reaction Path Model

Another gas generation model is the reaction path model. This model considered a much larger number of possible reactions that could take place within the WIPP repository. Although it was still an equilibrium reaction model, it could account for the different paths that a sequence of reactions could follow. Input and output for the model was completed, together with a multi-component gas transport scheme (see Subsection 7.2.13), but the reaction path model itself has not been implemented and will not be used in the re-certification compliance calculations.

4.14 Linear Equation Solver

Each iteration step in the Newton-Raphson method requires the solution of a system of linear equations. Linear equation solvers fall into two general categories: direct or elimination type solvers and iterative solvers. Algorithms for direct solvers involve a finite number of arithmetic steps to produce the solution. Solution error in a direct solver occurs from round-off error in the arithmetic operations, which is a result of the finite word length representation of any number on a computer. BRAGFLO is written with double precision word length which produces floating point number representation of 64 bits or approximately 15 significant digits on a single word length machine such as the DEC Alpha. BRAGFLO has available a direct solver which uses LU-decomposition.

For large-scale problems accumulation of round-off error in a direct solver can swamp the true solution. Also storage and computation time may become prohibitive for direct solvers. Iterative

solvers are generally advantageous over direct solvers when the problem size becomes large. There are many iterative solvers found in the numerical literature. BRAGFLO includes a successive over relaxation (SOR) solver. Iterative solvers have the disadvantage that the solution depends on the convergence of an iterative procedure. For this reason direct solvers are more simplistic in concept and application.

For performance assessment work the original LU-decomposition method is used exclusively. It has been found from experience that the iterative solver (SOR) is not robust enough to successfully solve many of the performance assessment problems.

A description of the LU-decomposition algorithm will be presented. The method will be demonstrated with a small (4×4 matrix) example. The objective is to write the coefficient matrix (Jacobian matrix) as a product of two matrices,

$$\mathbf{LU} = \mathbf{A} \tag{161}$$

where \mathbf{L} is lower triangular (has non-zero elements only on the main diagonal and below) and \mathbf{U} is upper triangular (has non-zero elements only on the main diagonal and above). It is further possible to require the diagonals of \mathbf{L} to be equal to one. If $\mathbf{A} = (a_{ij})$, $\mathbf{L} = (\alpha_{ij})$ and $\mathbf{U} = (\beta_{ij})$, then for the case of a 4×4 matrix the decomposition would look like

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{21} & 1 & 0 & 0 \\ \alpha_{31} & \alpha_{32} & 1 & 0 \\ \alpha_{41} & \alpha_{42} & \alpha_{43} & 1 \end{bmatrix} \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} & \beta_{14} \\ 0 & \beta_{22} & \beta_{23} & \beta_{24} \\ 0 & 0 & \beta_{33} & \beta_{34} \\ 0 & 0 & 0 & \beta_{44} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \tag{162}$$

For example, it can be checked by matrix multiplication that the following is an LU-decomposition of the given 4×4 matrix:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 0 & -2 & -2 \\ 0 & 0 & 0 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -2 & 1 & 1 & 1 \\ 0 & 3 & 1 & 1 \\ 1 & 4 & 2 & 6 \end{bmatrix}$$

If the LU-decomposition of the matrix \mathbf{A} is known then the solution of the system of equations $\mathbf{Ax} = \mathbf{b}$ can be written as

$$\mathbf{Ax} = (\mathbf{LU})\mathbf{x} = \mathbf{L}(\mathbf{Ux}) = \mathbf{b}. \tag{163}$$

The solution is obtained by solving for the vector \mathbf{y} such that

$$\mathbf{Ly} = \mathbf{b} \tag{164}$$

and then solving

$$\mathbf{Ux} = \mathbf{y}. \tag{165}$$

The advantage of decomposing one linear set of equations into two successive sets of equations is that the solution of a triangular set of equations is an easy substitution calculation. Recall for the Modified Newton-Raphson method the Jacobian matrix is not updated every iteration; while, the right-hand side of the system of equations is recalculated each iteration. Once the LU-

decomposition of the Jacobian matrix is obtained, the Newton-Raphson iteration step is accomplished by solving the system $\mathbf{L}\mathbf{y} = \mathbf{b}$ with updated right-hand side vector \mathbf{b} by applying the forward substitution algorithm

$$y_1 = \frac{b_1}{\alpha_{11}} \quad (166)$$

$$y_i = \frac{1}{\alpha_{ii}} \left[b_i - \sum_{j=1}^{i-1} \alpha_{ij} y_j \right] \quad i = 2, 3, \dots, N \quad (167)$$

and then solving the system $\mathbf{U}\mathbf{x} = \mathbf{y}$ with the back substitution algorithm

$$x_N = \frac{y_N}{\beta_{NN}} \quad (168)$$

$$x_i = \frac{1}{\beta_{ii}} \left[y_i - \sum_{j=i+1}^N \beta_{ij} x_j \right] \quad i = N-1, N-2, \dots, 1. \quad (169)$$

Given the coefficient matrix \mathbf{A} consider the computation of the decomposition matrices \mathbf{L} and \mathbf{U} . The (i,j) th entry in matrix \mathbf{A} will be the inner product of the i th row of \mathbf{L} with the j th column of \mathbf{U} . If the triangular structure of \mathbf{L} and \mathbf{U} are considered, then the resulting product is described by the two cases,

$$\sum_{k=1}^i \alpha_{ik} \beta_{kj} = a_{ij} \quad i = 1, \dots, j \quad (170)$$

$$\sum_{k=1}^j \alpha_{ik} \beta_{kj} = a_{ij} \quad i = j+1, \dots, N \quad (171)$$

Crout's algorithm (Maron, 1982) solves the equations for the α 's and β 's by arranging the equations in a certain order. The algorithm is sequential over columns from 1 to N . For the j th column the β_{1j} to β_{jj} are computed from linear system (170) by

$$\beta_{ij} = a_{ij} - \sum_{k=1}^{i-1} \alpha_{ik} \beta_{kj} \quad \text{for } i = 1, \dots, j \quad (172)$$

followed by the solution of $\alpha_{j+1,j}$ to α_{Nj} from linear system (171) by

$$\alpha_{ij} = \frac{1}{\beta_{jj}} \left(a_{ij} - \sum_{k=1}^{j-1} \alpha_{ik} \beta_{kj} \right) \quad \text{for } i = j+1, \dots, N. \quad (173)$$

The following example will demonstrate that the α 's and β 's that occur on the right-hand side of equations (172) and (173) are already determined by the time they are needed.

Within BRAGFLO the LU-decomposition is done within the band structure of the Jacobian matrix. This is crucial for efficient computation. Therefore, the above algorithms must be modified to work only within the bandwidth of the Jacobian matrix. Further, only the band structure is stored in the BRAGFLO treatment. This allows considerable saving in the storage

requirement. Finally, BRAGFLO implements a partial pivoting (row interchanges) which reduces the round-off errors in the arithmetic and is essential for the numerical stability of Crout's method.

Now consider the example with

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -2 & 1 & 1 & 1 \\ 0 & 3 & 1 & 1 \\ 1 & 4 & 2 & 6 \end{bmatrix} \quad (174)$$

Starting with the first column we solve for $\beta_{11} = 1$ from equation (172) where the sum is taken to mean zero. Equation (173) is then used to solve sequentially for $\alpha_{21} = -2$, $\alpha_{31} = 0$, and $\alpha_{41} = 1$. We now proceed to the second column and from equation (172) compute sequentially $\beta_{12} = 1$, $\beta_{22} = 3$. Now from equation (173) we compute $\alpha_{32} = 1$ and $\alpha_{42} = 1$. This procedure is continued for the 3rd and 4th columns with the resulting \mathbf{L} and \mathbf{U} given by the example stated earlier in this section.

Now suppose the solution of the system $\mathbf{Ax} = \mathbf{b}$ is required given right-hand side vector $\mathbf{b} = (4, 1, 5, 13)^T$. We first solve the system $\mathbf{Ly} = \mathbf{b}$ by the forward substitution algorithm. The system is

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \\ 5 \\ 13 \end{bmatrix}$$

Forward substitution from the first equation to the fourth equation yields $\mathbf{y} = (4, 9, -4, 4)^T$. We then solve the system $\mathbf{Ux} = \mathbf{y}$. The system is

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 0 & -2 & -2 \\ 0 & 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 4 \\ 9 \\ -4 \\ 4 \end{bmatrix}$$

Back substitution from the fourth equation to the first equation yields $\mathbf{x} = (1, 1, 1, 1)^T$.

4.15 Model Geometry

The mesh used in the BRAGFLO simulations incorporates radial flow phenomena at large distances from the repository and includes the full accessible volume available for multiphase flow. Time and cost constraints currently preclude a full three-dimensional representation of the repository and surrounding strata, so a two-dimensional approximation to the actual geometry is made, as described in WIPP PA Department (1992b).

4.16 Well Models

Well behavior is described by an inflow performance relation:

$$q_l = -\frac{(PI)\rho_l k_{rl}}{\mu_l} (P_l - P_{wf}), \quad (175)$$

where

l	=	phase index ($l = w, g$),
q_l	=	phase mass flow rate [kg/s],
P_l	=	phase pressure [Pa],
P_{wf}	=	flowing wellbore pressure [Pa],
PI	=	well productivity index [m^3],
ρ_l	=	phase density [kg/m^3],
μ_l	=	phase viscosity [Pa s],
k_{rl}	=	phase relative permeability.

The material balance requires the mass rate for each phase. If a well is operated as rate-specified, the inflow performance equation determines the flowing wellbore pressure, although BRAGFLO does not do this calculation. For this reason, BRAGFLO does not use the PI and P_{wf} values for rate-specified wells, although values are required on input. If the well is operated as pressure-specified, the rate is computed from the inflow performance relation. The required input parameters for either a rate- or pressure-specified well is found in the Subsection 7.2.5.

The well type as specified in the input file determines the well operation. The operation by well type is as follows:

- INJQ: The well injects ($q_l > 0$) or produces ($q_l < 0$) at a specified rate.
- INJP: The well injects at a specified flowing wellbore pressure. If the inflow performance relation predicts $q_l < 0$, then the rate is set to zero.
- PROD: The well produces at a specified flowing wellbore pressure. If the inflow performance relation predicts $q_l > 0$, then the rate is set to zero.

BRAGFLO does not allow a well with completion in multiple grid blocks. However, BRAGFLO does allow multiple wells in a single grid block. The information describing well location, number of wells in a grid block, and the time period over which each well is in operation is specified in the input file.

4.17 Special Materials

BRAGFLO has four special material types that have unique capabilities. These have evolved to handle situations encountered in modeling the WIPP, so they have names that apply to regions included in models of the WIPP, but actually have fairly general applicability. The materials are referred to as:

- Waste,
- DRZ (Disturbed Rock Zone),
- Reset
- Borehole.

4.17.1 Waste Material

In Waste materials, and only in Waste, can chemical reactions take place. Another special capability unique to Waste is simulation of creep closure, in which the porosity decreases over time, the rate depending on the rate of gas production and the pressure within the Waste. Porosity can change in any material as a result of pressure-dependent compressibility, but the change is generally quite small. In contrast, the porosity change resulting from creep closure of the Waste can be very large, changing from an initial 66% porosity to as low as 9% porosity. Only in Waste can there be an *initial* mass of radionuclides, the transport and decay of which can be modeled in any region as long as there was some amount initialized in the Waste. Finally, during the operational period in the WIPP when excavations are open to the atmosphere and any brine seepage is removed by means of ventilation or pumping, the initial brine pressure and saturation in the Waste can be specified to be different from the initial conditions. Then, at some later time the conditions in the Waste can be reset to the specified initial conditions.

4.17.2 Disturbed Rock Zone (DRZ) Material

Certain materials and flow conditions are required to be reset at the time the repository obtains closure. In the DRZ material, if the porosity has increased at the time the initial conditions are reset the brine volume is assumed to remain fixed over that change, and the brine saturation is adjusted to account for the increased pore volume. Gas is assumed to fill the additional pore space. The gas appears instantaneously, *i. e.*, it does not flow from any other cell, is not introduced by well injection, and is not created by way of chemical reaction. The pressure in this material at reset time is specified by input. This material arose from a need to simulate the disturbed rock zone surrounding excavations. The time-dependent behavior of disturbed halite is not well understood, but it is considered likely that the porosity will be greater by the time the repository is filled and sealed. This behavior is currently modeled very simply as an instantaneous increase in porosity with the additional pore space filled with gas that, in reality, would have flowed in from the adjacent excavated regions through cracks and borings. More than one DRZ material can be used, each with a different reset pressure. In modeling the WIPP the pressure is reset to 1 atm (101.325 kPa), the same as in the Waste so that the newly-introduced gas in the DRZ does not expand and unrealistically flow into the Waste.

4.17.3 "Reset" Material

In this material, conditions will be reset to the initial conditions. This differs from DRZ material in that both saturation and pressure are reset. In contrast, in DRZ material, the saturation is adjusted to maintain a fixed brine volume and the pressure is reset to a specified value, rather than to the initial pressure. These materials arose in modeling the WIPP from the need to simulate backfilled regions, which are initially excavations, but become backfill. Because the backfilled and sealed regions may cover a large number of grid blocks, these new conditions are most easily provided with the original initial conditions.

4.17.4 Borehole Material

In this material, the solute concentration and solute mass are reset to zero when an intrusion borehole opens. This simulates the removal of radionuclides in both solid and dissolved phases

when a drill cuts through the waste. It is a minor adjustment, but easily accomplished in BRAGFLO, so it is done just to make the results reflect reality slightly more accurately. It is used only when nuclide transport is activated. Nuclide transport is not qualified for use in WIPP compliance calculations and is not tested.

In BRAGFLO, a subroutine RESETMID has been added which resets the saturation, pressure, and concentrations in a material at the time of a material change. This routine was designed for the Borehole material at the time of an intrusion but can be used on other materials as well. The input parameters for this subroutine are read in through the input file, in the subroutine READMAT.

In the BRAGFLO main program at the completion of a time step, BRAGFLO checks to see whether the current time is equal to a time (TIMEBORE) at which the saturation, pressure and concentrations are supposed to be reset in a borehole. If yes, then the subroutine RESETMID is called; RESETMID is called before the material change is made in the subroutine MATERIALS. The subroutine RESETMID then checks each block to determine if its material is a material (MATBORE) to be reset at the current time. If yes, then the pressure is reset to PORSET and the saturation is reset to SORESET. If the flag ICHM is set equal to one (in the input file) then all concentrations of CPR, iron, iron corrosion products, and MgO products are set equal to zero in that material. Finally the capillary pressure, relative permeability, gas pressure, and dissolved gas terms are reset based on the new saturation and pressure.

4.18 Smooth Transition during Material Changes

In BRAGFLO Version 5.0, material changes such as drilling intrusions into the waste area were treated as instantaneous changes in the grid materials. This was equivalent to restarting the code at the time of the material change but with initial conditions that were equal to the state of the previous material at the time immediately before the material change. Although certain material changes occur over very short time-scales, such as an intrusion, we do not believe that instantaneous changes are necessarily the right way to numerically handle all of these events.

BRAGFLO Version 6.02 has a subroutine SMOOTHPERM which smoothly changes the permeability, and thus the capillary pressure with time during a material change. In the input file, the user chooses the initial material number (contained in the array MATSP), a final material number (contained in the array MATSPF), a time at which the material change ends (contained in the array TEND), and the time over which the material change occurs (contained within the array TCHANGE). The user also inputs the coefficients a_i of the polynomial used to smooth transitions

$$\ln(k) = \ln(k_i) + [\ln(k_f) - \ln(k_i)] \sum_{j=0}^7 a_j \left(\frac{t - t_i}{\Delta t} \right)^j \quad \text{for } t_i \leq t \leq t_f \quad (176)$$

where k_i is the initial permeability at time $t_i = TEND - TCHANGE$, k_f is the final permeability, and $\Delta t = TCHANGE$ is the time over which the change occurs.

4.19 Gas Dissolution Models

Dissolution of gas in brine can be modeled in BRAGFLO. A bubble point tracking treatment is available but is untested and its use is not recommended. A Henry's law treatment is also available. Additional details and input for these models are described in Subsection 7.2.9. Gas dissolution will not be included in the WIPP re-certification compliance calculations.

5.0 Capabilities and Limitations of the Software For the WIPP Application

BRAGFLO is the two-phase (brine and gas) finite difference program used to study the fluid flow within the WIPP repository site. The BRAGFLO code is an essential part of the probabilistic modeling necessary for performance assessment of the WIPP site. BRAGFLO Version 6.02 has more capabilities than are necessary for the WIPP PA application. The implementation of BRAGFLO Version 6.02 for the WIPP PA has the following capabilities and limitations:

1. The WIPP PA implementation of BRAGFLO assumes two fluid phases: a liquid phase (brine) and a gas phase (H_2) (Subsection 4.8).
2. In the WIPP PA implementation of BRAGFLO fluid phases are assumed to be immiscible. (Subsection 4.8).
3. In the WIPP PA implementation of BRAGFLO the liquid phase consists of one component, brine. Dissolution of gas in the brine phase is not considered.
4. In the WIPP PA implementation of BRAGFLO the gas phase consists of one component, H_2 . Water vapor in the gas phase is not considered. The primary component of the gas generation process is H_2 (Subsection 4.13)
5. The WIPP PA implementation of BRAGFLO has the capability of computing relative permeability and capillary pressure using several different empirical relations. Choice of the characteristic curves is controlled by the user (Subsection 4.9).
6. The WIPP PA implementation of BRAGFLO allows for coupling to the mechanical system (rock matrix) through the introduction of a variable rock compressibility (Subsection 4.10).
7. The fracture treatment in the WIPP PA implementation of BRAGFLO allows for pressure induced alterations to the porosity by introducing a pressure-dependent porosity (Subsection 4.10).
8. In the WIPP PA implementation of BRAGFLO fracture treatment further allows for change in the fracture material permeability (section 4.10).
9. Representation of the creep closure within the WIPP PA implementation of BRAGFLO is accomplished by a change in the formation porosity. This porosity function or porosity surface will be time dependent and is also driven by pressure. The resulting closure information comes from a geomechanical simulation using the structural mechanics code SANTOS (Subsection 4.11).
10. The WIPP PA implementation of BRAGFLO corrects gas permeability for the Klinkenberg effect (Subsection 4.12).
11. Well models in the WIPP PA implementation of BRAGFLO allow simulation of gas or brine injection or production (Subsection 4.16).
12. Within the WIPP PA implementation of BRAGFLO there are chemical reactions which consume brine and generate gas. The WIPP PA implementation of BRAGFLO accounts for these reactions by using the Average Stoichiometry Model, which,

- assumes that all reaction rates are zero order (independent of reactant or product concentration). However, the WIPP PA implementation of BRAGFLO recognizes a different reaction rate if the solid reactant is in contact with liquid brine (inundated condition) or if the solid reacts with brine in the gas phase (humid condition) (Subsection 4.13).
13. The WIPP PA implementation of BRAGFLO assumes that the directions of the permeability tensor are aligned with the reservoir coordinate axis; that is, $\theta = 0$ (Subsection 4.3).
 14. The WIPP PA implementation of BRAGFLO evaluates brine density assuming its fluid compressibility is constant (Subsection 4.4).
 15. The WIPP PA implementation of BRAGFLO uses the Redlich-Kwong-Soave equation of state to relate gas density to pressure (Subsection 4.4).
 16. The WIPP PA implementation of BRAGFLO treats viscosity constant for both water and gas (Subsection 4.4).
 17. The WIPP PA implementation of BRAGFLO assumes a no-flow Neumann type boundary condition at all exterior grid boundaries (Subsection 4.4).
 18. The WIPP PA implementation of BRAGFLO uses a fully implicit formulation to solve the material balance equations (Subsection 4.5).
 19. The WIPP PA implementation of BRAGFLO uses a first order difference quotient approximation for the Jacobian evaluation (Subsection 4.6).
 20. In the WIPP PA implementation of BRAGFLO the user can specify from input directives the frequency of the Jacobian evaluation in the Newton-Raphson iteration (Subsection 4.6).
 21. For both storage and computational considerations the linear equation solver should take advantage of the banded structure. The WIPP PA implementation of BRAGFLO uses the banded LU solver (Subsection 4.14).
 22. To minimize the bandwidth, the WIPP PA implementation of BRAGFLO orders the grid blocks so that sequential indexing proceeds first in the shortest grid direction, then in the longest grid direction (Subsection 4.7).
 23. The WIPP PA implementation of BRAGFLO is written with double precision word length which produces floating point number representation of 64 bits or approximately 15 significant digits on a single word length machine such as the DEC Alpha. The only qualified solver is the LU-decomposition (Subsection 4.14).
 24. The WIPP PA implementation of BRAGFLO implements a partial pivoting (row interchanges) which reduces the roundoff errors in the arithmetic and is essential for the numerical stability of Crout's method (Subsection 4.14).

6.0 User Interactions with the Software

To exercise BRAGFLO, the BRAGFLO command (.COM) file must specify the desired input and output files. The following files must be specified:

1. The BRAGFLO input control (.INP) file for the sampled vector. This file is the ASCII input file that controls BRAGFLO; it is generated by PREBRAG, the code immediately upstream from BRAGFLO (Figure 29).
2. The input file containing the closure sureface data (.CSD). This file is an ASCII input file that is read by BRAGFLO if creep closure is to be simulated (i.e. "CLOSURE" .EQ. .TRUE on Line 10.2 of the input file). If creep closure is not to be simulated a dummy file must be included even though this dummy file will not be read, (see Figure 29). The user is responsible for the creation of the .CSD file. It is not generated by PREBRAG.
3. The BRAGFLO binary output (.BIN) file for the sampled vector. This file is the primary results file that is converted by POSTBRAG (Figure 29) into standard .CDB format. Interrogation of the .BIN file is facilitated by using POSTBRAG and ALGEBRA which provide for using varous analysis tools.
4. The BRAGFLO ASCII output (.OUT) file for the sampled vector. This file echoes input and provides user-readable output and QA information.
5. The BRAGFLO summary (.SUM) file for the sampled vector. This file contains a limited amount of summary information on results at each time step.
6. The BRAGFLO restart output (.ROT) file for the sampled vector. Enough information is stored in this binary file to permit restarting BRAGFLO if execution is halted.
7. The BRAGFLO restart input (.RIN) file for the sampled vector. This binary file, a copy of the .ROT file, is read at the beginning of a restart run.

The name of the restart input file may be specified, even though BRAGFLO runs for the WIPP calculations do not presently use it.

The above files are specified in the command (.COM) file that runs BRAGFLO. The file names are already entered into the DEFINE lines of the .COM file. A sample .COM file with the six specified file names follows:

```
$ DEFINE BF2_UIF$INPUT BF2_TEST7_V001.INP
$ DEFINE BF2_UIF$INPUTCS BF2_TEST7_V001.CSD
$ DEFINE BF2_DBG$OUTPUT BF2_TEST7_V001.OUT
$ DEFINE BF2_DBG$SUMMARY BF2_TEST7_V001.SUM
$ DEFINE BF2_BIN$OUTPUT BF2_TEST7_V001.BIN
$ DEFINE BF2_IN$RESTART BF2_TEST7_V001.RIN
$ DEFINE BF2_OUT$RESTART BF2_TEST7_V001.ROT
```

If so desired, the user can modify those file names by editing the DEFINE lines.

Information Only

If the user wishes to run BRAGFLO interactively, he or she can enter the following command after the VMS \$ prompt, followed by a carriage return:

```
@[name of .COM command file]
```

If the user wants to run BRAGFLO in "batch" mode, he or she can enter the following command after the VMS "\$" prompt, followed by a carriage return:

```
SUBMIT/QUEUE=SYS$BATCH [name of .COM command file]
```

Both options are shown in Figure 30. Regardless of the approach, BRAGFLO executes as directed by the input control .INP file, the closure surface data input .CSD file, and outputs the Files 3, 4, 5, 6, and 7, as shown in Figure 30.

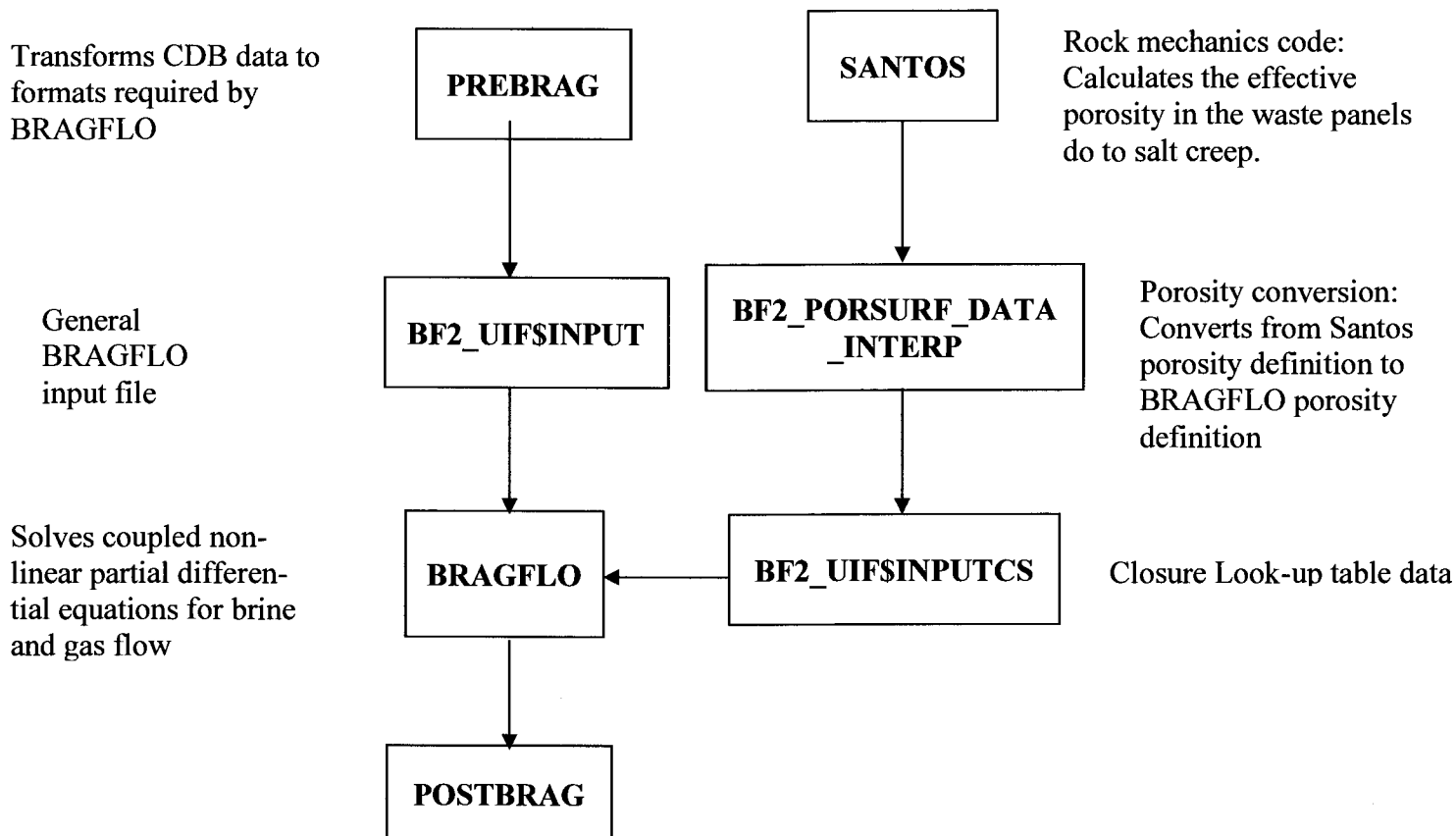


Figure 29. Sample computational flow diagram for BRAGFLO, highlighting flow to and from BRAGFLO.

```
$BRAGFLO
>Submit/QUEUE=SYS$BATCH [>com file name]
or
>@[name of .COM command file]
```

```
$DEFINE BF@_UIF$INPUT BF2_TEST0_V001.INP
$DEFINE BF@_UIF$INPUTCS BF2_TEST0_V001.CSD
$DEFINE BF@_UIF$INPUT BF2_TEST0_V001.OUT
$DEFINE BF@_UIF$INPUT BF2_TEST0_V001.SUM
$DEFINE BF@_UIF$INPUT BF2_TEST0_V001.BIN
$DEFINE BF@_UIF$INPUT BF2_TEST0_V001.RIN
$DEFINE BF@_UIF$INPUT BF2_TEST0_V001.ROT
```

File 1
 File 2
 File 3
 File 4
 File 5
 File 6
 File 7

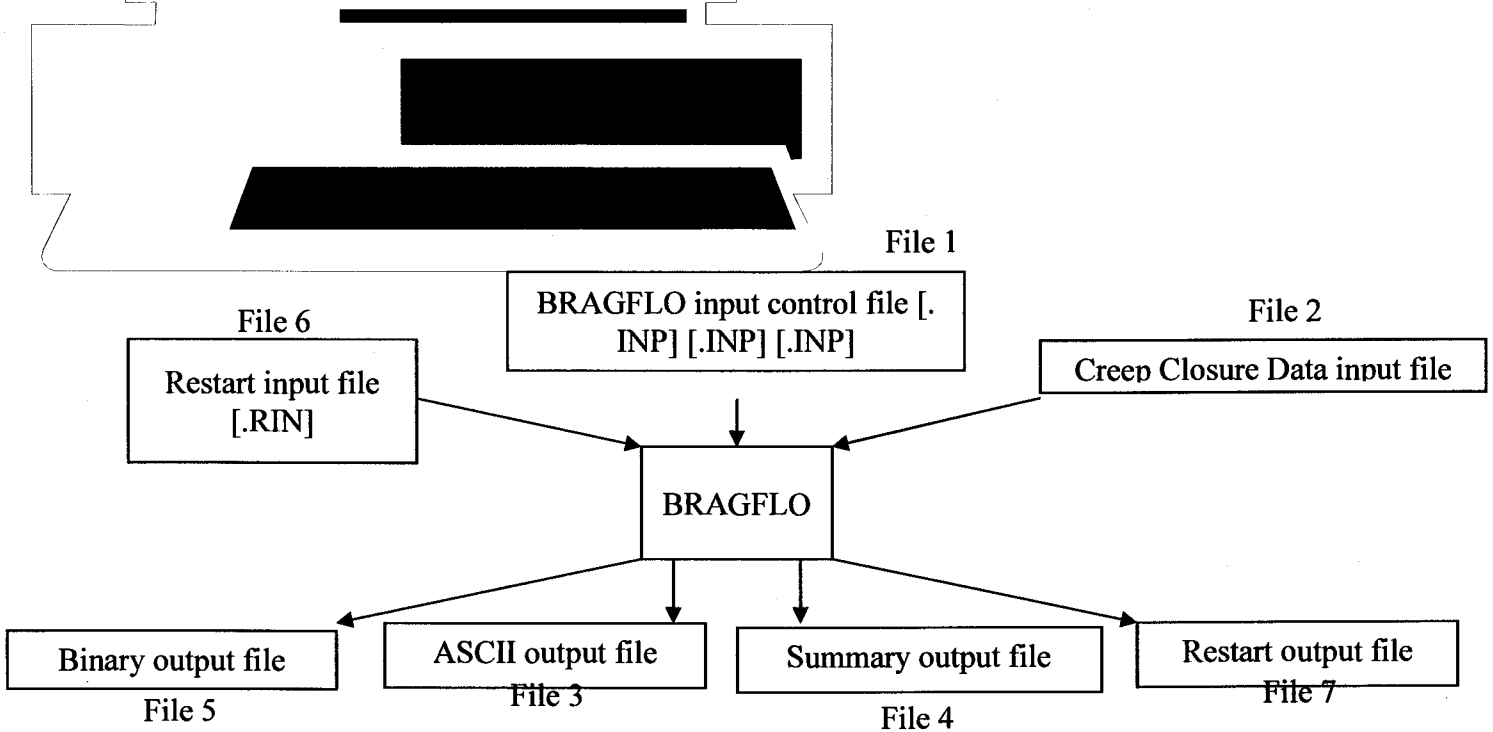


Figure 30. User-required file specifications for BRAGFLO.

7.0 Description of input files

BRAGFLO requires two user specified input files. The first input file is the BRAGFLO input control file. This input file is described in detail in Subsection 7.2. The second input file is the creep closure look-up table data input file. This input file is described in detail in Subsection 7.3.

7.1 Parameter Statement

BRAGFLO uses one INCLUDE file, BF2_PARAMS.INC, containing a single PARAMETER statement that sets dimensions on many of the arrays used in BRAGFLO. (Where the term "PARAMETER statement" is used in this manual, it refers to the statement in BF2_PARAMS.INC.) An example of the INCLUDE file follows:

```

C
C   NOTE:  Value of MDIM = 3*(NEQ*[MIN(MX*MY, MX*MZ, MY*MZ)+1]-1)+1
C           Value of IBWM = 3*MAX(MX*MY, MX*MZ, MY*MZ)+1
C
C   INTEGER
1   MX           , MY           , MZ           , MG           ,
2   NEQ         , MGNEQ        , MDIM        , NPHASE       ,
3   NWTIME      , NW           , NWPERGRID   , MMAT         ,
4   NPINT       , NCOMP        , MGAS        , MRAD         ,
5   MRXYZ       , MAXPRNTASC  , MAXPRNTBIN  , MAXPRNTRST
C
C   INTEGER
1   MAXMATTIMES, NWTIMEP      , NDTFIXMAX   , MAXMATTIMP   ,
2   NDTFIXMAXP , NSDATA          , NTDATA      , MKLOS        ,
3   MMON       , MWST           , MDRZ        , NVPR         ,
4   MXHIV     , MVHIV          , IBWM        , MRWXYZ       ,
5   MWXYZ     , MGVAR          , MSPEC       , NDIRMAX
C
C   PARAMETER (MX=210, MY=120, MZ=1, MG=MX*MY*MZ, NEQ=2, MGNEQ=MG*NEQ,
1   MDIM=244, NPHASE=2, NWTIME=10, NW=50, NWPERGRID=2, MMAT=80,
2   NPINT=10000, NCOMP=3, MGAS=6, MRAD=1, MRXYZ=MRAD*MG,
3   MAXPRNTASC=100, MAXPRNTBIN=100, MAXPRNTRST=100,
4   MAXMATTIMES=20, NWTIMEP=NWTIME+1, NDTFIXMAX=50,
5   MAXMATTIMP=MAXMATTIMES+1, NDTFIXMAXP=NDTFIXMAX+1,
6   NSDATA=13, NTDATA=214, MKLOS=4, MMON=9, MWST=2, MDRZ=1,
7   NVPR=112+3*MWST*(1+MRAD), MXHIV=15000, MVHIV=MG, IBWM=8401,
8   MRWXYZ=MRAD*MWST*MG, MWXYZ=MWST*MG, MGVAR=10, MSPEC=23,
9   NDIRMAX=204)
  
```

The parameters that can be changed by the user are listed here. Note that all of these parameters are maximum values. They can be set to be larger than required for the problem being run, but to minimize memory requirements, the smallest values needed to run the problem should be used. No values less than one should be used.

Table 4. Variables used in BF2_PARAMS.INC

Parameter	Description
-----------	-------------

MX	Maximum number of grid blocks in the <i>x</i> -direction; can be greater than the actual number of grid blocks in the problem to be run.
MY	Maximum number of grid blocks in the <i>y</i> -direction; can be greater than the actual number of grid blocks in the problem to be run.
MZ	Maximum number of grid blocks in the <i>z</i> -direction; can be greater than the actual number of grid blocks in the problem to be run.
MDIM	Minimum bandwidth of the Jacobian matrix; the value should be calculated using the formula: $MDIM = 3 * (NEQ * [MIN (MX * MY, MX * MZ, MY * MZ) + 1] - 1) + 1$
NWTIME	Maximum number of times that well properties will be changed.
NW	Maximum number of wells to be specified at any given time.
NWPERGRID	Maximum number of wells in any grid block.
NMAT	Maximum number of materials regions.
MRAD	Maximum number of radionuclides allowed in the transport, decay, and radiolysis calculation.
MAXPRNTASC	Maximum number of times at which an ASCII output dump can be specified.
MAXPRNTBIN	Maximum number of times at which a binary output dump can be specified.
MAXPRNTRST	Maximum number of times at which a restart can be specified.
MAXMATTIMES	Maximum number of times at which a new material map can be specified.
NDTFIXMAX	Maximum number of times that the time step can be fixed.
MMON	Maximum number of monitor grid blocks that can be specified.
MWST	Maximum number of waste regions allowed.
MDRZ	Maximum number of DRZ regions allowed.
MXHIV	Maximum total number of history variables allowed. Includes 10 time- and performance-related history variables; therefore, must be ≥ 10 .
MVHIV	Maximum number of history variables per output distribution (<i>e.g.</i> , brine pressure or gas saturation).
IBWM	Maximum bandwidth for Jacobian used in solution of multi-component gas transport model within BRAGFLO; value to be used is computed from the formula: $IBWM = 3 * MAX (MX * MY, MX * MZ, MY * MZ) + 1$ If gas transport is not being modeled, IBWM should be set to 1 to save large amounts of storage.
NDIRMAX	Maximum number of grid blocks in which Dirichlet boundary conditions can be specified.

Several parameters are set in the PARAMETER statement that should not or cannot be changed. These are described below so the user will know why they should not be altered, and, if they are inadvertently changed, how they can be reset to their correct values.

Table 5. Constants for BF2_PARAMS.INC

Parameter	Required Value	Description
NEQ	2	Number of equations being solved in BRAGFLO.
NPHASE	2	Number of immiscible fluid phases.
NPINT	10000	Number of pressure intervals at which gas density is evaluated when using the lock-up table to obtain gas density.
NCOMP	3	Number of components in all phases. Includes gas, brine, and gas dissolved brine.
MGAS	6	Number of gases for which equation of state parameters are included in BRAGFLO (H ₂ , CO ₂ , CH ₄ , N ₂ , O ₂ , and H ₂ S).
NSDATA	13	Number of gas-generation-rate entries in creep closure surface data.
NTDATA	214	Number of time entries in creep closure surface data.
MKLOS	4	Number of creep closure surfaces available in BRAGFLO.
MGVAR	10	Number of "global" variables printed out to binary and ASCII output files.
MSPEC	23	Maximum number of species to be used in the reaction path model.

7.2 Input Control File

As is explained in Section 6.0, the input control file for BRAGFLO is created by PREBRAG based on user inputs to PREBRAG. Even though the input control file for BRAGFLO is not technically user-specified, it is still important to understand and is therefore explained in detail in this user's manual.

The input file is composed of several sections, each dealing with different types of input. Within each section, input parameters control specific areas of the simulation. Input generally consists of a line of description or informative comments followed, on the next line, by one or more parameter values. The descriptive line can be any 132 characters. It is intended solely to make the input file easier to read and be understood by the user. None of the information on any of these descriptive lines is used for program control. The content of these lines is entirely at the discretion of the user and will have no effect whatsoever on how the program runs. The line can even be blank, if the user wishes, but there must be a line, informative or blank, and only one line, everywhere that one is indicated. An example input file is provided in Appendix A.

The order of the input is fixed, *i. e.*, each line of input must appear in exactly the order described in below. Any deviation from this order will cause BRAGFLO to abort or run incorrectly.

Many input values have units associated with them, examples being time and initial pressures. BRAGFLO generally allows input to be in either of two systems of units: SI or English. The choice is up to the user, but one system must be used consistently for all input parameters that have units. The description of each input parameter includes in brackets the units that can be used for that parameter, with the SI units given first and the English units second. If the parameter has no units, none is shown. In a few instances, only SI units are allowed. If no English units are mentioned in the description of the parameter, then English units are not allowed for that particular parameter. Further details concerning units are given in Subsection 7.2.3.

The input control file consists of the following sections, each dealing with different types of inputs:

1. startup and time control
2. output control parameters
3. mesh description parameters
4. well parameters and boundary conditions
5. initial conditions
6. numerical control parameters
7. material maps and material properties
8. fluid properties
9. chemical reaction parameters
10. creep closure parameters
11. radionuclide transport and decay parameters (Not used or qualified)
12. multi-component gas transport parameters (Not used or qualified).

7.2.1 PREBRAG QA Information

BRAGFLO, versions 4.00 and beyond allows QA information on PREBRAG to be placed into the .CDB file that is created when POSTBRAG processes the BRAGFLO output. This is accomplished by including this information in the BRAGFLO input file created by PREBRAG. Inclusion of this information is optional, in order to maintain compatibility with input files for earlier versions. If PREBRAG is used to set up the BRAGFLO input file, this information is written automatically to the BRAGFLO input file.

Line 0.1. PREBRAG QA flag.

If PREBRAG QA information is to follow, then the first nonblank characters on this line must be the character string:

****QA****

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Any number of blanks (up to 125) may precede this character string, and the rest of the line (up to 132 characters) can be blank or contain any characters or descriptions that the user wishes to use; but none of the information on this line will be saved & this line serves only as a flag.

If the characters ‘**QA**’ are not the first nonblank characters on this line, then it is assumed that PREBRAG QA information does not follow, and this line is assumed to be the title of the run, Line 1.1 (see next subsection, 7.2.2). In this case, no more input from this section can follow, or BRAGFLO will abort.

Line 0.2. Name of program.

The first nonblank characters on this line should be the string:

PREBRAG

Any number of blanks (up to 125) may precede this character string, and the rest of the line (to a total of 132 characters) can be blank or may contain any characters or descriptions that the user wishes to use, but none of that information will be saved; only the string ‘PREBRAG’ will be written to output files.

If the characters ‘PREBRAG’ are not the first nonblank characters on this line, then it is assumed that the input in this section is not PREBRAG QA information, and no PREBRAG QA information will be written to the output files. However, it is still necessary to include all of the lines in this section (Lines 0.1 - 0.6). If any of Lines 0.2 - 0.6 is completely blank, BRAGFLO will abort.

If this line does begin with ‘PREBRAG’, then the information on the next four lines will be written to the BRAGFLO output files.

Line 0.3. PREBRAG version number.

The first 8 characters starting with the first nonblank character must be the version number of PREBRAG used to set up the input file, *e. g.*, ‘6.00’. If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

Line 0.4. PREBRAG revision date.

The first 8 characters starting with the first nonblank character must be the revision date of PREBRAG used to set up the input file, *e. g.*, ‘01/19/96.’ If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

Line 0.5. PREBRAG run date.

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The first 8 characters starting with the first nonblank character must be the date on which PREBRAG was run to set up the input file, *e. g.*, '01/25/96'. If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

Line 0.6. PREBRAG run time.

The first 8 characters starting with the first nonblank character must be the time at which PREBRAG was run to set up the input file, *e. g.*, '11:13:44'. If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

The first 7 lines of the input file will typically appear as in the following example:

```
**QA**  
  
PREBRAG      -- Program name  
  
8.02  -- PREBRAG version number  
  
11/29/12    -- PREBRAG revision date  
  
11/30/12    -- PREBRAG run date  
  
11:13:44    -- PREBRAG run time  
  
Title of the run (Line 1.1)
```

7.2.2 Startup and Time Control

In this section, parameters that initialize the size of the problem and control the simulation time are input.

Line 1.1. Title of run.

This is a descriptive title for the simulation being run. This title is saved and printed to the output files, but otherwise has no effect on the performance of BRAGFLO.

Line 1.2. Descriptor. Logical flags indicating files to be used.

One-line (up to 132 characters) descriptor for the following parameters:

Line 1.3. LWASC, LWBIN, LWSUM, LWRST, LRRST.

Input each flag in free format as a T, .TRUE., F, or .FALSE., separated by one or more spaces or by commas.

LWASC: Flag indicating whether an ASCII output file is to be written.
LWBIN: Flag indicating whether a binary output file is to be written.
LWSUM: Flag indicating whether an ASCII summary output file is to be written.
LWRST: Flag indicating whether a binary restart output file is to be written.
LRRST: Flag indicating whether a binary restart input file is to be read. If this flag is .TRUE., then a restart input file for this run must exist in the same directory as the input [.INP] file. This file is created by copying a restart output [.ROT] file from an initial run into a [.RIN] file having the same root name as the input file used in the restart run. (Although it is best for traceability reasons for all files used in both initial runs and in restart runs to have the same root name, it is not necessary in order for the restart to run correctly.)

RESTART CAPABILITY IS NOT QA'D OR USED FOR WIPP COMPLIANCE CALCULATIONS.

Line 1.4. Descriptor. Model type and grid size parameter.

One-line (up to 132 characters) descriptor for the following parameters:

Line 1.5. MODTYPE, NX,NY,NZ.

MODTYPE: Number of dimensions being used for this run. Although BRAGFLO is a fully three-dimensional code, many shortcuts are taken that speed up execution if the problem being run is only one-dimensional ($NY = NZ = 1$) or two-dimensional ($NZ = 1$). MODTYPE is given a value of 1, 2, or 3, depending on whether the problem is 1-, 2-, or 3-dimensional, respectively. If a value less than 1 or greater than 3 is input, the program will abort with the following message printed to the screen:

```
*** MODTYPE Error in READSTARTUP ***
```

The ASCII output file provides additional information:

```
**FATAL ERROR in Input: MODTYPE = <input value>
```

```
**MODTYPE must be 1, 2, or 3.
```

NX: Number of grid blocks in the x-direction.

NY: Number of grid blocks in the y-direction.

NZ: Number of grid blocks in the z-direction. NX, NY, and NZ must be less than or equal to MX, MY, and MZ, respectively, (these are specified in the PARAMETER statement),

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and they must all be greater than zero. If not, BRAGFLO will abort with the following message printed to the screen:

```
*** Size error in READSTARTUP; invalid NX, NY, or NZ
The ASCII output file provides additional information:
```

```
** FATAL ERROR in Input:      NX,NY,NZ = <input values>
```

```
** Maximum values dimensioned:  MX,MY,MZ = <values set in PARAMETER statement>
```

```
** Minimum values allowed:      MX,MY,MZ =      1      1      1
```

Coordinate system. BRAGFLO uses a right-handed coordinate system in which the origin is at the front lower left corner of the region being modeled. In this system, the x -direction increases to the right, the y -direction increases into the page, and the z -direction increases upward. Gravity acts in the negative z -direction. The grid can be reoriented (for example, to make the y -direction vertical) with input described in Subsection 7.2.4 (Mesh Parameters). This will be discussed in more detail in Subsection 7.2.4.

Line 1.6. Descriptor. Simulation time limits.

Line 1.7. START, FINISH, MAXITF.

START: Start time for the simulation [s or days]. START can be negative; if so, certain special material properties can be changed at time zero. More details can be found in Subsection 7.2.8 (Material Properties).

FINISH: End time for the simulation [s or days].

MAXITF: Maximum number of time steps allowed in this run. This is the only means for limiting how long the simulation will run. WIPP Performance Assessment simulations typically require about 1000 time steps to complete a 10,000-yr simulation, depending on convergence criteria selected (Subsection 7.2.7). On a few occasions, more than 10,000 steps have been required. A value of MAXITF = 10000 is normally used; if more steps are required, the run can be restarted from where it ended at the 10000th step, because a restart record is always written at the end of a run, provided that LWANS = .TRUE. In a restart run that is to continue from the MAXITFth step, the new input file must have a value for MAXITF that is greater than the MAXITF in the original input file.

Line 1.8. Descriptor. Time step controls.

Line 1.9. DELT, DELTMIN, DELTMAX, DTIMEMAX, ITIMECNTRL, TSWITCH.

DELT: Initial time step [s or days]. Recommended value: 864. s (1/10 day).

DELTMIN: Minimum time step allowed [s or days]. Recommended value: 864. s (1/10 day).

DELTMAX: Maximum time step allowed [s or days]. Recommended value: 1.728×10^9 s (20,000 days or about 55 yr.).

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DTIMEMAX: Maximum fractional increase in time step that will be allowed when auto time step control is used [dimensionless]. A value of 1.0 would, in effect, turn off auto time step control. No check is made to ensure that a value greater than 1.0 is used. A value too close to 1.0, *e. g.*, 1.1, is generally inefficient, not taking full advantage of the tendency for pressures and flows eventually to equilibrate and thereby allow larger time steps. A value that is too large, greater than 2.0, is also inefficient because the solution will fail to converge much more frequently, resulting in wasted calculations as the time step size must be reduced and the time step repeated. The value used for DELTFACTOR (Subsection 7.2.6, Line 6.24) should be taken into consideration in selecting a value for DTIMEMAX. Recommended value: 1.5.

ITIMECNTRL: Flag for automatic time step control . Recommended value: 1.

= 0: A fixed time step of DELT will be used throughout the simulation.

= 1: Auto time step control will be used. Variable changes vary greatly throughout a typical simulation. Auto time step control allows large time steps to be taken when little is happening, but forces small steps to be used when rapid changes are occurring.

TSWITCH: Value of gas saturation that determines when to switch from relative to absolute change in gas saturation for calculating time step size when auto time step control is used (ITIMECNTRL=1). When the current value of gas saturation is greater than TSWITCH, the time step algorithm uses the relative change in saturation over the previous time step; otherwise, it uses the absolute change in gas saturation. Valid range of input value: 0 - 1. Recommended value: 0.01. In some instances, BRAGFLO will run faster when TSWITCH is turned off by using an input value of TSWITCH = 1.

Line 1.10. Descriptor. Time step changes.

Line 1.11. NDTFIX.

NDTFIX: Number of times at which the time step will be reset to a specified value, overriding the time step computed by the auto time step control. This feature allows computing time to be saved when major changes in material properties at some point in simulation time are likely to cause the auto time step control to cut back the time step repeatedly. By reducing the time step manually, fewer unsuccessful calculations will be performed. If the auto time step control is not being used (ITIMECNTRL = 0), this capability is not used, but some value must still be input for NDTFIX; a value of 0 is recommended. If NDTFIX < 0, BRAGFLO will behave as though NDTFIX = 0. If NDTFIX > NDTFIXMAX (set in PARAMS.INC), the run will abort with a message printed to the screen:

```
*** ERROR in READSTARTUP: NDTFIXMAX needs to be larger;
```

```
NDTFIX = <input value>
```

```
*** NDTFIX error in READSTARTUP ***
```

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The next line (1.12) is repeated NDTFIX times, each line with two numbers. If NDTFIX = 0, no lines are input for these two parameters. If ITIMECNTRL = 0 (*i. e.*, no auto time step control), but NDTFIX > 0, then NDTFIX lines of TIMEDTFIX and DTFIX must still be input, even though they will not be used.

Line 1.12. TIMEDTFIX(K), DTFIX(K).

TIMEDTFIX: Simulation time at which the time step will be reset [s or days].

DTFIX: New time step size to be used in the first time step after TIMEDTFIX is exceeded [s or days].

7.2.3 Output Control Parameters

This section describes input that controls output to the three output files: ASCII, binary, and restart files.

Line 2.1. Descriptor. Output interval specification; units used in input and output.

Line 2.2. IPRTYPEASC, IPRTYPEBIN, IPRTYPERST, UNITSI, UNITSO.

IPRTYPEASC: ASCII output control option.

IPRTYPEBIN: Binary output control option.

IPRTYPERST: Restart output control option.

Three options are available. Additional input is required for each option, and the type of additional input for each option differs.

0: Output at first, last, and fixed frequency of time steps.

1: Output at first and last time step and at fixed time intervals.

2: Output at specified times.

Printing at a fixed frequency of time steps (option 0) offers the advantage of more frequent output over a given time span when rapid changes are occurring and less output when changes are slower. This results when auto time step control is in effect, and the time step is small when changes are rapid and large when changes are small. This option is generally used only for output to the binary output file. Specifying output at selected times (option 2) or at fixed time intervals (option 1) is useful when comparisons of different runs will be made. These two options are usually used for the ASCII and restart output, where less frequent output is desired. The binary output file is intended to be the primary repository for results because more data can be stored more compactly than in the ASCII output. An important output feature in BRAGFLO is that whenever any results are printed to the ASCII file or to the restart file, they are also printed at the same time to the binary output file. Thus, the binary file contains the complete record of all results that have been printed to any output file.

UNITSI: Units used in the input (CHARACTER*8 variable). Options are: 'SI' or 'ENGLISH'. Recommended: 'SI'. The input is read in free format, so the input character string must be enclosed in tick marks.

UNITSO: Units used in the output (CHARACTER*8 variable). Options are: 'SI' or 'ENGLISH'. Recommended: 'SI'. The input character string must be enclosed in tick marks.

The same system of units must be used consistently throughout the input. Only these units can be used in the input:

Table 6. Conversion factors.

Quantity	SI units	English units	Conversion Factor (multiply by value in English units to obtain value in SI units)
Length	m	ft	0.3048
Mass	kg	lb	0.4535237
Time	s	day	86400
Temperature	K	°R	5/9
Amount of substance	gm-mol (mol)	lbmol	$2.2049564333683113 \times 10^{-3}$
Area	m ²	ft ²	0.09290304
Volume	m ³	ft ³	0.028316846592
Pressure	Pa	psi	6894.757293168362
Mass flow rate	kg/s	lb/day	$5.2499116898148148 \times 10^{-6}$
Concentration rate change	kg/(s·m ³)	lb/(day · ft ³)	0.018539888164305717
Density or concentration	kg/m ³	lb/ft ³	16.01846337396014
Velocity	m/s	ft/day	$3.527777777777778 \times 10^{-6}$
Volumetric rate	m ³ /s	ft ³ /day	3.2774128×10^{-7}
Viscosity	Pa·s	cP	0.001
Productivity index	m ³	bbbl · cP/ (day · psi)	$2.6688839796530887 \times 10^{-13}$
Slope of solution gas-brine ratio vs. pressure	Pa ⁻¹	ft ³ /(bbbl·psi)	$2.5832324345269173 \times 10^{-5}$
Slope of viscosity vs. pressure	s	cP/psi	$1.4503773773020921 \times 10^{-7}$
Permeability	m ²	darcy	$9.8692326671601282 \times 10^{-13}$

Subsequent input for output control depends on the input value selected for IPRTYPEASC, IPRTYPEBIN, and IPRTYPERST. ASCII output is dealt with first.

7.2.3.1 ASCII Output Controls.

Line 2.3. Descriptor. ASCII output time or frequency control parameters.

If IPRTYPEASC (Line 2.2) = 0 (output at fixed time step frequency):

Line 2.4. IPRNTASC.

IPRNTASC: ASCII output time step frequency.

If IPRTYPEASC (Line 2.2) = 1 (output at fixed time interval):

Line 2.4: TMEINTASC, SPTMEASC, FPTMEASC.

TMEINTASC: Time interval [s or days]

SPTMEASC: Starting output time [s or days]

FPTMEASC: Final output time [s or days]

If IPRTYPEASC (line 2.2) = 2 (output at specified times):

Line 2.4: NPTMEASC.

NPTMEASC: Number of specified times.

Line 2.4.1:Descriptor. "User Requested Printout Times"

Line 2.4.2: TIMESASC (NPTMEASC values).

TIMESASC: Specified output times [s or days]

7.2.3.2 Binary output controls.

Line 2.5. Descriptor. Binary output time or frequency control parameters.

If IPRTYPEBIN (Line 2.2) = 0 (output at fixed time step frequency):

Line 2.6. IPRNTBIN.

IPRNTBIN: Binary output time step frequency.

If IPRTYPEBIN (line 2.2) = 1 (output at fixed time intervals):

Line 2.6. TMEINTBIN, SPTMEBIN, FPTMEBIN.

TMEINTBIN: Binary output time interval [s or days].

SPTMEBIN: Starting time for binary output [s or days].

FPTMEBIN: Final output time for binary output [s or days].

If IPRTYPEBIN (Line 2.2) = 2 (output at specified times):

Line 2.6. NPTMEBIN.

NPTMEBIN: Number of output times specified.

Line 2.6.1. Descriptor. Output times.

Line 2.6.2. TIMESBIN (NPTMEBIN values).

TIMESBIN: Specified binary output times [s or days]

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7.2.3.3 Restart Output Controls.

The restart capability in BRAGFLO enables a run to be restarted from the point where the restart output is written. This feature is useful when debugging a case that is known to run into problems after much computing time has elapsed. It is also useful when conditions are changed part way through a base case; then, the base case can be run all the way to completion, with restarts written at specified times, and sub-cases can then be run starting from the restarts, rather than starting from the beginning, thereby saving much computing time. The restart file contains only enough information to enable BRAGFLO to resume from where the restart was written, including values of the dependent variables, certain cumulative variables, and current settings for flags that get changed over the course of a run. A regular input file is still needed to provide all the information normally obtained from an input file. The restart capability is discussed in detail in Subsection 7.2.14.

NOTE: RESTART CAPABILITY IS NOT TO BE USED FOR WIPP COMPLIANCE CALCULATIONS.

Line 2.7. Descriptor. Restart output time or frequency control parameters.

If IPRTYPERST (Line 2.2) = 0 (restart output at fixed time step frequency):

Line 2.8. IPRNTRST.

IPRNTRST: Restart output time step frequency.

If IPRTYPERST (Line 2.2) = 1 (restart output at fixed time intervals):

Line 2.8. TMEINTRST, SPTMERST, FPTMERST.

TMEINTRST: Restart output time interval [s or days]

SPTMERST: Starting time for restart output [s or days]

FPTMERST: Final time for restart output [s or days]

If IPRTYPERST (Line 2.2) = 2 (restart output at specified times):

Line 2.8. NPTMERST.

NPTMERST: Number of times to specify restart output.

Line 2.8.1. Descriptor. Restart output times.

Line 2.8.2. TIMESRST (NPTMERST values).

TIMESRST: Specified restart output times [s or days].

Element Variables. The next inputs are the ASCII and binary print control flags. These flags indicate which of at least 115 element variables are printed to the output files. Element variables are defined as any variable that has a time-varying value at each grid block. These are listed in Table 7. The number of element variables available to be printed out depends on the number of waste regions in the mesh (defined in Subsection 7.2.8) and the number (if any) of radionuclides being tracked in the transport calculation. There are 115 element variables that are always

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available, none of which is associated with radionuclide transport. Of these 115 variables, 45 (numbers 66-110) are associated with the reaction-path gas-generation model, which has been partially implemented but is not available for use in the current version of BRAGFLO. Any of the reaction path model variables can be printed out, but their values are all zero. The total number available is $NVPR = 115 + 3 \times MWST \times (1 + MRAD)$, where MWST is the number of waste regions, and MRAD is the number of radionuclides involved in transport and decay.

Line 2.9. Descriptor. ASCII print flags.

Line 2.10. NPRNTA (NVPR values).

NPRNTA: Flag to indicate output of element variables to the ASCII output file.

0 = Do *not* print this element variable to the ASCII output file.

1 = Do print this element variable to the ASCII output file.

Line 2.11. Descriptor. Binary print flags. Unlike almost all other descriptor lines in the BRAGFLO input file, this line cannot be blank. If it is blank, BRAGFLO will abort. Any non-blank character(s) may be used.

Line 2.12. NPRNTB (NVPR values).

NPRNTB: Flag to indicate output of element variables to the binary output file.

0 = Do *not* print this element variable to the binary output file.

1 = Do print this element variable to the binary output file.

History Variables. For purposes of the BRAGFLO input, a history variable is defined as any variable listed in Table 7, at a specified grid block location. History variables are printed at every time step, unlike the rest of the ASCII and binary printout, which is generally not printed at every time step, but rather at multiple time steps or at intervals specified in the input, as described above. History variables are printed only to the binary output file, never to the ASCII output file. The purpose for history variables is to allow accurate post-processing. For example, integration of brine flow past some boundary can be done in post-processing to give cumulative flows that are as accurate as if they were computed internally to BRAGFLO. Earlier versions of BRAGFLO performed some of this integration, but, without extremely complex input, it was not possible to keep the code general and not specific to a particular mesh. Without history variables, post-processing can only be done using the element variables, which are usually output at multi-step intervals. Then, variables that change rapidly over a short period of time cannot be integrated accurately.

Line 2.13. Descriptor. History variables.

Unlike almost all other descriptor lines in the BRAGFLO input file, this line cannot be blank. If it is blank, BRAGFLO will abort. Any non-blank character(s) may be used.

Line 2.14. NHIV.

NHIV: Total number of element variables (from the list in Table 7) that will be printed as history variables. This is the number of sets of variables to be read from input.

If NHIV = 0, no history variables will be printed out, and no more history variable input will be read from input.

If NHIV > 0, then read NHIV sets of lines 2.15 and 2.16:

Line 2.15. LH, NGBHIV, Text Label (i.e. NAME=BRINE PRESUURE).

LH: Element variable number from Table 7.

NGBHIV: Number of grid blocks to be printed as history variables for variable number LH.

Table 7. Element variables available for printout in BRAGFLO.

No.	CAMCON Element Variable Name	Description	SI Unit
1	PRESBRIN	Brine pressure	Pa
2	PRESGAS	Gas pressure	Pa
3	POTO	Brine density $\times g \times$ potentiometric head	Pa
4	POTG	Gas density $\times g \times$ potentiometric head	Pa
5	PBUB	Brine bubble pressure	Pa
6	POROS	Porosity	m ³ void/m ³ rock
7	RELPERMB	Relative permeability to brine	dimensionless
8	RELPERMG	Relative permeability to gas	dimensionless
9	DENBRINE	Brine density	kg/m ³
10	DENGAS	Gas density	kg/m ³
11	PERMBRX	Permeability to brine, <i>x</i> -direction	m ²
12	PERMBRY	Permeability to brine, <i>y</i> -direction	m ²
13	PERMBRZ	Permeability to brine, <i>z</i> -direction	m ²
14	PERMGASX	Permeability to gas, <i>x</i> -direction	m ²
15	PERMGASY	Permeability to gas, <i>y</i> -direction	m ²
16	PERMGASZ	Permeability to gas, <i>z</i> -direction	m ²
17	SATBRINE	Brine saturation	fraction void volume
18	SATGAS	Gas saturation	fraction void volume

No.	CAMCON Element Variable Name	Description	SI Unit
19	CBRBR	Brine component of brine phase	mass frac brine phase
20	CGASBR	Gas component of brine phase	mass frac brine phase
21	WELLBRIN	Time-averaged well brine flow rate	m ³ /s (@ ref. conds)
22	WELLGAS	Time-averaged well gas flow rate	m ³ /s (@ ref. conds)
23	CWELLBR	Cumulative well brine flow	m ³ /s (@ ref. conds)
24	CWELLGAS	Cumulative well gas flow	m ³ /s (@ ref. conds)
25	VELDBRX	Brine Darcy velocity, x-direction	m/s
26	VELDBRY	Brine Darcy velocity, y-direction	m/s
27	VELDBRZ	Brine Darcy velocity, z-direction	m/s
28	VELDGASX	Gas Darcy velocity, x-direction	m/s
29	VELDGASY	Gas Darcy velocity, y-direction	m/s
30	VELDGASZ	Gas Darcy velocity, z-direction	m/s
31	FLOWBRX	Time-avg. inter-block brine flow, x- direction	m ³ /s (@ ref. conds)
32	FLOWBRY	Time-avg. inter-block brine flow, y- direction	m ³ /s (@ ref. conds)
33	FLOWBRZ	Time-avg. inter-block brine flow, z- direction	m ³ /s (@ ref. conds)
34	FLOWGASX	Time-avg. inter-block gas flow, x- direction	m ³ /s (@ ref. conds)
35	FLOWGASY	Time-avg. inter-block gas flow, y- direction	m ³ /s (@ ref. conds)
36	FLOWGASZ	Time-avg. inter-block gas flow, z- direction	m ³ /s (@ ref. conds)
37	MASSBALB	Relative Brine mass balance	dimensionless
38	MASSBALG	Relative Gas mass balance	dimensionless
39	CORRATI	Inundated corrosion rate-simple model	gm-mol/s
40	CORRATH	Humid corrosion rate-simple model	gm-mol/s
41	BIORATI	Inundated biodegradation rate-simple model	gm-mol/s
42	BIORATH	Humid biodegradation rate-simple model	gm-mol/s
43	FEOH2_SR	Iron hydroxide sulfidation rate-simple model	gm-mol/s
44	FE_SR	Iron sulfidation rate-simple model	gm-mol/s
45	MGO_HR	MgO hydration rate-simple model	gm-mol/s
46	MGOH2_CR	Mg(OH) ₂ carbonation rate-simple model	gm-mol/s
47	MGO_CR	MgO carbonation rate-simple model	gm-mol/s
48	HYMAG_CR	Hydromagnesite conversion rate-simple model	gm-mol/s

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No.	CAMCON Element Variable Name	Description	SI Unit
49	H2RATE	H ₂ generation rate–simple model	kg/(s·m ³)
50	BRINRATE	Brine consumption rate–simple model	kg/(s·m ³)
51	FERATE	Fe consumption rate–simple model	kg/(s·m ³)
52	CELLRATE	Biodegrad consumption rate–simple model	kg/(s·m ³)
53	FEOH2R	Fe(OH) ₂ generation rate–simple model	kg/(s·m ³)
54	FESR	FeS generation rate–simple model	kg/(s·m ³)
55	MGOR	MgO generation rate–simple model	kg/(s·m ³)
56	MGOH2R	Mg(OH) ₂ generation rate–simple model	kg/(s·m ³)
57	HYMAGR	Hydromagnesite generation rate-simple model	kg/(s·m ³)
58	MGCO3R	MgCO ₃ generation rate–simple model	kg/(s·m ³)
59	FECONC	Fe concentration–simple model	kg/m ³
60	CELLCONC	Biodegradables concentration–simple model	kg/m ³
61	FEOH2C	Fe(OH) ₂ concentration–simple model	kg/m ³
62	FESC	FeS concentration–simple model	kg/m ³
63	MGOC	MgO concentration–simple model	kg/m ³
64	MGOH2C	Mg(OH) ₂ concentration–simple model	kg/m ³
65	HYMAGC	Hydromagnesite concentration-simple model	kg/m ³
66	MGCO3C	MgCO ₃ concentration–simple model	kg/m ³
67	SALTC	Salt concentration–simple model	kg/m ³
68	PORSOLID	Normalized volume of solids produced	dimensionless
69	H2_R ¹	H ₂ generation rate–reaction path model	kg/(s·m ³)
70	CO2_R ¹	CO ₂ generation rate–reaction path model	kg/(s·m ³)
71	CH4_R ¹	CH ₄ generation rate–reaction path model	kg/(s·m ³)
72	N2_R ¹	N ₂ generation rate–reaction path model	kg/(s·m ³)
73	H2S_R ¹	H ₂ S generation rate–reaction path model	kg/(s·m ³)
74	O2_R ¹	O ₂ generation rate–reaction path model	kg/(s·m ³)
75	H2O_R ¹	H ₂ O generation rate–reaction path model	kg/(s·m ³)
76	H2SO4_R ¹	H ₂ SO ₄ generation rate–reaction path model	kg/(s·m ³)
77	HNO3_R ¹	HNO ₃ generation rate–reaction path model	kg/(s·m ³)
78	[C ₆ H ₁₀ O ₅]/6_R ¹	Biodegrad consumption rate–reaction path model	kg/(s·m ³)
79	FE_R ¹	Fe generation rate–reaction path model	kg/(s·m ³)
80	FES2F_R ¹	FeS ₂ generation rate–reaction path model	kg/(s·m ³)
81	FES20_R ¹	FeS ₂ generation rate–reaction path model	kg/(s·m ³)
82	FECO3F_R ¹	FeCO ₃ generation rate–reaction path	kg/(s·m ³)

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No.	CAMCON Element Variable Name	Description	SI Unit
		model	
83	FECO3O_R ¹	FeCO ₃ generation rate–reaction path model	kg/(s·m ³)
84	FEOH2_R ¹	Fe(OH) ₂ generation rate–reaction path model	kg/(s·m ³)
85	FEOOH_R ¹	FeO(OH) generation rate–reaction path model	kg/(s·m ³)
86	FE3O4_R ¹	Fe ₃ O ₄ generation rate–reaction path model	kg/(s·m ³)
87	FES_R ¹	FeS generation rate–reaction path model	kg/(s·m ³)
88	CAO_R ¹	CaO generation rate–reaction path model	kg/(s·m ³)
89	CAOH2_R ¹	Ca(OH) ₂ generation rate–reaction path model	kg/(s·m ³)
90	CACO3_R ¹	CaCO ₃ generation rate–reaction path model	kg/(s·m ³)
91	H2_RAD_R ¹	H ₂ generation rate–radiolysis	kg/(s·m ³)
92	H2_C ¹	H ₂ concentration–reaction path model	kg/(s·m ³)
93	CO2_C ¹	CO ₂ concentration–reaction path model	kg/m ³
94	CH4_C ¹	CH ₄ concentration–reaction path model	kg/m ³
95	N2_C ¹	N ₂ concentration–reaction path model	kg/m ³
96	H2S_C ¹	H ₂ S concentration–reaction path model	kg/m ³
97	O2_C ¹	O ₂ concentration–reaction path model	kg/m ³
98	H2O_C ¹	H ₂ O concentration–reaction path model	kg/m ³
99	H2SO4_C ¹	H ₂ SO ₄ concentration–reaction path model	kg/m ³
100	HNO3_C ¹	HNO ₃ concentration–reaction path model	kg/m ³
101	[C ₆ H ₁₀ O ₅]/6_C ¹	Biodegradables concentration–reaction path model	kg/m ³
102	FE_C ¹	Fe concentration–reaction path model	kg/m ³
103	FES2F_C ¹	FeS ₂ concentration–reaction path model	kg/m ³
104	FES2O_C ¹	FeS ₂ concentration–reaction path model	kg/m ³
105	FECO3F_C ¹	FeCO ₃ concentration–reaction path model	kg/m ³
106	FECO3O_C ¹	FeCO ₃ concentration–reaction path model	kg/m ³
107	FEOH2_C ¹	Fe(OH) ₂ concentration–reaction path model	kg/m ³
108	FEOOH_C ¹	FeO(OH) concentration–reaction path model	kg/m ³
109	FE3O4_C ¹	Fe ₃ O ₄ concentration–reaction path model	kg/m ³
110	FES_C ¹	FeS concentration–reaction path model	kg/m ³
111	CAO_C ¹	CaO concentration–reaction path model	kg/m ³
112	CAOH2_C ¹	Ca(OH) ₂ concentration–reaction path model	kg/m ³
113	CACO3_C ¹	CaCO ₃ concentration–reaction path model	kg/m ³

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No.	CAMCON Element Variable Name	Description	SI Unit
114	H2 RAD C ¹	H ₂ concentration–radiolysis	kg/m ³
115	H2OFLOWI ¹	Water inflow rate	kg/s
116	BMI1TOT ¹	Total isotope mass from Waste Region 1	kg
117	BC1TOT ¹	Total isotope conc. from Waste Region 1	kg/m ³
118	SM1TOT ¹	Total solid isotope mass from Waste Region 1	kg
119	BM1PU240 ¹	Mass of isotope 1 (Pu240) from Waste Region 1	kg
120	BM1U236 ¹	Mass of isotope 2 (U236) from Waste Region 1	kg
121	BM1TH232 ¹	Mass of isotope 3 (Th232) from Waste Region 1	kg
122	BC1PU240 ¹	Conc. of isotope 1 from Waste Region 1	kg/m ³
123	BC1U236 ¹	Conc. of isotope 2 from Waste Region 1	kg/m ³
124	BC1TH232 ¹	Conc. of isotope 3 from Waste Region 1	kg/m ³
125	SM1PU240 ¹	Solid mass of isotope 1 from Waste Region 1	kg
126	SM1U236 ¹	Solid mass of isotope 2 from Waste Region 1	kg
127	SM1TH232 ¹	Solid mass of isotope 3 from Waste Region 1	kg

1) Not Used or QA'd for WIPP compliance calculations.

Note: Variables 1 - 115 are, by default, available in any run. Variables 116 and greater depend on the values of MWST and MRAD. This list is for MWST = 1, MRAD = 3 (Pu240, U236, and Th232), which results in a total of $NVPR = 115 + 3 \times MWST \times (1 + MRAD) = 127$ element variables.

Line 2.16. IIHIV, JJHIV, KKHIV (NGBHIV sets).

IIHIV: I-index for grid block location for the history variable.

JJHIV: J-index for grid block location for the history variable.

KKHIV: K-index for grid block location for the history variable.

Monitor Blocks. BRAGFLO prints out certain summary data to the screen and to the .SUM file at each time step to provide the user with continuous information on the how the run is progressing. This summary includes two lines showing simulation time along with time step and global mass balance information (described more fully in Subsection 9.3). In addition, the summary

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allows the user to monitor values of certain element variables at specified grid blocks. These monitor blocks are intended solely to monitor progress, rather than to provide data for post-processing or other later use, so only a few grid blocks should be selected where significant changes are likely to occur or where the behavior is representative of an entire region. Typically, one to three monitor blocks are selected. Because this information is printed both to the screen (or to a log file if run in batch) and to the .SUM file at every time step, the amount of information printed out can become large in a long run if too many monitor blocks are selected. The maximum number of blocks allowed is MMON, which is set in the PARAMETER statement.

Line 2.17. Descriptor. Monitor block parameters.

Line 2.18. MONITOR.

MONITOR: LOGICAL Flag for monitoring key parameters at a specified grid block.

If MONITOR = .TRUE., then read the next two lines (and possibly more, depending on the values read); otherwise, go to Subsection 7.2.3.

Line 2.19. Descriptor. Number of monitor blocks.

Line 2.20. NMON.

NMON: Number of monitor blocks to be specified. NMON should be less than 100, because the monitor block number printout is formatted I2. If NMON > MMON (where MMON is set in the PARAMETER statement), BRAGFLO will abort with a message is printed to the screen:

```
*** ERROR: Too many Monitor Blocks in Input:
          Specified: NMON = <NMON input value>
          Maximum:   MMON = <MMON value set in PARAMETER state-
ment>

*** Monitor error in READPRTYPE ***
```

Line 2.21. Descriptor. Monitor block locations.

Read NMON repetitions of Line 2.22.

Line 2.22. IMONITOR, JMONITOR, KMONITOR

IMONITOR: I-index of grid block to be monitored.
JMONITOR: J-index of grid block to be monitored.
KMONITOR: K-index of grid block to be monitored.

7.2.4 Mesh Description Parameters

BRAGFLO provides several options for inputting the mesh. With these options, a simple mesh can be easily set up with very little input, yet very complex meshes can still be specified, with correspondingly more detailed input. BRAGFLO uses a rectilinear grid; defining the mesh

requires specifying the Δx (DXGRID), Δy (DYGRID), and Δz (DZGRID), and the elevation (DEPTH) for each grid block. How much of this information has to be input depends on which input option is selected.

Line 3.1. Descriptor. Grid data flags.

Line 3.2. IDXFLAG, IDYFLAG, IDZFLAG, IDEPTHFLAG.

IDXFLAG: Specifies how grid block width Δx (DXGRID) is to be read.

IDYFLAG: Specifies how grid block width Δy (DYGRID) is to be read.

IDZFLAG: Specifies how grid block width Δz (DZGRID) is to be read.

IDEPTHFLAG: Specifies how grid block elevations (DEPTH) are to be read.

IDXFLAG = 0: DXGRID does not vary; input one value of DXGRID.

= 1: DXGRID varies in I-direction; input NX values of DXGRID.

IDYFLAG = 0: DYGRID does not vary; input one value of DYGRID.

= 1: DYGRID varies in I-direction; input NX values of DYGRID.

= 2: DYGRID varies in J-direction; input NY values of DYGRID.

IDZFLAG = 0: DZGRID does not vary; input one value of DZGRID.

= 1: DZGRID varies in I-direction; input NX values of DZGRID.

= 2: DZGRID varies in J-direction; input NY values of DZGRID.

= 3: DZGRID varies in K-direction; input NZ values of DZGRID.

= 4: DZGRID varies in I- and J-directions; input NX x NY values of DZGRID.

IDEPTHFLAG = 0: Elevation does not vary; input one value of DEPTH.

= 1: Elevation varies in I-direction; input NX values of DEPTH.

= 2: Elevation varies in J-direction; input NY values of DEPTH.

= 3: Elevation varies in K-direction; input NZ values of DEPTH.

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- = 4: Elevation varies in I- and J-directions; input NX x NY values of DEPTH.
- = 5: Elevation varies in I- and K-directions; input NX x NZ values of DEPTH.
- = 6: Elevation varies in J- and K-directions; input NY x NZ values of DEPTH.
- = 7: Elevation varies in I-, J-, and K-directions; input NX x NY x NZ values of DEPTH.
- = -1: Elevation varies in I-direction; have BRAGFLO calculate values of DEPTH.
- = -2: Elevation varies in J-direction; have BRAGFLO calculate values of DEPTH.
- = -3: Elevation varies in K-direction; have BRAGFLO calculate values of DEPTH.
- = -4: Elevation varies in I- and J-directions; have BRAGFLO calculate values of DEPTH.
- = -5: Elevation varies in I- and K-directions; have BRAGFLO calculate values of DEPTH.
- = -6: Elevation varies in J- and K-directions; have BRAGFLO calculate values of DEPTH.
- = -7: Elevation varies in I-, J-, and K-directions; have BRAGFLO calculate values of DEPTH.

If the input value for any of these flags is outside the range listed above, BRAGFLO will abort, with messages printed to the screen indicating what the problems are. The final messages printed are:

```
Number of FATAL errors in READMESH = <number of errors>
```

```
*** FATAL geometry input errors in READMESH ***
```

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Subsequent input depends on the values of the geometry flags. There are four sets of input, one each for inputting DXGRID, DYGRID, DZGRID, and DEPTH.

DXGRID input

Line 3.3. Descriptor. DXGRID input.

If IDXFLAG (Line 3.2) = 0:

Line 3.4. DXCONST.

DXCONST: Uniform grid block Δx -dimension [m or ft].

If IDXFLAG (line 3.2) = 1:

Line 3.4. (DXGRID(I,1,1), I=1, NX).

DXGRID(I,1,1): Grid block Δx -dimensions, varying in the I-direction [m or ft].

BRAGFLO does not allow DXGRID to vary in the J- or K-directions; thus, only values for DXGRID in the I-direction need (and can) be input.

DYGRID input

Line 3.5. Descriptor. DYGRID input.

If IDYFLAG (Line 3.2) = 0:

Line 3.6. DYCONST.

DYCONST: Uniform grid block Δy -dimension [m or ft].

If IDYFLAG (Line 3.2) = 1:

Line 3.6. (DYGRIDI(I), I=1, NX).

DYGRIDI(I): Grid block Δy -dimensions, varying only in the I-direction [m or ft].

If IDYFLAG (Line 3.2) = 2:

Line 3.6. (DYGRIDJ(J), J=1, NY).

DYGRIDJ(J): Grid block Δy -dimensions, varying only in the J-direction [m or ft].

BRAGFLO does not allow Δy to vary in the K-direction, nor in the I- and J-directions simultaneously.

DZGRID input.

Line 3.7. Descriptor. DZGRID input.

If IDZFLAG (Line 3.2) = 0:

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Line 3.8. DZCONST.

DZCONST: Uniform grid block Δz dimensions [m or ft].

If IDZFLAG (Line 3.2) = 1:

Line 3.8. (DZGRIDI(I), I=1, NX).

DZGRIDI(I): Grid block Δz -dimensions, varying only in the I-direction [m or ft].

If IDZFLAG (Line 3.2) = 2:

Line 3.8. (DZGRIDJ(J), J=1, NY).

DZGRIDJ(J): Grid block Δz -dimensions, varying only in the J-direction [m or ft].

If IDZFLAG (Line 3.2) = 3:

Line 3.8. (DZGRIDK(K), K=1, NZ).

DZGRIDK(K): Grid block Δz -dimensions, varying only in the K-direction [m or ft].

If IDZFLAG (Line 3.2) = 4:

Line 3.8. ((DZGRIDIJ(I,J), I=1, NX), J=1, NY).

DZGRIDIJ(I,J): Grid block dimensions, varying in both I- and J-directions [m or ft].

BRAGFLO does not allow DZGRID to vary simultaneously in all three directions.

IDEPTHFLAG input

Line 3.9. Descriptor. IDEPTHFLAG input.

Input values are elevations above the origin to the center of grid blocks. Positive values increase with elevation, indicating grid block center elevations above the elevation of the origin. If IDEPTHFLAG is greater than zero, user-specified values of DEPTH are entered. If IDEPTHFLAG is less than zero, elevations will be calculated from input inclinations.

If IDEPTHFLAG (Line 3.2) = 0:

Line 3.10. DEPTHCONST.

DEPTHCONST: Uniform elevation in all I-, J-, and K-directions [m or ft]. Using a value for IDEPTHFLAG of zero is physically realistic only if the problem is one- or two-dimensional, and NX, NY, or NZ, or two of these, is 1. However, a uniform elevation can be specified for a fully three-dimensional problem or for a two-dimensional problem with a vertical cross-section. The effect, which is sometimes desired, is to “turn off” gravity, because there is no difference in elevation between any adjacent layers in the mesh.

If IDEPTHFLAG (Line 3.2) = 1:

Line 3.10: (DEPTHI(I), I=1, NX).

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DEPTHI(I): Elevations to grid block centers, varying only in the I-direction [m or ft].

If IDEPTHFLAG (Line 3.2) = 2:

Line 3.10: (DEPTHJ(J), J=1, NY).

DEPTHJ(J): Elevations to grid block centers, varying only in the J-direction [m or ft].

If IDEPTHFLAG (Line 3.2) = 3:

Line 3.10. (DEPTHK(K), K=1, NZ).

DEPTHK(K): Elevations to grid block centers, varying only in the K-direction [m or ft].

If IDEPTHFLAG (Line 3.2) = 4:

Line 3.10. ((DEPTHIJ(I,J), I=1, NX), J=1, NY).

DEPTHIJ(I,J): Elevations to grid block centers, varying in both I- and J-directions [m or ft].

If IDEPTHFLAG (Line 3.2) = 5:

Line 3.10. ((DEPTHIK(I,K), I=1, NX), K=1, NZ).

DEPTHIK(I,K): Elevations to grid block centers, varying in both I- and K-directions [m or ft].

If IDEPTHFLAG (Line 3.2) = 6:

Line 3.10. ((DEPTHJK(J,K), J=1, NY), K=1, NZ).

DEPTHJK(J,K): Elevations to grid block centers, varying in both J- and K-directions [m or ft].

If IDEPTHFLAG (Line 3.2) = 7:

Line 3.10. (((DEPTH(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

DEPTH(I,J,K): Elevations to grid block centers, varying in all three directions [m or ft].

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If IDEPTHFLAG (Line 3.2) < 0: Elevations will be calculated from inclination input. Certain rules must be carefully followed to achieve the proper orientation of the mesh. Start with a right-handed coordinate system, with the origin at $(x,y,z) = (0,0,0)$ in the center of the front lower left corner block. The x -direction increases to the right; the y -direction increases into the page; and the z -direction increases upward. Translate the mesh so that the new origin is at the center of grid block (I ORIG, J ORIG, K ORIG). Next, set the elevation at the center of this grid block to ZERODEPTH. Finally, rotate the mesh about the axes in the following order: 1) Positive rotation about the original x -axis; 2) Positive rotation about the original y -axis; 3) Positive rotation about the original z -axis. The "original" axes are the axes as they exist after the elevation is set to ZERODEPTH; in other words, the axes of rotation do not change after each rotation.

Line 3.10. I ORIG, J ORIG, K ORIG, ZERODEPTH, THETAX, THETAY,
THETAZ.

I ORIG: I-index of origin block.

J ORIG: J-index of origin block.

K ORIG: K-index of origin block.

ZERODEPTH: Elevation of origin block [m or ft].

THETAX: Angle of positive right-handed rotation about the x -axis
[degrees].

THETAY: Angle of positive right-handed rotation about the y -axis
[degrees].

THETAZ: Angle of positive right-handed rotation about the z -axis
[degrees].

If IDEPTHFLAG (Line 3.2) = -1:

Elevation varies only in I-direction; there must be only one layer in the K-direction. In this case, BRAGFLO allows only rotation about the original y -axis. The only value used from Line 3.10 is THETAY; all other inputs are ignored, but appropriate placeholder values (three integers and four real numbers) must be input.

If IDEPTHFLAG (Line 3.2) = -2:

Elevation varies only in J-direction; there must be only one layer in the K-direction. BRAGFLO allows only rotation about the original x -axis. The only value used from Line 3.10 is THETAX; all other inputs are ignored, but appropriate placeholder values (three integers and four real numbers) must be input.

If IDEPTHFLAG (Line 3.2) < -2:

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Elevation can vary in all three directions. This is the most general case, and it is used whenever IDEPTHFLAG < -2. Other specialized cases, for IDEPTHFLAG = -3 to -6, analogous to IDEPTHFLAG = +3 to +6, are not yet implemented in BRAGFLO, so any value of IDEPTHFLAG between -3 and -7, inclusive, is treated as IDEPTHFLAG = -7.

7.2.5 Well Parameters and Boundary Conditions

BRAGFLO is capable of simulating wells that are completed within the formations or porous media being modeled. A well is either an injection well or a production (or withdrawal) well. Each type of well can be treated as a constant-pressure well or as a constant flow rate well.

In a constant-pressure well, fluids (gas and brine) are injected or produced at whatever rate is necessary to maintain the specified pressure. The amount of each phase that is injected or produced is proportional to the saturation of each phase in the grid block containing the well.

A constant-pressure well is useful for simulating constant-pressure boundary conditions, and, in earlier versions of BRAGFLO, this was the only means of maintaining a truly fixed boundary pressure. In the current version, constant-pressure boundary conditions can be specified directly, so wells are no longer used for that purpose.

In a constant-flow injection or production well, the rate of injection or production of each phase is specified, and the pressure in the grid block containing the well fluctuates accordingly. Injection and production wells are useful for simulating sources and sinks, for example, generation of gas by a chemical reaction.

In BRAGFLO, a well exists only in a single grid block. In reality, a well might be completed (*i. e.*, open to the surrounding formation) over a range of depths, which might encompass more than one grid block in the mesh. To simulate such a well using BRAGFLO, multiple wells must be used, one for each grid block in which the well is completed. More than one well may exist in a grid block. Each well in a grid block must be specified individually in the input. All wells are assumed to be located at the center of the grid block. (In fact, BRAGFLO, as a cell-centered finite difference code, considers all properties and influences as occurring at the centers of grid blocks.) It is currently not possible in BRAGFLO for wells to interact directly; for example, fluids withdrawn from one well cannot be injected in another well. Furthermore, injection and production rates are fixed over the specified time period; they cannot be varied over time, except in finite increments as specified explicitly in the input, and they cannot be made to vary as a function of any other rates or processes simulated in BRAGFLO. They depend solely, although implicitly, on the brine pressure and gas saturation within the grid block in which the wells are completed.

Specified well conditions remain in effect only until the next time at which conditions in any well are changed. For example, suppose two constant-pressure wells are specified initially, and a third well, a constant-flow well, is to be added after 1000 years. If only the third well is specified at 1000 years, the two constant-pressure wells will be turned off at 1000 years. If these two wells are to continue to be in effect after 1000 years, their conditions must be specified at 1000 years (along with the third well) as well as at the start of the run. Wells are turned off simply by specifying another time when conditions go into effect, but without specifying any conditions for those wells.

Constant-pressure (Dirichlet) boundary conditions can be specified directly, instead of being simulated by means of constant-pressure wells. BRAGFLO assumes all external mesh boundaries to be no-flow boundaries. Although constant-pressure wells can usually hold the pressure constant in any grid cell where they are applied, numerical problems are sometimes encountered. Using wells also requires that productivity indexes (PIWELL-Line 4.6) be judiciously chosen. If PIWELL is too small, the pressure will not be held exactly constant; if PIWELL is too big, numerical difficulties are exacerbated. When gas dissolution is being simulated, constant-pressure wells may not work at all. Specifying Dirichlet boundary conditions can eliminate these problems. The user has the option of fixing either the brine pressure or the gas saturation, or both, in any grid block in the mesh.

Dirichlet boundary conditions are in effect during the entire run. They cannot be turned on or off at various times the way wells can.

Line 4.1. Descriptor. Well parameters.

Line 4.2. NWELLTIMES.

NWELLTIMES: Number of times to specify well conditions. If NWELLTIMES is greater than NWTIME (which is set in the PARAMETER statement in BF2_PARAMS.INC), BRAGFLO will abort with the message:

In READWELL, NWTIME needs to be larger.

```
NWELLTIMES = <NWELLTIMES input value>
```

```
*** Well time errors in READWELL ***
```

The following input is repeated NWELLTIMES.

Line 4.3. WELLTIME, NWELLS.

WELLTIME: Time when conditions go into effect [s or days]. Conditions specified at this time remain in effect only until the next WELLTIME. In order for a well to remain in effect after the next WELLTIME, the description and conditions for that well (Lines 4.4, 4.5, and 4.6) must be repeated at the next WELLTIME. If this information is *not* repeated at the next WELLTIME, the well is, in effect, turned off at that time.

NWELLS: Number of grid blocks containing wells at this WELLTIME.

The following input is repeated NWELLS times.

Line 4.4. IWELLNODE, JWELLNODE, KWELLNODE, NWELLSPERGRID.

IWELLNODE: I-index of grid block containing the well(s).

JWELLNODE: J-index of grid block containing the well(s).

KWELLNODE: K-index of grid block containing the well(s).

NWELLSPERGRID: Number of wells that exist in this grid block.

The following input is repeated NWELLSPERGRID times.

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Line 4.5. WELLTYPE.

WELLTYPE: Type of well. This is a CHARACTER*4 variable. It is input in free format, with *no* enclosing tick marks and any number of leading spaces, in contrast to earlier versions of BRAGFLO, which used a formatted read statement. The available options are:

INJP: Pressure-controlled (or constant-pressure) injection well.

INJQ: Flow-rate-controlled injection well.

PROD: Production well.

NONE: None of the above. This is the initial value for WELLTYPE; if not changed by an input value, a well that is otherwise fully specified by input will be ignored and has no effect.

Line 4.6. QGWELL, QOWELL, PIWELL, PW.

QGWELL: Gas mass flow rate [kg/s or lb/day].

QOWELL: Brine mass flow rate [kg/s or lb/day].

PIWELL: Injectivity or productivity index [m^3 or (bbl cP)/(day psi)]. Recommended value: $1.0 \times 10^{-6} \text{ m}^3$, to achieve constant pressure (PO = PW), as when wells are used to maintain a specified boundary condition.

PW: Flowing down-hole well bore pressure [Pa or psi].

The productivity index, PIWELL, is a function of grid block dimensions, permeability, and borehole diameter that allows accurate simulation of well behavior when a small-diameter borehole is completed within a large grid block. To simulate the pressure drop from the formation immediately surrounding a borehole into the borehole, the productivity index must be calibrated to actual measurements of pressure and flow rates. In the WIPP PA, wells are generally used only to maintain fixed pressures at the boundaries of a mesh, rather than to simulate the actual behavior of a well. (Since Dirichlet boundary conditions were implemented, wells are now seldom used at all.) In this case, accurate simulation of the pressure behavior in the vicinity of the well is unimportant, and a large productivity index (say, $1.0 \times 10^{-6} \text{ m}^3$) is used so that the pressure in the grid block is the same as specified for the borehole. Because the productivity index is dependent on grid block dimensions, a "large" value in one grid block may not be large enough in another. However, for grid blocks as large as $15 \text{ km} \times 60 \text{ km} \times 100 \text{ m}$, a productivity index of $1.0 \times 10^{-6} \text{ m}^3$ [$3.7 \times 10^{12} \text{ bbl cP}/(\text{day psi})$] provides the desired equal pressures in the well borehole and the grid block.

Line 4.7. Descriptor. Constant brine pressure and gas saturation boundary conditions.

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Line 4.8. DIRICHLET, NO_DIRGRID.

DIRICHLET: Logical flag (T or F) indicating that Dirichlet boundary conditions will be used.

NO_DIRGRID: Number of grid blocks in which Dirichlet boundary conditions will be applied.

If DIRICHLET is .FALSE., no additional well or boundary condition data are input.
If DIRICHLET is .TRUE., the following input is repeated NO_DIRGRID times.

Line 4.9. IR,JR,KR,DIRGRIDP,DIRGRIDS,DIR_PRES,DIR_SATB.

IR: I-index of grid block in which Dirichlet boundary conditions are applied.

JR: J-index of grid block in which Dirichlet boundary conditions are applied.

KR: K-index of grid block in which Dirichlet boundary conditions are applied.

DIRGRIDP: Logical flag (T or F) indicating that a constant brine pressure is to be used.

DIRGRIDS: Logical flag (T or F) indicating that a constant gas saturation is to be used.

DIR_PRES: Brine pressure specified to be constant [Pa].

DIR_SATB: Brine saturation specified to be constant. Because BRAGFLO solves for gas saturation, it is actually the gas saturation that will be held constant. However, to be consistent with the initial condition input, where brine saturation is input, brine saturation is specified here, rather than gas saturation.

Note: DIR_PRES and DIR_SATB must be identical to the initial values, PIINIT (IR,JR,KR) and SOINIT (IR,JR,KR), respectively (see next subsection). Otherwise, BRAGFLO will run incorrectly. BRAGFLO does not check to be sure that DIR_PRES and DIR_SATB are the same as the initial; it is up to the user to ensure that this is true.

7.2.6 Initial Conditions

Initial conditions must be input for brine pressure, brine saturation, iron concentration, and cellulosics concentration.

Line 5.1. Descriptor. Brine pressure initial conditions.

Line 5.2. (((PINIT(I,J,K), I=1, NX), J=1, NY), K=1, NZ).
PINIT: Initial brine pressure [Pa or psi].

Line 5.3. Descriptor. Brine saturation initial conditions.

Line 5.4. (((SOINIT(I,J,K), I=1, NX), J=1, NY), K=1, NZ).
SOINIT: Initial brine saturation [dimensionless].

Line 5.5. Descriptor. Iron concentration initial conditions.

Line 5.6. (((CONCFE(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

CONCFE: Initial iron concentration [kg/m^3 or lb/ft^3].

Line 5.7. Descriptor. Cellulosics concentration initial conditions.

Line 5.8. (((CONCBIO(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

CONCBIO: Initial cellulosics concentration [kg/m^3 or lb/ft^3].

Line 5.9. Descriptor. MgO concentration initial conditions.

Line 5.10. (((CONCMGO(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

CONCMGO: Initial magnesium oxide concentration [kg/m^3 or lb/ft^3].

It is sometimes desirable to calculate, rather than input, certain initial conditions, an example being the initial brine pressure distribution in formations surrounding the WIPP repository. In this example, other initial conditions, such as the brine pressure within the repository and initial concentrations of reactants (iron and cellulosics), still need to be specified in the input, even though pressures outside the repository are calculated. BRAGFLO accommodates this need to calculate initial conditions of only some variables in only part of the mesh by means of a somewhat convoluted interaction between special materials specifications and starting times.

If a run begins at time $\text{START} \geq \text{TIMEICRESET}$ (described in Subsection 7.2.8, Line 7.24; generally, $\text{TIMEICRESET} = 0$.), BRAGFLO uses only the initial conditions specified in Lines 5.1-5.8 above. This use of initial conditions is straightforward and uncomplicated, being the obvious way that initial conditions are expected to be used.

If a run begins at time $\text{START} < \text{TIMEICRESET}$, only some of the initial conditions are used at time START , while other initial conditions from Lines 5.1-5.8 are used at time TIMEICRESET . In this case, initial pressures, PINIT , will be used in all regions *except Waste regions* at time START . Initial brine saturations, SOINIT , will also be used in all regions *except Waste regions* at time START . Reactant concentrations, CONCFE , CONCBIO and CONCMGO are not used until after TIMEICRESET ; furthermore, reactions that affect the values of CONCFE , CONCBIO and CONCMGO occur only in *Waste regions*, which are undefined prior to TIMEICRESET .

At TIMEICRESET , brine pressures *only in Reset Material regions* are set to PINIT . At the same time, brine saturations *only in Reset Material regions* are set to SOINIT . Because CONCFE , CONCBIO , and CONCMGO are unaffected before TIMEICRESET , both of these variables have initial values as specified in Lines 5.6 and 5.8 at time START as well as at time TIMEICRESET .

7.2.7 Numerical Control Parameters

Parameters input in this section allow the user to control the numerical behavior of BRAGFLO. These parameters affect the accuracy of solutions and can have major effects on computing time. The equations solved in BRAGFLO are highly nonlinear, and the discretized equations are solved using an iterative Newton-Raphson technique. The control parameters govern the rate of convergence of the solution procedure, as well as the degree of precision to be achieved in the solution. The Newton-Raphson procedure involves computing a Jacobian matrix, which is the most computationally intensive step in the solution. The control parameters allow the user to specify the frequency at which the Jacobian is recalculated. The Jacobian is always computed at

the beginning of each time step. It can be calculated as frequently as each iteration within a time step (at great computational expense), or after every so many iterations.

Line 6.1. Descriptor. Physical realism constraints.

Line 6.2. DEPLIMIT(1), DEPLIMIT(2), SATLIMIT.

DEPLIMIT(1): Limit allowed on gas saturation outside the physically realistic range of 0.0 to 1.0. The solution will not be rejected provided: $1.0 + \text{DEPLIMIT}(1) > S_g > -\text{DEPLIMIT}(1)$. Otherwise, the time step size will be reduced and the time step will be repeated. Note that this is only the first of several criteria that must be met before a solution is finally accepted. "Slightly unrealistic" values of gas saturation can (and generally must) be tolerated; if DEPLIMIT(1) is too small, or zero, BRAGFLO will likely struggle excessively (and consume large amounts of computing time) without appreciably improving the solution. Recommended value: $\text{DEPLIMIT}(1) = 0.2$.

DEPLIMIT(2): Lower limit allowed on brine pressure [Pa or psi]; primarily intended to catch large negative values of pressure. The solution will be accepted provided: $\text{PO} > \text{DEPLIMIT}(2)$. If $\text{PO} \leq \text{DEPLIMIT}(2)$, the time step size will be reduced and the time step will be repeated. As with DEPLIMIT(1), DEPLIMIT(2) should not be set too stringently. These two limits are intended simply to reject the solutions that are beyond hope before any more computational effort is expended on them. Recommended value: -1.0×10^8 Pa.

SATLIMIT: Limit on gas saturation solution beyond which a solution will not be accepted; inter-step iterations will continue using the same Δt (*i. e.*, the solution is not accepted, but Δt is not reduced) even if DEPLIMIT(1) is satisfied if: $1.0 + \text{SATLIMIT} > S_g > -\text{SATLIMIT}$ provided that $\text{DEPLIMIT}(1) > \text{SATLIMIT}$. Non-convergence occurs once S_g violates the SATLIMIT constraint. This is intended to be a more stringent limit than DEPLIMIT(1), but it is up to the user to ensure that $\text{DEPLIMIT}(1) > \text{SATLIMIT}$. Recommended value: 1.0×10^{-3} .

Line 6.3. Descriptor. Limits on variable changes for auto time step control.

These parameters are used in the auto time step control algorithm. They affect the efficiency of BRAGFLO by allowing larger time steps when the variables (gas saturation and brine pressure) are changing slowly. If auto time step is turned off, these parameters are not used, but they must still be input.

Line 6.4. DELTADEPNORM(1), DELTADEPNORM(2).

DELTADEPNORM(1): Relative change in gas saturation across a time step; used to control size of next time step. Input value is the largest relative change in gas saturation in the time step just completed such that the new time step will be the same as the current time step. Using a smaller input value will cause smaller increases in the new time step for a given relative change in gas saturation or reduce the relative change in gas saturation that will be allowed in order to achieve a given increase in time step size. Using a larger input value will have the opposite effect. Recommended value: 0.3.

DELTADEPNORM(2): Absolute change in brine pressure across a time step [Pa or psi]; used to control size of next time step. Input value is the largest absolute change in brine pressure in the time step just completed such that the new time step will be the same as the current time step. Using a smaller input value will cause smaller increases in the new time step for a given absolute change in brine pressure or reduce the absolute change in brine pressure that will be allowed in order to achieve a given increase in time step size. Using a larger input value will have the opposite effect. Recommended value: 5.0×10^5 Pa.

Line 6.5. Descriptor. Maximum absolute variable changes.

Line 6.6. DDEPMAX(1), DDEPMAX(2).

DDEPMAX(1): Maximum absolute gas saturation change allowed over a time step. If a greater change in gas saturation occurs, the time step is repeated using a smaller time step. Recommended value: 1.0. (This allows gas saturation to change from 0.0 to 1.0 in a single step, the most that is physically possible, in effect turning off this control except when unphysical gas saturations are obtained.)

DDEPMAX(2): Maximum absolute pressure change allowed over a time step. If a greater change in brine pressure occurs, the time step is repeated using a smaller time step [Pa or psi]. Recommended value: 1.0×10^7 Pa.

Line 6.7. Descriptor. Newton-Raphson normal convergence criteria.

Line 6.8. ICONVTEST.

ICONVTEST: Flag specifying whether *either* or *both* convergence criteria must be satisfied before a solution is considered to have converged. Recommended value: 1. requiring both convergence criteria to be met should result in a more accurate solution. However, prohibitively small time steps are sometimes required because the convergence tests tend to over-emphasize the importance of small grid blocks in which small changes can result in relatively large mass balance errors. To get BRAGFLO to run to completion when such problems occur, it may be necessary to relax one of the criteria that must be met. Generally, this has been found to have little impact on gross results. However, in some instances, important short-lived transient results can differ greatly depending on whether either or both convergence criteria are met. Therefore, whenever possible, ICONVTEST = 1 should be used.

= 0: Satisfy *either* EPSNORM or FTOLNORM. (described next, on Lines 6.10 and 6.14).

= 1: Satisfy *both* EPSNORM and FTOLNORM. (described next, on Lines 6.10 and 6.14).

Line 6.9. Descriptor. Maximum change in variables for normal convergence.

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Line 6.10. EPSNORM(1), EPSNORM(2).

EPSNORM(1): Number of digits of accuracy to the right of the decimal in the change in gas saturation. This parameter limits the change in gas saturation when saturations are very small, in which case DDEPMAX(1) is too easily satisfied. Recommended value range: 2 to 5 with a best estimate of 3.

EPSNORM(2): Maximum *relative* change in brine pressure allowed over a time step. This parameter provides control over brine pressure changes when the pressure is small and DDEPMAX(2) (the maximum *absolute* change) is too easily satisfied. Recommended value range: 1.0×10^{-5} to 1.0×10^{-2} with a best estimate of 1.0×10^{-3} .

Line 6.11. Descriptor. Loosened Newton-Raphson convergence criteria.

Occasionally, BRAGFLO encounters great difficulty in converging to a solution. If a solution has not been obtained at a particular time step after numerous time step reductions, it is quite likely that further time step reductions will not improve the solution sufficiently to satisfy the normal convergence criteria, EPSNORM(1) and EPSNORM(2). One option at this point is for BRAGFLO to abort. The user would then rerun the problem after adjusting one or more of the control parameters and hope for better results. However, it is often the case that BRAGFLO's difficulties are temporary, and that if it can get past the trouble spot, it will complete the run without further major difficulties. Thus, a second option has been built into BRAGFLO to handle those occasions when repeated time step reductions fail to provide convergence: The convergence criteria are temporarily relaxed. These relaxed criteria are applied after user-specified IJACSWITCH time step reductions have occurred, and they continue to be applied only until convergence is obtained at that time step. After IJACRESET time steps, and at all subsequent time steps, the normal convergence criteria are used. This capability makes BRAGFLO a little more robust, enabling it to complete runs that would otherwise abort and require input modifications before rerunning, at only a minor cost in overall accuracy. This feature becomes important when carrying out large number of runs in automated batch systems. It can be turned off by setting all input values of the loosened criteria equal to the normal criteria. Caution is advised when using this feature because large mass balance errors can be introduced which may not be apparent in a cursory examination of the results. THIS FEATURE HAS NOT BEEN TESTED OR QA'D FOR USE IN WIPP COMPLIANCE CALCULATIONS. IT WILL NOT BE USED FOR WIPP COMPLIANCE CALCULATIONS.

Line 6.12. EPSLOOSE(1), EPSLOOSE(2).

EPSLOOSE(1): Same meaning as EPSNORM(1); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1 to 4 with a best estimate of 2.

EPSLOOSE(2): Same meaning as EPSNORM(2); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1.0×10^{-1} to 1.0×10^{-4} with a best estimate of 1.0×10^{-2} .

Line 6.13. Descriptor. Normal right-hand-side function (or residual) criteria.

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BRAGFLO solves a pair of simultaneous mass balance equations: $F_1 = 0$ (gas mass balance), and $F_2 = 0$ (brine mass balance). Because the nonlinear equations are solved numerically and iteratively, F_1 and F_2 are generally not zero. The deviation from zero is the residual, or mass balance error. Ideally, iterations will continue until the residuals are zero, but, in practice, the best that can be hoped for is to get “close” to zero. Discretization errors, round-off errors, discontinuous functional dependencies, property functions with discontinuous derivatives, and non-linearities all contribute to making convergence to truly zero residuals unattainable. The degree of closeness of the residuals to zero that is acceptable is input as the tolerances FTOLNORM(1) and FTOLNORM(2).

Line 6.14. FTOLNORM(1), FTOLNORM(2).

FTOLNORM(1): [kg gas in residual/kg gas in grid block]. For gas saturation, the value of the residual is normalized by dividing by the amount of gas present in the grid block, $\phi(\rho_g S_g + C_{gb} \rho_b S_b)$, where ϕ is the porosity, ρ_g and ρ_b are the gas and brine densities at local conditions, S_g and S_b are the gas and brine saturations, and C_{gb} is the mass fraction of gas in the brine phase ($C_{gb} = 0.0$ if no dissolved gas is present). The minimum of this normalized residual value is compared with FTOLNORM(1). If ICONVTEST = 0 and the normalized residual is less than FTOLNORM(1), convergence is accepted regardless of EPSNORM(1). If ICONVTEST = 1, the normalized residual must be less than FTOLNORM(1) and EPSNORM(1) must be satisfied in order for the solution to be accepted. Recommended value range: 1.0×10^{-1} to 1.0×10^{-6} with a best estimate of 1.0×10^{-2} .

FTOLNORM(2): [kg brine in residual/kg brine in grid block]. For brine pressure, the value of the residual is normalized by dividing by the amount of brine present in the grid block, $\phi C_{bb} \rho_b S_b$, where ϕ is the porosity, C_{bb} is the mass fraction of brine in the brine phase ($C_{bb} = 1.0$ if no dissolved gas is present), ρ_b is the brine density at local conditions, and S_b is the brine saturation. The minimum of this normalized minimum residual value is compared with FTOLNORM(2). If ICONVTEST = 0 and the normalized residual is less than FTOLNORM(2), convergence is accepted regardless of EPSNORM(2). If ICONVTEST = 1, the normalized residual must be less than FTOLNORM(2) and EPSNORM(2) must be satisfied in order for the solution to be accepted. Recommended value range: 1.0×10^{-1} to 1.0×10^{-6} with a best estimate of 1.0×10^{-2} .

Line 6.15. Descriptor. Loosened right-hand-side function criteria. . THIS FEATURE HAS NOT BEEN TESTED OR QA'D FOR USE IN WIPP COMPLIANCE CALCULATIONS.

Line 6.16. FTOLLOOSE(1), FTOLLOOSE(2).

FTOLLOOSE(1): Relaxed value of normalized residual for gas saturation below which convergence is accepted regardless of EPSLOOSE(1); used after IJACSWITCH time step reductions have occurred [kg gas in residual/kg gas in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1} .

FTOLLOOSE(2): Relaxed value of normalized residual for brine pressure below which convergence is accepted regardless of EPSLOOSE(2); used after IJACSWITCH time step

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reductions have occurred [kg brine in residual/kg brine in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1} .

Line 6.17. Descriptor. Multi-component gas constituent transport convergence tolerances.

Line 6.18. EPSGAS(1), EPSGAS(2), EPSGAS(3), EPSGAS(4).

EPSGAS(1): Smallest negative value allowed in the amount of each gas component in a grid block [gm-mol]. If input as a positive number, BRAGFLO sets it negative.

EPSGAS(2): Largest change in a molar concentration of a gas component that is allowed over a Newton-Raphson iteration [gm-mol/m³].

EPSGAS(3): Smallest value of molar concentration that is considered to be nonzero. Used to ensure that, in calculating the relative change in molar concentration, a zero or essentially zero value is not used [gm-mol/m³].

EPSGAS(4): Maximum relative change in gas component molar concentration allowed over a Newton-Raphson iteration [dimensionless].

Line 6.19. Descriptor. Equation solver selection.

Line 6.20. CHSOLVER.

CHSOLVER: This is a CHARACTER*3 variable indicating the solver to be used. It is input in free format, with *no* enclosing tick marks and any number of leading spaces. The available options are:

LU: Original LU-decomposition solver, a direct (non-iterative) solver. This is the solver most frequently used in WIPP PA work. Its principal advantage is its great robustness: unless the Jacobian matrix is truly singular (which generally indicates flawed input or a conceptual model error), a solution (*i. e.*, inversion of the given Jacobian) is virtually guaranteed. The main disadvantages are large storage requirements and slow speed, which makes large meshes (such as realistic three-dimensional problems) impractical.

LP: Another LU-decomposition solver from Linpack, a non-proprietary package of linear algebra routines. Essentially identical to the original LU solver, this solver first calculates a condition number, which indicates the degree of singularity of the Jacobian. If the condition number is too small, the LP solver concludes that the matrix is singular and aborts the run, in contrast to the original LU solver, which will continue with the solution unless the Jacobian determinant is exactly zero. The parameters and mesh used by WIPP PA often result in Jacobians that are very nearly singular at times during a run, so the LP solver is generally not used because it aborts too readily. However, the LP solver is sometimes useful for debugging. It has been disabled in BRAGFLO Version 6.0 because the massive Jacobian array is rewritten into another array, nearly doubling the memory required to run BRAGFLO. It may be reactivated easily in future versions. If the LP solver is selected, the program will abort with a message printed to the screen:

```
*** Abort in READCNTRL; LP solver not available.
```

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THE LP SOLVER IS NOT QA'D AND WILL NOT BE USED FOR WIPP COMPLIANCE CALCULATIONS.

MG: Multigrid solver. This is a sophisticated, state-of-the-art high-speed iterative solver. In addition to speed (compared to direct solvers), this solver has the advantage of all iterative solvers in that the storage requirements are far less than for direct solvers, making large three-dimensional simulations possible. However, the multigrid solver originally implemented in BRAGFLO was limited to two dimensions and suffered from a lack of robustness that was intolerable in WIPP PA, where *all* runs must be completed. This option is currently not available, pending development of a robust three-dimensional multigrid solver. Although prospects are poor that a multigrid solver will eventually work in BRAGFLO, the shell for selecting this solver has been retained. If it is selected, the program will abort with a message printed to the screen:

```
*** Abort in READCNTRL; MG solver not available.
```

THE MULTIGRID SOLVER IS NOT QA'D AND WILL NOT BE USED FOR WIPP COMPLIANCE CALCULATIONS.

LSOR: Point successive over-relaxation (SOR) solver. This is another iterative solver, which, like the multigrid solver, lacks robustness. It should work on simple problems or large problems using uniform grid blocks and smoothly varying material properties.

THE LSOR SOLVER WILL NOT BE USED FOR WIPP COMPLIANCE CALCULATIONS.

Line 6.21. Descriptor. Iteration limits; scaling options.

Line 6.22. ITMAX, IRESETMAX, IJACINPUT, LSCALE, P_SCALE, LVARSWTCH.

ITMAX: Maximum number of Newton-Raphson iterations per time step. Recommended value: 10.

IRESETMAX: Maximum number of time step size reductions allowed at any time step should non-convergence problems be encountered. If this number is exceeded, the run is aborted; this is the only way a BRAGFLO run will cleanly abort (aside from input errors). Note that the time steps obtained as a result of time step reductions following non-convergence are not restricted in size by the input parameter DELTMIN (Line 1.9). It is possible for a time step smaller than DELTMIN to be obtained that results in convergence after fewer than IRESETMAX time step reductions. This can only occur when non-convergence causes time steps to be reduced below DELTMIN. In this case, the next time step will automatically be reset to DELTMIN. Convergence requiring time steps smaller than DELTMIN may occur repeatedly and has the potential for causing BRAGFLO to stall out, consuming great quantities of computing time using impractically small time steps by sidestepping the normal time step minimum through this one loophole. However, it has been found that when BRAGFLO has difficulties resulting in

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repeated use of time steps smaller than DELTMIN, either these problems are resolved by taking just a couple of time steps smaller than DELTMIN, or they cause IRESETMAX to be exceeded. Recommended value: 40.

IJACINPUT: Default iteration interval frequency for updating the Jacobian. The Jacobian is always evaluated at the start of each time step. Reevaluating the Jacobian at each Newton-Raphson iteration within a time step will, at least in theory, result in the fastest convergence to a solution. However, in some instances, convergence may be just as fast even when the Jacobian is evaluated only before the first iteration. Because evaluating the Jacobian is the most computationally intensive step in the solution, it is highly desirable to do this as infrequently as possible. On the other hand, reevaluating every iteration is more likely to give a solution, especially in difficult problems, whereas doing this, say, just once each time step (every 40 iterations), can sometimes cause the solution to diverge, resulting in more computational effort than simply reevaluating every iteration. Recommended value: 1.

LSCALE: Logical flag specifying whether to scale the Jacobian and the right hand side. Scaling may reduce round-off errors that cause numerical problems when working with near-singular matrices, which is often the case in WIPP PA. Recommended value: T.

P_SCALE: When LSCALE = T, the Jacobian and right hand side are divided by P_SCALE to reduce the singularity of the Jacobian when the degree of singularity is exacerbated by round-off errors. Whether LSCALE = T or F, a value must be input here; when LSCALE = F, P_SCALE is read in but is not used. Recommended value: 1.0×10^7 Pa.

LVARSWTCH: Logical flag specifying whether variable switching will be allowed. This flag can be set to T only if dissolved gas is being modeled and Henry's law is to be used (IDGAS = 2). The gas solubility options are described in Subsection 7.2.8. When Henry's law gas solubility is used, LVARSWTCH *should* be set to T; this is not a requirement, but BRAGFLO may not run well or at all if variable switching is not allowed (set to F) when IDGAS = 2. When LVARSWTCH = T, the dependent variables may be automatically changed when the gas phase disappears, from the normal set of gas saturation and brine pressure (S_g and P_o) to P_o and P_o . P_o is the equilibrium Henry's law gas pressure, defined as the gas pressure that would exist if a gas phase were present given the mole fraction of gas that is currently dissolved in the brine. Because gas can dissolve in brine, it is possible for the gas phase to disappear, but a gas component will remain in the liquid phase. When this happens, it is no longer possible to keep track of the amount of gas dissolved in brine because the dissolved gas is no longer in equilibrium with gas in the (nonexistent) gas phase. Instead of solving two equations (gas mass balance and brine mass balance) for two unknowns (S_g and P_o), BRAGFLO will be trying unsuccessfully to solve just one equation, the brine mass balance, for two unknowns, since the gas mass balance is identically zero as a result of S_g being zero. This will cause the run to abort or to flounder, struggling hopelessly by cutting back time steps. The solution to this difficulty is to change the dependent variable from gas saturation to a pseudo-pressure, P_o , which is directly proportional to the mass or mole fraction of gas dissolved in brine:

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$$P_a = x_g H,$$

where: x_g = mole fraction of gas dissolved in brine,

H = Henry's law constant [Pa/mol fraction gas in solution].

When a gas phase is present, P_a is identical to P_g . When a single liquid phase is present, P_a is the gas pressure that would exist in equilibrium with the dissolved gas if a gas phase were present. In this manner, BRAGFLO can still use the gas mass balance equation as one of the two equations being solved, but solves, in effect, for the nonzero dissolved gas mass fraction instead of the zero gas saturation. When LVARSWTCH = T, this switching of the dependent variables is done automatically and is transparent to the user, except that informational messages are printed to the screen and to the summary [.SUM] file to indicate when the variables are switched and at which grid blocks. If LVARSWTCH = F when Henry's law is used to model gas dissolution, BRAGFLO will run smoothly only if a gas phase is always present. Unless this situation can be assured of holding true for the full duration of the run, LVARSWTCH = T should be used. *This feature has not been extensively tested.*

Line 6.23. Descriptor. Upstream weighting frequencies; time step reduction factor; averaging methods for relative permeabilities and mass fractions.

Line 6.24. IUPRPFLAG, IUPMFFLAG, DELTFACTOR, ITRAVE, IMFRAVE.

IUPRPFLAG: Frequency of updating the inter-time step upstream weighting direction for relative permeabilities. The upstream weighting direction can be changed only when the Jacobian is reevaluated; thus, IUPRPFLAG is not simply the number of Newton-Raphson iterations between updating the upstream direction, but rather the number of Jacobian evaluations between updates. For example, if IJACINPUT (Line 6.22) = 3 (Jacobian reevaluated every third iteration) and IUPRPFLAG = 3, then the upstream direction for relative permeability is updated every 9 iterations. *This option has not been extensively tested*, but it appears that the upstream direction should not be changed every iteration, nor every other iteration (assuming IJACINPUT (Line 6.22) = 1), because this may cause the solution to oscillate and fail to converge. Recommended value: same as ITMAX (Line 6.22), which effectively turns this option off, anchoring the upstream direction at the first iteration. If convergence difficulties suggest that this option may improve convergence, a value of 3 should be tried first.

IUPMFFLAG: Frequency of updating the inter-time step upstream weighting direction for mass fractions. As with relative permeabilities, the upstream weighting direction can be changed only when the Jacobian is reevaluated. IUPMFFLAG the number of Jacobian evaluations between updates. This option will have an effect only if the dissolved gas option is activated (see Section 7.2.9); without dissolved gas, the mass fraction of gas dissolved in brine is always zero everywhere, and the mass fraction of brine component in the brine phase is always 1.0 everywhere, so the upstream direction is not only fixed, but has no impact on the solution. *Although this option is available, it has not been tested sufficiently to know if it has any significant effect on convergence behavior. Until it has been tested more thoroughly, this option should not be used. IT WILL NOT BE USED IN WIPP COMPLIANCE CALCULATIONS.* Recommended value: same as ITMAX (Line

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6.22), which turns this option off, anchoring the upstream direction at the first iteration. A value must be input even if the dissolved gas option is not activated.

DELTFACOR: Time step reduction factor when non-convergence occurs. Recommended value: 0.5.

ITRAVE: Transmissivity averaging method at block interfaces. Recommended value: 1.
ITRAVE = 0: Use arithmetic average. This method is untested.
ITRAVE = 1: Use harmonic average.

IMFRAVE: Method for averaging mass fractions at block interfaces when dissolved gas option is activated. A value must be input even if the dissolved gas option is not activated. Recommended value: 0.

IMFRAVE = 0: Use upstream value of mass fractions.
IMFRAVE = 1: Use harmonic average.

Line 6.25. Descriptor. Jacobian reevaluation control parameters. These parameters are invoked when difficulties arise that cause the time step to be cut back repeatedly, potentially causing the run to abort. The options permit the frequency of Jacobian reevaluation to be changed, convergence tolerances to be relaxed, and upstream directions to be updated at different frequencies. These changes remain in effect for a specified number of time steps before the original set of control parameter values is reinstated.

Line 6.26. **IJACSWITCH, IJACMIN, IJACRESET, IUPRPLOOSE, IUPMFLOOSE.**

IJACSWITCH: Number of time step reductions allowed before the new set of control parameters is temporarily invoked. This parameter controls when the Jacobian starts to be reevaluated every IJACMIN iterations instead of every IJACINPUT (Line 6.22) iterations, the looser convergence tolerances are invoked, and upstream direction update frequencies are changed. Recommended value: 10.

IJACMIN: Number of iterations allowed before the Jacobian is reevaluated after IJACSWITCH time step reductions have occurred; the Jacobian is now reevaluated every IJACMIN iterations. Reevaluating the Jacobian more frequently (if IJACINPUT > 1) can sometimes promote convergence when BRAGFLO is encountering difficulties. Although many iterations can be performed in much less computing time than is required for a single evaluation of the Jacobian, convergence is often achieved with a single iteration after reevaluation. If IJACINPUT > 1, this parameter alone should be changed first, before tolerances are loosened or upstream direction frequencies are changed, because this parameter generally has the greatest impact on convergence. Recommended value: 1.

IJACRESET: Number of time steps during which IJACMIN, looser tolerances, and modified upstream direction update frequencies remain in effect following a time step in which IJACSWITCH time step reductions occurred. When BRAGFLO is having severe difficulties, reevaluating the Jacobian more frequently for a few time steps can help it through the difficult period. However, such trouble spots are usually of short duration, so more frequent reevaluations should not be continued indefinitely if not necessary. Looser convergence tolerances should also not be used any longer than necessary because, strict-

ly speaking, the accuracy of the entire run is only as good as the looser tolerances, even though they were used only a few small time steps. Recommended value: 2.

IUPRPLOOSE: Frequency of updating the upstream direction for relative permeabilities. This is the “looser tolerances” value of IUPRPFLAG, and is used for IJACRESET time steps. *This option has not been tested, so its use is not recommended. IT WILL NOT BE USED IN WIPP COMPLIANCE CALCULATIONS.* Use a value equal to or greater than ITMAX, which turns this option off.

IUPMFLOOSE: Frequency of updating the upstream direction for mass fractions. This is the “looser tolerances” value of IUPMFFLAG, and is used for IJACRESET time steps. *This option has not been tested, so its use is not recommended. IT WILL NOT BE USED IN WIPP COMPLIANCE CALCULATIONS.* Use a value equal to or greater than ITMAX, which turns this option off.

Line 6.27. Descriptor. Relative changes for Jacobian elements.

Line 6.28. DH(1), DH(2).

DH(1): Relative change in gas saturation for Jacobian element derivative calculations. Because the equations being solved are so nonlinear, DH should be as small as possible without losing numerical precision. Recommended value: 1.0×10^{-8} .

DH(2): Relative change in brine pressure for Jacobian element derivative calculations. Recommended value: 1.0×10^{-8} .

Line 6.29. Descriptor. Minimum absolute change for Jacobian elements.

Line 6.30. HMIN(1), HMIN(2).

HMIN(1): Minimum absolute gas saturation change allowed for Jacobian element derivative calculations. This limit prevents the variable change calculated using the *relative* change factor DH from becoming too small when the saturation is small. Recommended value: 1.0×10^{-10} .

HMIN(2): Minimum absolute brine pressure change allowed for Jacobian element derivative calculations [Pa or psi]. Recommended value: 0.01 Pa.

7.2.8 Material Maps and Material Properties

This section describes input that establishes material properties for each grid block. A material type grid map is input in which each grid block is assigned a material type index. This map applies during a specified time period. A series of material maps covers the duration of the run, allowing material properties in each grid block to change for discrete periods of time. Following the material maps, certain special materials are input; for these materials, specialized submodels apply, the most important example being Waste, in which chemical reactions occur that can occur in no other material. Material properties are input next. These include two-phase flow parameters, permeabilities, reference-condition porosities, and compressibilities. Finally, flags and parameters for submodels simulating fracturing and Klinkenberg effect are input.

Line 7.1. Descriptor. Number of material maps.

Line 7.2. NMATTIMES.

NMATTIMES: Number of times to specify a material map. NMATTIMES must be less than or equal to MAXMATTIMES, set in the PARAMETER statement. If NMATTIMES is less than one or greater than MAXMATTIMES, no error message will be printed, but BRAGFLO will abort sooner or later.

Lines 7.3 - 7.6 are repeated NMATTIMES times.

Line 7.3. Descriptor. Start times.

Line 7.4. TIMEMAT.

TIMEMAT: Starting time at which the material map that follows is in effect [s or days]. If the first TIMEMAT is later than START, the starting time for the run, no error message is printed, but any results obtained before BRAGFLO aborts will be unpredictable and unreliable.

Line 7.5. Descriptor. Material map.

Line 7.6. (((IMAT(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

IMAT(I,J,K): Material type number for grid block (I,J,K). This number is associated later with the material properties input. BRAGFLO finds the minimum and maximum material type numbers in all NMATTIMES maps and assumes that the total number of materials, NMAT, is equal to the maximum value found in the maps. If any IMAT(I,J,K) is less than 1 or greater than MMAT (set in the PARAMETER statement), BRAGFLO will abort after printing the offending minimum or maximum value of IMAT, with the following message printed to the screen:

```
*** Aborted:  Input material type error in READMAT ***
```

One or more material type numbers between 0 and NMAT may, at the user's option, be omitted from the material maps without causing any problem. However, material properties (starting at Line 7.31 below) must be input for NMAT materials, regardless of how many material numbers are actually used in the maps. For example, if the maps have only two material types, numbered 2 and 8, properties for 8 materials must be input, even though the properties for only two of the eight materials will actually be used. Normally, NMAT materials would actually be used.

Line 7.7. Descriptor. Material names. The following line is repeated NMAT times.

The information on each line is not used in any way in BRAGFLO. It is intended solely to provide space within the input file to help the user identify each material type

Line 7.8. LABEL.

LABEL: Dummy CHARACTER*132 variable. Must be read in, but is not used.

Special Materials.

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BRAGFLO has four special material types that have unique capabilities. These have evolved to handle situations encountered in modeling the WIPP, so they have names that apply to regions included in models of the WIPP, but actually have fairly general applications. The materials are referred to as: Waste, DRZ (Disturbed Rock Zone), "Reset" materials, and Borehole.

Waste Material.

In Waste materials, and only in Waste, can chemical reactions take place. Specifically, corrosion of iron can occur, which consumes iron and water and produces hydrogen; microbial degradation of cellulose can occur; this reaction consumes cellulose and produces hydrogen, and, if indicated in the input (described later), can also consume or produce water. Hydration and carbonation of MgO can occur as described above in Subsection 4.13.5.

Another special capability unique to Waste is simulation of creep closure, in which the porosity decreases over time, the rate depending on the rate of gas production and the pressure within the Waste. Porosity can change in any material as a result of pressure-dependent compressibility, but the change is generally quite small. In contrast, the porosity change resulting from creep closure of the Waste can be very large.

Only in Waste can there be an *initial* mass of radionuclides, the transport and decay of which can be modeled in any region as long as there was some amount initialized in the Waste. Finally, to be able to simulate an operational period in the WIPP, during which excavations are open to the atmosphere and any brine seepage is removed by means of ventilation or pumping, the initial brine pressure and saturation in the Waste can be specified to be different from the initial conditions described in Subsection 7.2.6. Then, at some later time (TIMEICRESET), the conditions in the Waste can be reset to the initial conditions specified in Subsection 7.2.6.

There is one important constraint in how Waste regions are specified. If there are to be NWST regions that will contain waste (MAT_WASTEI), there must also be NWST Waste regions (MAT_WASTE) to "deposit" into these regions to be filled with Waste. Additionally, each NWST MAT_WASTE material index numbers must be unique even though the same Waste properties are desired to be placed in the NWST MAT_WASTEI regions. For example, assume $NWST = 2$ and the 2 MAT_WASTEI regions are empty excavations described by materials number 4 and 5 of the materials table defined in the section "Material Property Data", below (see lines 7.41 to 7.46). Also suppose that at some time during the simulation defined by TIMEICRESET in line 7.24, above, that Waste properties, defined by material 6 are to replace the MAT_WASTEI materials, 4 and 5. Since two MAT_WASTE material numbers are required and since these material identifiers must be unique, then an additional material must be specified in the table (lines 7.41 to 7.46) say material 7 even though it has the same properties as material 6, the original Waste material. Therefore, in this example $NWST = 2$, $MAT_WASTEI(1) = 4$, $MAT_WASTEI(2) = 5$, $MAT_WASTE(1) = 6$, and $MAT_WASTE(2) = 7$. An error check is performed in BRAGFLO Version 6.0 to make sure NWST unique MAT_WASTE material identifiers are provided. If they are not BRAGFLO will abort with an error message printed to the screen and to the .SUM file. No such check is done in earlier versions of BRAGFLO.

Line 7.9. Descriptor. Waste regions.

Line 7.10. NWST.

NWST: Number of Waste regions.

If $NWST \leq 0$, the next two lines (7.11 and 7.12) are omitted. If $NWST > MWST$ (set in the PARAMETER statement), the run will abort.

Line 7.11. Descriptor. Definition of Waste regions.

Line 7.12. (MAT_WASTEI(I), I=1, NWST), (MAT_WASTE(I), I=1, NWST).

MAT_WASTEI: Material type index of the material at time START that will *become* Waste at time TIMEICRESET. Prior to TIMEICRESET, materials designated as MAT_WASTEI have no special characteristics and receive no special treatment. It is necessary to know which regions are eventually going to become Waste regions, however, to calculate what will be the Waste region volume, because this information must be known before any initial conditions are printed or any other calculations are done.

MAT_WASTE: Material type index of Waste *after* TIMEICRESET. Porosity will be calculated using the creep closure sub-model only for this material type (provided that model is turned on; input controlling this sub-model will be discussed later, in Section 10). Corrosion and biodegradation reactions occur only in this material. There should be a one-to-one correspondence between MAT_WASTEI(I) and MAT_WASTE(I); NWST values of each are read in.

Disturbed Rock Zone (DRZ) Material.

In this material, if the porosity increases at time TIMEICRESET, the brine volume is assumed to remain fixed over that change, and the brine saturation is adjusted to account for the increased pore volume. Gas is assumed to fill the additional pore space. The gas appears instantaneously; there is no source for this gas, *i. e.*, it does not flow from any other cell, is not introduced by well injection, and is not created by way of chemical reaction. It just appears suddenly to occupy newly created pore volume. The pressure in this material at TIMEICRESET is specified by input as PRES DRZ. This material arose from a need to simulate the disturbed rock zone surrounding excavations in halite. The time-dependent behavior of disturbed halite is not well understood, but it is considered likely that the porosity will be greater by the time the repository is filled and sealed. This behavior is currently modeled very simply as an instantaneous increase in porosity at TIMEICRESET, with the additional pore space filled with gas that, in reality, would have migrated in from the adjacent excavated regions through cracks and borings. More than one DRZ material can be used, each with a different reset pressure (PRES DRZ). In modeling the WIPP, a single DRZ material is generally used, and the pressure is reset to PRES DRZ = 1 atm (101.325 kPa), the same as in the Waste at TIMEICRESET, so that the newly-introduced gas in the DRZ does not expand and unrealistically flow into the Waste.

Line 7.13. Descriptor. DRZ regions.

Line 7.14. NDRZ.

NDRZ: Number of DRZ material regions.

If $NDRZ \leq 0$, the next two lines (7.15 and 7.16) are omitted. If $NDRZ > MDRZ$ (set in the PARAMETER statement), the run will abort.

Line 7.15. Descriptor. DRZ materials.

Line 7.16. (MAT_DRZ(I), I=1, NDRZ), (MAT_DRZNEW(I), I=1, NDRZ).

MAT_DRZ: Original DRZ material type index number, from the first material map.

MAT_DRZNEW: The DRZ material type index number for the material map starting at time TIMEICRESET (input later); in this material type at time TIMEICRESET, saturations will be adjusted and pressures will be reset to PRES DRZ (input later).

“Reset” Material.

In this material, conditions will be reset to the initial conditions specified in Subsection 7.2.6. This differs from DRZ material in that both saturation and pressure are reset at time TIMEICRESET, and they are reset to the Subsection 7.2.6 conditions. In contrast, in DRZ material, the saturations are adjusted to maintain a fixed brine volume and the pressure is reset to PRES DRZ, rather than to the Subsection 7.2.6 initial pressure. These materials arose in modeling the WIPP from the need to simulate backfilled regions, which are initially excavations, but become backfill at TIMEICRESET. In this case, the conditions calculated just prior to TIMEICRESET are inconsequential, and new specified conditions reflecting newly-emplaced backfill and seals are needed; because the backfilled and sealed regions may cover a large number of grid blocks, these new conditions are most conveniently provided in the original conditions in Subsection 7.2.6.

Line 7.17. Descriptor. “Reset” materials.

Line 7.18. NMATRESET.

NMATRESET: Number of material regions where initial conditions will be reset at time TIMEICRESET to the original initial conditions.

If $NMATRESET \leq 0$, the next two lines (7.19 and 7.20) are omitted. If $NMATRESET > NMAT$, the run will abort.

Line 7.19. Descriptor. “Reset” materials.

Line 7.20. (MATRESET(I), I=1, NMATRESET).

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MATRESET: Material type index numbers for materials in which the brine pressure, PO, and brine saturation, SO, will be reset to the original (Subsection 7.2.6) initial conditions, PINIT and SOINIT, respectively. Waste material index numbers should be included here if PO and SO are to be reset. The material index numbers used should be for the last material map *prior* to TIMEICRESET; this map may be (and generally is) the first map specified (at time START), but if more than one map is specified prior to TIMEICRESET, use the last map immediately before TIMEICRESET.

Borehole Material.

In this material, the solute concentration and solute mass are reset to zero when an intrusion borehole opens. This simulates the removal of radionuclides in both solid and dissolved phases when a drill cuts through the waste. It is a minor adjustment, but easily accomplished in BRAGFLO, so it is done just to make the results reflect reality slightly more accurately. It is used only when transport is activated. However, if transport is not being modeled, lines 7.21 and 7.22 must still be input, although MAT_BOREHOLE can be any number from 0 to NMAT and is not used.

Line 7.21. Descriptor. Borehole material.

Line 7.22. MAT_BOREHOLE.

MAT_BOREHOLE: Material type index number for borehole material, if transport is activated (see Section 11). If transport is not activated, MAT_BOREHOLE can be any number from 0 to NMAT, but a number must still be input.

Special Material Control and Reset Parameters.

Line 7.23. Descriptor. Reset control parameters.

Line 7.24. TIMEICRESET, ICWASTE.

TIMEICRESET: Time when initial conditions are reset [s or days]. Normally = 0. Used only when START is less than zero. Negative times (START<0) are used in WIPP PA simulations to cover the operational period of the WIPP, prior to the start of the regulatory compliance period, which begins at time zero. The primary objective of using these negative times is to enable realistic pressure distributions in the formations surrounding the WIPP repository to be calculated without doing this in a separate run. Designation of times as positive or negative is largely a question of semantics. All calculations could start at time zero, cover, say, a 20-year operational period and extend to 10,020 years total to cover the 10,000-year compliance period. However, then the plotting and other post-processing would need to deal with a time period of 20 to 10,020 years, instead of the more clearly understandable period of 0 to 10,000 years specified in regulations. Using negative times for the operational period, and omitting this period from plots and re-

ports, makes discussions of the results simpler and more in line with compliance regulations.

No results are printed to the output files until TIMEICRESET. The initial conditions that are always printed to both the ASCII and binary output files are the conditions at TIMEICRESET, *after* all the special materials have been reset to their respective initial conditions.

If TIMEICRESET = START, the ICWASTE must be 0. Otherwise, BRAGFLO will abort with the message:

ICWASTE: Flag to indicate that waste initial conditions will differ from the initial conditions specified in Subsection 7.2.6. This flag overrides any implied reset control indicated by material type indexes in Lines 7.9 - 7.22, but these lines must still be input.

= 1: Initial conditions specified by POWASTEIC and SOWASTEIC (input next) will be used at time START instead of PINIT and SOINIT (from Subsection 7.2.5).

= 0: Initial conditions PINIT and SOINIT will be used at time START.

ICWASTE must be 0 when TIMEICRESET = START.

*** ICWASTE error in READMAT.

If ICWASTE is not 0 or 1, BRAGFLO will neither abort nor warn of an error, but results may be unpredictable.

Line 7.25. Descriptor. Pressure initial conditions.

Line 7.26. (POWASTEIC(I), I=1, NWST).

POWASTEIC(I): Brine pressure in Waste region I at time START, uniform throughout Waste region I [Pa or psi]. Used only when ICWASTE = 1, but NWST values must still be input even if ICWASTE = 0.

Line 7.27. Descriptor. Saturation initial conditions.

Line 7.28. (SOWASTEIC(I), I=1, NWST).

SOWASTEIC: Brine saturation in Waste region I at time START, uniform throughout Waste region I. Used only when ICWASTE = 1, but NWST values must still be input even if ICWASTE = 0.

Line 7.29. Descriptor. Reset DRZ pressure.

Line 7.30. (PRESDRZ(I), I=1, NDRZ).

PRESDRZ(I): Brine pressure to which DRZ region I will be reset at time TIMEICRESET [Pa or psi].

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Line 7.31 Descriptor. Number of times the borehole is to be reset

Line 7.32 NBORERESET

NBORERESET: Number of times at which a borehole (or other material) is to be reset to a new pressure and saturation. See Subsection 4.17.4 for a description of the subroutine RESETMID and how it is used. For example if two separate materials were to be reset at two different material changes, then NBORERESET = 2.

If NBORERESET = 0, then the following lines are not entered

Line 7.33 Descriptor. NBORETIME(I), NMATBORE(I), MATBORE(I,NMATBORE), I = intrusion time index

The following line is entered NBORERESET times

Line 7.34 NBORETIME(I), NMATBORE(I), MATBORE(I,NMATBORE)

NBORETIME: Index of the material change at which a borehole (or other material) is to be reset to a new pressure and saturation. $1 \leq \text{NBORETIME} \leq \text{NMATTIMES}$.

NMATBORE: Number of materials to be changed at the intrusion time.

(MATBORE(I),I=1,NMATBORE): Material type numbers that are to be reset at NBORETIME.

Line 7.35 Descriptor. Borehole reset pressure.

The following line is entered NBORERESET times

Line 7.36 PORESET(I). I = intrusion index.

PORESET(I): Reset pressure [Pa or psi] for the materials identified in Line 7.34. All materials identified in MATBORE(I) are reset to PORESET(I) for a given intrusion index. Each material cannot be reset to a different pressure.

Line 7.37 Descriptor. Borehole reset saturation.

The following line is entered NBORERESET times

Line 7.38 SORESET(I). I = intrusion index.

SORESET(I): Reset saturation [dimensionless] for the materials identified in Line 7.34. All materials identified in MATBORE(I) are reset to SORESET(I) for a given intrusion index. Each material cannot be reset to a different saturation.

Line 7.39 Descriptor. ICHEM.

The following line is entered NBORERESET times

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Line 7.40 ICHEM(I). I = intrusion index.

ICHEM: Flag which determines whether concentrations of Fe, cellulose, and MgO are set to zero after an intrusion. If ICHEM = 1 then concentrations are set to zero, otherwise they are not.

Material Property Data.

In this section, material properties are input for each of the NMAT materials in the material map. Properties used include relative permeability and capillary pressure model parameters, intrinsic permeability values, porosities, and compressibilities.

Line 7.41. Descriptor. Relative permeability and capillary pressure model parameters.

If some material type numbers less than NMAT are not actually used in any material maps, NMAT property values must still be read in. If there are fewer than NMAT lines of property data, BRAGFLO will abort as a result of an input error while trying to read character data into INTEGER and REAL variables.

The next line is repeated NMAT times.

Line 7.42. I, XLAMDA(I), SBR(I), SGR(I).

I: Material type number.

XLAMDA(I): Pore-size distribution parameter, λ , for Brooks-Corey and van Genuchten-Parker relative permeability and capillary pressure models. The van Genuchten-Parker model uses a parameter, m , which is obtained from the Brooks-Corey parameter, λ :

$$m = \lambda / (1 + \lambda).$$

SBR(I): Residual brine saturation, S_{br} .

SGR(I): Residual gas saturation, S_{gr} . The original Brooks-Corey and van Genuchten-Parker models do not use a residual gas saturation, but a value must still be input.

Line 7.43. Descriptor. More relative permeability and capillary pressure model parameters.

The next line is repeated NMAT times.

Line 7.44. I, SBMIN(I), POMIN(I), PCMAX(I), PCT_A(I), PCT_EXP(I), KRP(I), KPC(I), KPT(I).

I: Material type number.

SBMIN(I): Minimum brine saturation when using capillary pressure model number $KPC(I) = 3$. It is otherwise not used; however, a value must still be read in, and $SBMIN(I) > SBR(I)$. If $SBMIN(I) < SBR(I)$, BRAGFLO will abort, even if $KPC(I) \neq 3$. Recommended value: $1.05 \times SBR(I)$.

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POMIN(I): Minimum brine pressure [Pa or psi]. Used to adjust capillary pressure when capillary pressure model KPC(I) = 3 is used. If KPC(I) \neq 3, POMIN(I) is not used and any value can be input for POMIN(I); however, some value must be input regardless of the capillary pressure model used. If KPC(I) = 3, a value of POMIN(I) = 1.01325×10^5 Pa is recommended.

PCMAX(I): Maximum capillary pressure that can be used when capillary pressure model KPC(I) = 2 or 3 is used [Pa or psi]. A value of PCMAX(I) = 1.0×10^8 Pa is recommended. If KPC(I) = 1, 4, or 5, a value must still be read in, but PCMAX(I) is not used.

PCT_A(I): Constant, a , in function relating threshold capillary pressure, P_{ct} , to permeability, k :

$P_{ct} = a k^\eta$. Gives P_{ct} for the Brooks-Corey models. In the van Genuchten-Parker model, a capillary pressure constant, P_o , is used; it is calculated in BRAGFLO by equating the capillary pressure from each of the two models at an effective saturation, S_e , of 0.5 and solving the expression for P_o . [$S_e = (S_b - S_{br})/(1 - S_{br})$]. [Pa]

PCT_EXP(I): Exponent, η , in function relating threshold capillary pressure, P_{ct} , to permeability [dimensionless].

KRP(I): Relative permeability model number:

- = 1: van Genuchten-Parker model; modified to use a nonzero residual gas saturation.
- = 2: Original Brooks-Corey model.
- = 3: Brooks-Corey model, modified to use a residual gas saturation in calculating the effective saturation for both wetting and non-wetting phase relative permeabilities.
- = 4: Brooks-Corey model, modified to use a residual gas saturation in calculating the effective saturation for the non-wetting phase relative permeability only.
- = 5: Linear relative permeabilities: $k_{rb} = S_{eg}$; $k_{rg} = 1 - S_{eg}$, where:
 $S_{eg} = (S_b - S_{br})/(1 - S_{gr} - S_{br})$ is the effective saturation using residual gas saturation.
- = 6: Linear relative permeabilities: $k_{rb} = S_e$; $k_{rg} = S_{eg}$, where S_{eg} is the same as given above for KRP(5), and $S_e = (S_b - S_{br})/(1 - S_{br})$ is the effective saturation without the gas saturation dependence.
- = 7: Linear relative permeabilities: $k_{rb} = k_{rg} = 1$.
- = 8: Original van Genuchten-Parker model, with zero residual gas saturation.
- = 11: Linear relative permeabilities between residual saturation and residual saturation plus a tolerance. See equations (131)-(133) and the supporting text in Subsection 4.9 for a complete description. The additional parameter tol needed for this model is given below in Line 7.48.
- = 12: Brooks-Corey model, modified to use S_{min} instead of the residual brine saturation. See equation (130) and the supporting text in Subsection 4.9 for a

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complete description. The additional parameters needed for this model are given below in Lines 7.48 and BLAH.

Note that models 9, and 10 are not QA'd and will not be used or discussed here.

KPC(I): Capillary pressure model number:

- = 1: No special treatment. Numerical problems may occur as brine saturation approaches residual brine saturation and capillary pressure tends to infinity. Below residual brine saturation, the capillary pressure is zero.
- = 2: Fixed maximum capillary pressure of PCMAX(I), thereby avoiding potential problems that might be encountered using KPC(I) = 1. BRAGFLO computes a minimum brine saturation at which the capillary pressure equals PCMAX; below this minimum brine saturation, the capillary pressure is PCMAX. This model is recommended.
- = 3: Variable maximum capillary pressure. This model has not been fully tested, and its theoretical basis is uncertain. Use this model at your own risk.
- = 4: Capillary pressure fixed at PTHRESH(I), which may be zero.
- = 5: Linear capillary pressures.

KPT(I): Flag indicating whether threshold capillary pressure will be continuously updated as a function of dynamically varying permeability or fixed in time for a given material.:

- = 0: Threshold capillary pressure is fixed in time for material I; computed in BRAGFLO using the function: $P_{ct} = a k^\eta$, as described above for PCT_A(I) and PCT_EXP(I). The intrinsic permeability in the x -direction, XKX(I) (input on Line 7.36), is used for k .
- = 1: Threshold capillary pressure varies in time for material I; computed in BRAGFLO using the function: $P_{ct} = a k^\eta$, as described above for PCT_A(I) and PCT_EXP(I). Brine permeability in the x -direction is used for k ; it varies as a function of time-dependent porosity in materials that undergo fracturing or creep closure. Fracturing is described below starting at Line 7.37. Creep closure is discussed in Subsection 7.2.10.

Line 7.45. Descriptor. Intrinsic properties.

The next line is repeated NMAT times.

Line 7.46. I, XKX(I), YKY(I), ZKZ(I), PORREFROCK(I), CROCK(I)

I: Material type number.

XKX(I): Intrinsic permeability of material I in the x -direction [m^2 or darcy].

YKY(I): Intrinsic permeability of material I in the y -direction [m^2 or darcy].

ZKZ(I): Intrinsic permeability of material I in the z -direction [m^2 or darcy].

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PORREFROCK(I): Porosity of material I at a reference pressure equal to the initial pressure, **PINIT**, which may be different in each grid block [fraction]. If material I is to undergo creep closure (see Subsection 7.2.10.), **PORREFROCK(I)** is not used unless material I is used before **TIMEICRESET**, when creep closure is not yet activated. If a material that will undergo creep closure is used before **TIMEICRESET**, an appropriate value of **PORREFROCK(I)** must be input. If such a material is not used until after **TIMEICRESET** (this is normally the case in **WIPP PA**), then the input value of **PORREFROCK(I)** is not used, and any value can be input. If creep closure is later turned off in this material because pressure or time limitations are exceeded, **BRAGFLO** resets **PORREFROCK(I)** at the value of porosity that exists at the time when closure is turned off; the reference pressure is reset at the same time and is equal to the current brine pressure in the material or grid block.

CROCK(I): Compressibility of material I at a reference pressure equal to the initial pressure, **PINIT** [Pa^{-1} or psi^{-1}].

Various checks are done on the material properties input. Errors or inconsistencies may cause **BRAGFLO** to abort with error messages printed to the screen and to the **.SUM** file.

Line 7.47 Descriptor. Tol and **SOCEFFMIN** for permeability models 11 and 12.

Line 7.48. **TOL**, **SOCEFFMIN**.

TOL: Tolerance over which the relative permeability changes from zero to 1 for **KRP** = 11. See equations (131)-(133) and the supporting text in Subsection 4.9 for a complete description.

SOCEFFMIN: Saturation below S_{\min} at which the Brooks-Corey model becomes singular (or capillary pressure is capped at **PCMAX** for **KPC** = 2). See equation (130) and the supporting text in Subsection 4.9 for a complete description.

Line 7.49. Descriptor. Number of materials to use the smooth permeability transition model. See Subsection 4.18 for a complete description of this module.

Line 7.50. **NMATSP**

NMATSP: Number of materials which will use the smooth permeability transition model. See Subsection 4.18 for a complete description of this module.

Line 7.51. Descriptor. **MATSP**, **MATSPF**, **TEND**, **TCHANGE**.

*The next line is repeated **NMATSP** times*

Line 7.52 **MATSP(I)**, **MATSPF(I)**, **TEND(I)**, **TCHANGE(I)**.

Information Only

MATSP(I): Starting material type number for the material in which to use the smooth permeability model. See Subsection 4.18 for a complete description of this module.

MATSPF(I): Final material type number that material **MATSP(I)** will become at the end of the smoothed permeability change. See Subsection 4.18 for a complete description of this module.

TEND(I): Time at which material **MATSP(I)** will have completed its smooth change to material **MATSPF(I)**. See Subsection 4.18 for a complete description of this module.

TCHANGE(I): Time over which the material change will occur. From **TCHANGE(I)** and **TEND(I)**, the time at which the material change begins **TINIT(I) = TEND(I) – TCHANGE(I)**. See Subsection 4.18 for a complete description of this module.

Line 7.53 Descriptor. NSMPRMC, SMPRMC.

The next line is repeated N_{MATSP} times

Line 7.54. NSMPRMC(I), SMPRMC(I).

NSMPRMC(I): Number of coefficients, i.e. order of the polynomial + 1, to be used in the smooth permeability model. See Subsection 4.18 for a complete description of this module.

(SMPRMC(I,J),J=1,NSMPRMC(I)): Coefficients a_j of the polynomial that smoothly changes permeability from that of the material **MATSP(I)** to that of **MATSPF(I)**. See equation (176) and the supporting text of Subsection 4.18 for a complete description. It is the user's responsibility to calculate these coefficients a priori. BRAGFLO does not calculate them for you.

Fracture Model.

A crude rock fracture model in BRAGFLO allows the porosity and permeability to increase in a fractured network as pore pressure increases above a threshold value. The implementation uses a pressure-dependent rock compressibility to determine fracture porosity. Permeability in the fractured layer is varied with porosity according to a power law function:

$$k = k_o \left[\frac{\phi_f}{\phi_o} \right]^n,$$

where k = fractured permeability [m^2];
 k_o = intact permeability [m^2];
 ϕ_f = fractured porosity [m^3 void/ m^3 rock];

Information Only

ϕ_o = intact porosity [m^3 void/ m^3 rock];
 n = exponent [dimensionless].

Line 7.55. Descriptor. Fracture model control.

Line 7.56. K FRACTURE.

K FRACTURE: Logical flag indicating whether the fracture model will be used and whether the fracture model parameters will be read in.

= .TRUE.: Use the fracture model in BRAGFLO and read in parameters.

= .FALSE.: Do not use the fracture model, and do not read in fracture model parameters.

Lines 7.57 -7.60 are input *only* if K FRACTURE = .TRUE.

Line 7.57. Descriptor. Number of materials in which the fracture model can be applied.

Line 7.58. NFRAC.

NFRAC: Number of materials in which the fracture model can be applied.

The following two lines are repeated NFRAC times.

Line 7.59. Descriptor. Fracture model parameters.

Line 7.60. I, FRPI(I), FRPF(I), FRPHIMAX(I), FRPRMEXP(I), IFRX(I), IFRY(I), IFRZ(I), LFPC(I).

I: Material type number for the material in which fracturing can occur.

FRPI(I): Pressure increment above the initial pressure, PINIT, at which fracturing will initially occur. [Pa or psi]. Typical value: 1.39×10^6 Pa.

FRPF(I): Pressure increment above the fracture initiation pressure (*i.e.*, increment above PINIT + FRPI), at which the fracture is fully-developed, *i. e.*, the porosity of the fractured material is at its maximum [Pa or psi]. Typical value: 2.5×10^6 Pa.

FRPHIMAX(I): [m^3 void/ m^3 rock] Maximum allowable fracture porosity. The pressure-dependent porosity will be limited to this value. Typical value: 0.10.

FRPRMEXP(I): Exponent, n , in the permeability-porosity power law relationship [dimensionless]. Typical value: 9.5.

IFRX(I): Flag to indicate whether x -direction permeability will be calculated for fractured material. Recommended value: 1.

= 1: Do calculate permeability for fractured material.

= 0: Permeability will remain the same as the intact permeability for material I.

Information Only

IFRY(I): Flag to indicate whether *y*-direction permeability will be calculated for fractured material. Recommended value: 0.

= 1: Do calculate permeability for fractured material.

= 0: Permeability will remain the same as the intact permeability for material I.

IFRZ(I): Flag to indicate whether *z*-direction permeability will be calculated for fractured material. Recommended value: 0.

= 1: Do calculate permeability for fractured material.

= 0: Permeability will remain the same as the intact permeability for material I.

LFPC(I): Flag to indicate whether to use constant pressure during fracturing model. Recommended value: F.

= T: Use constant pressure during fracturing model.

= F: Use original fracture model.

Klinkenberg Effect.

At low pressures and in low-permeability materials, the gas phase intrinsic permeability can be significantly higher than the liquid phase intrinsic permeability. This is the Klinkenberg effect. The gas or non-wetting phase permeability, k_{nw} , can be correlated to the brine or wetting phase permeability, k_w , by the Klinkenberg equation:

$$k_{nw} = k_w (1 + b / P)$$

where

k_w = brine phase intrinsic permeability [m^2],

P = brine pressure [Pa],

b = Klinkenberg coefficient [Pa]

$$= \text{BKLINK} \cdot (k_w)^{\text{EXPLINK}},$$

BKLINK = linear parameter in Klinkenberg equation [Pa],

EXPKLINK = exponent in Klinkenberg equation [dimensionless].

It is assumed in BRAGFLO that input values of intrinsic permeability (Line 7.46) are brine phase intrinsic permeabilities. If the Klinkenberg effect is modeled, gas phase intrinsic permeabilities are obtained from the Klinkenberg equation from the input values of brine phase intrinsic permeability. If the fracture model is also activated (Line 7.38; KFRACTURE = .TRUE.), brine phase intrinsic permeabilities are calculated first, using the fracture model parameters, and then gas phase intrinsic permeabilities are calculated using the Klinkenberg equation.

Information Only

Line 7.61. Descriptor. Klinkenberg effect control parameter.

Line 7.62. KLINK.

KLINK: Logical flag controlling use of Klinkenberg effect:
= .TRUE.: Do include Klinkenberg effect and read in the two parameters.
= .FALSE.: Do not include Klinkenberg effect and do not read in the two parameters.

Lines 7.45 and 7.46 are read in only if KLINK = .TRUE.

Line 7.63. Descriptor. Klinkenberg parameters.

Line 7.64. BKLINK, EXPKLINK.

BKLINK: Linear parameter in Klinkenberg equation [Pa].
Recommended value: 0.336 Pa.

EXPKLINK: Exponent in Klinkenberg equation [dimensionless].
Recommended value: -0.336.

7.2.9 Fluid Properties.

This section discusses input for fluid properties and parameters that control their use. BRAGFLO has two fluids: brine and gas. Brine is composed of water and an unspecified solute, the composition of which is of no consequence in BRAGFLO. The gas is a mixture of any of six gases: hydrogen (H₂), carbon dioxide (CO₂), methane (CH₄), nitrogen (N₂), oxygen (O₂), and hydrogen sulfide (H₂S). Brine is treated as an ideal fluid. Gases can be treated either as ideal gases or as real gases using the Redlich-Kwong-Soave equation of state. As an option, gas can dissolve in brine; using either a Henry's law treatment or an unreliable, untested bubble point calculation. THE DISSOLUTION OF GAS IN BRINE IS NOT SIMULATED IN WIPP COMPLIANCE CALCULATIONS. Additionally, as mentioned in section 5.0, the gas phase is assumed to be all H₂.

Line 8.0 Descriptor. Gravity Constant, GSTD, and Gas Constant, R.

Line 8.1 GSTD, R.

GSTD: Gravity Acceleration Constant at WIPP [m/s² or ft/day²]

R : Gas Constant [J/(gm-mol*K) or Btu/(lbmol*R)]

: A value of 8.314510 [J/(gm-mol*K)] is used.

Line 8.2. Descriptor. Reference conditions.

Line 8.3. TREF, PREF.

TREF: Reference temperature for standard densities [K or °R].

PREF: Reference pressure for standard densities [Pa or psi].

Line 8.4 Descriptor. Brine property parameters.

Line 8.5. SALT, DENOSC, KGSAT, IDGAS, BRCOMP, WMSALT, WMH2O.

SALT: Brine salinity [wt % solute].

DENOSC: Density of brine at reference conditions [kg/m³ or lb/ft³].

KGSAT: Flag to indicate initial gas content of brine:

= 0: Brine is initially gas-free.

= 1: Brine is initially saturated with gas. This is the recommended input value.

IDGAS: Flag to indicate treatment of dissolved gas in brine:

= 0: Gas does not dissolve in brine.

= 1: Gas does dissolve in brine, using bubble point tracking.

= 2: Gas does dissolve in brine, using Henry's law treatment.

BRCOMP: Brine compressibility, β [Pa⁻¹ or psi⁻¹]. The compressibility of WIPP brine is 2.5×10^{-10} Pa⁻¹. The equation BRAGFLO uses to evaluate brine density is:

$$\rho = \rho_o \exp[\beta(p - p_o)]$$

where:

p = brine pressure [Pa],

p_o = reference pressure, PREF (Line 8.2) [Pa],

ρ_o = brine density, DENOSC, at reference pressure [kg/m³].

WMSALT: Molecular weight of salt component of the brine [kg/gm-mol or lb/lbmol].
Assumed to have the molecular weight of NaCl.

Information Only

WMH2O : Molecular weight of water component of the brine [kg/gm-mol or lb/lbmol].

If IDGAS = 0 (Line 8.5), no additional gas dissolution parameters are read in; Do not enter lines 8.5.1-8.5.4. *THIS IS THE QUALIFIED OPTION FOR USE IN WIPP COMPLIANCE CALCULATIONS THE DISSOLUTION OF GAS IN BRINE IS NOT SIMULATED IN WIPP COMPLIANCE CALCULATIONS.*

If IDGAS = 1 (Line 8.5), input Lines 8.5.1, 8.5.2, 8.5.3, and 8.5.4: *THIS OPTION IS NOT QUALIFIED FOR USE IN WIPP COMPLIANCE CALCULATIONS AND WILL NOT BE USED IN WIPP COMPLIANCE CALCUALTIONS.*

Line 8.5.1. Descriptor. Gas solubility parameters.

The input parameters are coefficients in the empirical correlation relating gas solubility to gas partial pressure. This correlation is commonly used, but it is used in BRAGFLO specifically to account for the solubility of hydrogen in WIPP brine.

$$\ln x_g = D_0 + D_1 \ln P$$

where:

x_g = mole fraction of gas in solution in brine.

D_0 = adjustable fitting coefficient. For hydrogen dissolved in 5 N NaCl brine, $D_0 = 10.0789$.

D_1 = adjustable fitting coefficient. For hydrogen dissolved in 5 N NaCl brine, $D_1 = 0.8205$.

P = partial pressure of the gas of interest in the gas phase [MPa].

The bubble point tracking treatment used in BRAGFLO is believed to be flawed, and its use is not recommended. If a user wishes to investigate this feature, the logic can be retained while the bubble point tracking is effectively turned off by using input values for RSOD0 of -100. and RSOD1 of 5.

Line 8.5.2. SGBUBMIN, RSOD0, RSOD1.

SGBUBMIN: Minimum gas saturation required for calculating new bubble point. Recommended value: -1.0.

RSOD0: Gas solubility correlation coefficient, D_0 .

RSOD1: Gas solubility correlation coefficient, D_1 .

Line 8.5.3. Descriptor. Slopes of parameters at pressures greater than the bubble pressure.

Line 8.5.4. BSLOPE, RSLOPE, VSLOPE.

Information Only

BSLOPE: Slope of the brine formation volume factor versus pressure curve for undersaturated brine (pressure above initial brine bubble point pressure): d (formation volume factor) / dP [Pa^{-1} or psi^{-1}]. Recommended value: 0.

RSLOPE: Slope of the solution gas-brine ratio versus pressure curve for undersaturated brine (pressure above initial brine bubble point pressure): d (R_w) / dP [Pa^{-1} or $\text{ft}^3/(\text{bbl psi})$]. Recommended value: 0.

VSLOPE: Slope of the brine viscosity versus pressure curve for undersaturated brine (pressure above initial brine bubble point pressure):
 d (brine viscosity) / dP [s or cP/psi]. Recommended value: 0.

If $\text{IDGAS} = 2$ (Line 8.5), read Lines 8.4a and 8.4b. *THIS OPTION IS NOT QUALIFIED FOR USE IN WIPP COMPLIANCE CALCULATIONS AND WILL NOT BE USED IN WIPP COMPLIANCE CALCUALTIONS.*

Line 8.5.1. Descriptor. Henry's law constant.

Line 8.5.2. HENRYC.

HENRYC: Henry's law constant [Pa/mol fraction gas dissolved in brine]. If selected, i.e. when $\text{IDGAS} = 2$, a single value is used for all gases, independent of the actual composition, at a fixed temperature. WIPP PA uses 4.0×10^{10} Pa/mol fraction gas. BRAGFLO assumes that the dissolved gas is N_2 , regardless of the actual composition of the gas phase, which WIPP PA generally assumes to be pure H_2 . These conflicting assumptions are used because the gas found dissolved in native WIPP brines is mostly N_2 , whereas the gas generated in the waste, especially by anoxic corrosion of ferrous metals, is mostly H_2 . To deal with this situation correctly would require tracking multiple gas components in both the gas phase and in the brine phase. Although BRAGFLO is capable of tracking multiple components in the gas phase, it cannot currently do this in the brine phase, and the computational effort to do so cannot be justified to correct the small errors resulting from these assumptions.

Note: If $\text{IDGAS} = 2$, a value for $\text{LVARSWTCH} = \text{T}$ should be used; see Line 6.22.

Line 8.6. Descriptor. Fluid viscosities. BRAGFLO does not account for the effects of pressure and composition on viscosity. A single constant value each for brine viscosity and gas viscosity at a temperature, TREF, is read in.

Line 8.7. VISO, VISG.

Information Only

VISO: Brine viscosity [Pa s or cP].

VISG: Gas viscosity [Pa s or cP].

Line 8.8. Descriptor. Gas density flag.

Line 8.9. INTERPDENG.

INTERPDENG: Flag indicating how gas density will be calculated:

- = 1: Interpolate from table set up by BRAGFLO using the Redlich-Kwong-Soave equation of state. This is a very fast and efficient means for calculating gas density accurately, but it can be used only when a single pure gas is used.
- = 0: Calculate gas density using the Redlich-Kwong-Soave equation of state. This option provides the greatest accuracy and can be used with any combination of the six gases that can be modeled in BRAGFLO: H₂, CO₂, CH₄, N₂, O₂, and H₂S. However, it is by far the slowest method for calculating gas density. The gases that are available is severely limited because of the lack of binary interaction coefficients for other gases.
- = -1: Interpolate from table set up by BRAGFLO using the ideal gas law. This option is made available as a counterpart to INTERPDENG = 1, but because the ideal gas law is so simple and fast, setting up an interpolation table is generally not recommended.
- = -2: Use ideal gas law. This option is the fastest method for calculating gas density, but is not as accurate as the Redlich-Kwong-Soave equation of state. Other gases, in addition to the six currently available, could easily be added because the only data required is molecular weight. When using the multi-component gas transport option (Subsection 7.2.12), the ideal gas law should always be used because the transport model introduces enough inaccuracies that the substantial additional computing time required to use INTERPDENG = 0 is not justified.

If a single pure gas such as hydrogen is used, it is best to interpolate from a table, because it is much faster computationally. In this case, BRAGFLO sets up a table of calculated gas densities using the Redlich-Kwong-Soave equation of state at fixed pressure intervals of 10,000 Pa. The number of table entries is specified in the PARAMETER statement by the constant, NPINT. Intervals of 10,000 Pa provides a sufficiently smooth density curve versus pressure. If much larger intervals are used, results can be noticeably affected; pressure vs. time plots, for example, will acquire a staircase appearance and the results may be seriously in error. To ensure that table values cover the full range of expected pressures, NPINT must be large. It is currently set at NPINT = 10,000, giving a maximum table entry of 100 MPa. If memory is limited, this can be safely reduced to a more practical limit of, say, 20 MPa, or NPINT = 2,000. If pressures higher than the maximum table entry are encountered, BRAGFLO will extrapolate from the two highest entries. If the pressure, P_g , is between 0 and 10,000 Pa, the density is calculated as $(P_g/10000)$ times the density at 10,000 Pa. If the pressure is less than zero, the density is set to 1/10 of the density at 10,000 Pa.

If more than one gas is used, interpolation is not possible, and the full Redlich-Kwong-Soave (RKS) equation of state (EOS) (INTERPDENG = 0) must be solved each time a new density is needed.

If INTERPDENG \geq 0 then the RKS EOS has been selected. Assigned RKS parameters on line 8.18 to 8.29.

FOR WIPP COMPLIANCE CALCULATIONS ONE GAS COMPONENT IS ASSUMED AND THE INTERPOLATION OF THE RKS EOS OPTION IS USED, I.E. INTERPDENG=0.

Line 8.10. Descriptor. Gas composition.

Line 8.11. (YGAS(I), I=1, MGAS).

YGAS: Initial mole fraction of each of the MGAS gases currently available in BRAGFLO (MGAS = 6); set in the PARAMETER statement. If the gas transport option is used, this composition can change during the run. If gas transport is not used, this initial gas composition will remain fixed for all time. All MGAS entries are required even though, as in the case for the WIPP COMPLIANCE calculations only one gas component is considered.

YGAS(1) = mole fraction of H₂ [dimensionless].
YGAS(2) = mole fraction of CO₂ [dimensionless].
YGAS(3) = mole fraction of CH₄ [dimensionless].
YGAS(4) = mole fraction of N₂ [dimensionless].
YGAS(5) = mole fraction of H₂S [dimensionless].
YGAS(6) = mole fraction of O₂ [dimensionless].

Line 8.12. Descriptor. Gas component molecular weights.

Line 8.13 (MWGAS(I), I=1, MGAS)

WMGAS: Molecular weights of the 6 possible gas phase components allowed by BRAGFLO v5.0. The identification and ordering of the 6 components is specified above in the description of N1GAS, above. All MGAS entries are required even though, as in the case for WIPP compliance calculations only one gas component is considered.

MWGAS(1) = Molecular Weight of H₂ [kg/gm-mol or lb/lbmol].
MWGAS(2) = Molecular Weight of CO₂ [kg/gm-mol or lb/lbmol].
MWGAS(3) = Molecular Weight of CH₄ [kg/gm-mol or lb/lbmol].
MWGAS(4) = Molecular Weight of N₂ [kg/gm-mol or lb/lbmol].
MWGAS(5) = Molecular Weight of H₂S [kg/gm-mol or lb/lbmol].
MWGAS(6) = Molecular Weight of O₂ [kg/gm-mol or lb/lbmol].

Line 8.16 Descriptor. Number of gas components used and index number.

Information Only

Line 8.17 NGAS, N1GAS

NGAS: Number of gases actually being used in the problem.

N1GAS: Gas number from the current list: 1 = H₂, 2 = CO₂, 3 = CH₄, 4 = N₂, 5 = H₂S ,

6 = O₂. This is used only if NGAS = 1; otherwise, it can be any number. This parameter is used to simplify the gas density calculation when only one gas is present.

If INTERPDENG >= 0 then the RKS EOS has been selected. Assigned RKS parameters on line 8.18 to 8.29. This is the qualified option for WIPP compliance calculations.

If INTERPDENG < 0, skip to section 7.2.10.

Line 8.18 Descriptor. RKS specified- TC: for H₂, CO₂, CH₄, N₂, H₂S, O₂.

Line 8.19 (TC(I), I=1, MGAS)

TC: Critical temperatures of the 6 possible gas phase components allowed by BRAGFLO v5.0. The identification and ordering of the 6 components are specified above in the description of N1GAS, above. All MGAS entries are required even though, as in the case for WIPP compliance calculations only one gas component is considered.

TC(1) = Critical Temperature of H₂ [K or R].

TC(2) = Critical Temperature of CO₂ [K or R].

TC(3) = Critical Temperature of CH₄ [K or R].

TC(4) = Critical Temperature of N₂ [K or R].

TC(5) = Critical Temperature of H₂S [K or R].

TC(6) = Critical Temperature of O₂ [K or R].

Line 8.20 Descriptor. RKS specified- PC for H₂, CO₂, CH₄, N₂, H₂S, O₂.

Line 8.21 (PC(I), I=1, MGAS)

PC: Critical pressure of the 6 possible gas phase components allowed by BRAGFLO v5.0. The identification and ordering of the 6 components are specified above in the description of N1GAS, above. All MGAS entries are required even though, as in the case for WIPP compliance calculations only one gas component is considered.

PC(1) = Critical Pressure of H₂ [Pa or psi].

PC(2) = Critical Pressure of CO₂ [Pa or psi].

PC(3) = Critical Pressure of CH₄ [Pa or psi].

PC(4) = Critical Pressure of N₂ [Pa or psi].

PC(5) = Critical Pressure of H₂S [Pa or psi].

PC(6) = Critical Pressure of O₂ [Pa or psi].

Line 8.22 Descriptor. RKS specified- ACEN for H₂, CO₂, CH₄, N₂, H₂S, O₂.

Information Only

Line 8.23 (ACEN(I), I=1, MGAS)

ACEN: Acentric Factors for the 6 possible gas phase components allowed by BRAGFLO v5.0. The identification and ordering of the 6 components are specified above in the description of N1GAS, above. All MGAS entries are required even though, as in the case for WIPP compliance calculations only one gas component is considered.

ACEN(1) = Acentric factor for H₂ [dimensionless].
ACEN(2) = Acentric factor for CO₂ [dimensionless].
ACEN(3) = Acentric factor for CH₄ [dimensionless].
ACEN(4) = Acentric factor for N₂ [dimensionless].
ACEN(5) = Acentric factor for H₂S [dimensionless].
ACEN(6) = Acentric factor for O₂ [dimensionless].

Line 8.24 Descriptor. RKS specified- Special properties for H₂.

Line 8.25 TCH2, PCH2, WMH2

TCH2 = Special critical temperature for H₂ [K or R].
PCH2 = Special critical pressure for H₂ [Pa or psi].
WMH2) = Special molecular weight for H₂ [kg/gm-mol or lb/lbmol].

Line 8.26 Descriptor. RKS specified- OMEGAA and OMEGAB constants.

Line 8.27 OMEGAA OMEGAB

OMEGAA = RKS constant [dimensionless].
OMEGAB = RKS constant [dimensionless].

Line 8.28 Descriptor. RKS specified- Binary Interaction Parameters.

Line 8.29.1 to Line 8.29.12 ((AKIJ(I,J), I=1, MGAS), J=1, MGAS)

AKIJ: Binary Interaction Parameters for all of the binary interactions among the 6 possible gas phase components allowed by BRAGFLO Version 6.0. The identification and ordering of the 6 components are specified above in the description of N1GAS, above. All MGAS*MGAS entries are required even though, as in the case for WIPP compliance calculations only one gas component is considered.

Line 8.29.1 Descriptor. RKS specified- Binary Interaction Parameters for H₂

Line 8.29.2 AKIJ(1,1:MGAS) = Binary Interaction Parameter for H₂ [dimensionless].
H₂ interaction with H₂, CO₂, CH₄, N₂, H₂S, O₂, respectively.

Line 8.29.3 Descriptor. RKS specified- Binary Interaction Parameters for CO₂

Information Only

Line 8.29.4 AKIJ(1,1:MGAS) = Binary Interaction Parameter for CO₂ [dimensionless].
CO₂ interaction with H₂, CO₂, CH₄, N₂, H₂S, O₂, respectively.

Line 8.29.5 Descriptor. RKS specified- Binary Interaction Parameters for CH₄

Line 8.29.6 AKIJ(3,1:MGAS) = Binary Interaction Parameter for CH₄ [dimensionless].
CH₄ interaction with H₂, CO₂, CH₄, N₂, H₂S, O₂, respectively.

Line 8.29.7 Descriptor. RKS specified- Binary Interaction Parameters for N₂

Line 8.29.8 AKIJ(4,1:MGAS) = Binary Interaction Parameter for N₂ [dimensionless].
N₂ interaction with H₂, CO₂, CH₄, N₂, H₂S, O₂, respectively.

Line 8.29.9 Descriptor. RKS specified- Binary Interaction Parameters for H₂S

Line 8.29.10 AKIJ(5,1:MGAS) = Binary Interaction Parameter for H₂S [dimensionless].
H₂S interaction with H₂, CO₂, CH₄, N₂, H₂S, O₂, respectively.

Line 8.29.11 Descriptor. RKS specified- Binary Interaction Parameters for O₂

Line 8.29.12 AKIJ(6,1:MGAS) = Binary Interaction Parameter for O₂ [dimensionless].
O₂ interaction with H₂, CO₂, CH₄, N₂, H₂S, O₂, respectively.

7.2.10 Chemical Reaction Parameters

These parameters govern the chemical reactions that are modeled in BRAGFLO. THE AVERAGE STOICHIOMETRY MODEL IS THE QUALIFIED GAS GENERATION MODEL TO BE USED FOR WIPP COMPLIANCE CALCULATIONS. This is explained fully in Subsection 4.13. These reactions take place only in the Waste Areas. Cellulose is approximated by the pseudo- molecule,, [C₆H₁₀O₅/6], having a molecular weight of 27.023 x 10⁻³ [kg/gm-mol]. The gas produced or consumed in these reactions is assumed to have the physical properties of hydrogen.

Line 9.1. Descriptor.

Line 9.2. IGASVAR.

IGASVAR: Gas generation reaction flag:

= 0: No Fe or [C₆H₁₀O₅]/6 consumption and no gas generation.

Information Only

= 1: Fe and $[C_6H_{10}O_5]/6$ consumption with gas generation (Average Stoichiometry Model. This is the qualified option for WIPP compliance calculations.).

= 2: Reaction path gas generation model. (Not yet available).

If IGASVAR = 0, no more chemical reaction parameters are input; go to Section 7.2.11.

If IGASVAR = 1, lines 9.3 to 9.12 are required.

If IGASVAR = 2, skip to line 9.13.

Currently lines 9.19-9.22 have to be entered even if IGASVAR = 0.

THE AVERAGE STOICHIOMETRY MODEL IS THE QUALIFIED GAS GENERATION MODEL TO BE USED FOR WIPP COMPLIANCE CALCULATIONS.

Line 9.3. Descriptor. Reaction rate constants for brine-inundated conditions.

Line 9.4. RK(1), RK(2), LINTRIN

RK(1): Corrosion reaction rate constant under brine-inundated conditions $[gm\text{-mol Fe}/(s\ m^3)$ or $lbmol\ Fe/(day\ ft^3)$], unless LINTRIN = TRUE (see below) and then the units should be $[gm\text{-mol Fe}/(s\ kg)]$.

RK(2): Biodegradation reaction rate constant under brine-inundated conditions $[gm\text{-mol } [C_6H_{10}O_5]/6 / (s\ m^3)$ or $lbmol\ [C_6H_{10}O_5]/6 / (day\ ft^3)$], unless LINTRIN = TRUE (see below) and then the units should be $[gm\text{-mol } [C_6H_{10}O_5]/6 / (s\ kg)]$.

LINTRIN: Parameter to decide whether to use intrinsic or extrinsic rates.

= TRUE: Then the chemical rates are multiplied by the initial concentration of the consumed material, on a element by element basis. For example in CORSAT and CORHUM, RK(1) would be multiplied by the initial concentration of Fe in the element in which the rate is being calculated. In this case the units of RK(1) in the input file should be $[gm\text{-mol Fe}/(s\ kg)]$ and not $[gm\text{-mol Fe}/(s\ m^3)]$. This option is for iron corrosion, biodegradation, and MgO hydration and carbonation. The purpose of this option is to allow for different initial concentrations in each element of the BRAGFLO grid.

= FALSE: Then the rates are used as is, and should be entered in the input file in units of $[gm\text{-mol}/(s\ m^3)]$.

Line 9.5. Descriptor. Humid rate factors.

Line 9.6. HF(1), HF(2).

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HF(1): Factor multiplying RK(1) to get the corrosion reaction rate constant under humid conditions [dimensionless].

HF(2): Factor multiplying RK(2) to get the biodegradation reaction rate constant under humid conditions [dimensionless].

Line 9.7 Descriptor. Inundated and humid MgO hydration rates and hydromagnesite conversion rate.

Line 9.8 BRUCITEI, BRUCITEH, HYMAGCON

BRUCITEI: Inundated MgO hydration rate in units of [gm-mol MgO/(s m³)] or [lbmol Fe/(day ft³)], unless LINTRIN = TRUE in which case the units should be [gm-mol MgO/(s kg)] or [lbmol Fe/(day lb)].

BRUCITEH: Humid MgO hydration rate in units of [gm-mol MgO/(s m³)] or [lbmol Fe/(day ft³)], unless LINTRIN = TRUE in which case the units should be [gm-mol MgO/(s kg)] or [lbmol Fe/(day lb)].

HYMAGCON: Hydromagnesite conversion rate in units of [gm-mol MgO/(s kg)] or [lbmol Fe/(day lb)].

Line 9.9 Descriptor. RXH2S and RXCO2.

The next line is repeated NWST times

Line 9.10 RXH2S(I), RXCO2(I)

RXH2S(I): Moles of Iron sulfidized per mole of organic carbon consumed. See Subsection 4.13.3.

RXCO2(I): Moles of magnesium needed to carbonate one mole of CO₂. See Subsection 4.13.5.

Line 9.11 Descriptor. SMIN.

Line 9.12 SMIN

SMIN: Minimum brine saturation below which all chemistry ceases. This is discussed in Subsection 4.13.1. Recommend SMIN = 0.015.

Line 9.13 Descriptor. Reactant/product molecular weights, WM(1:4).

Line 9.14 (WM(I),I=1,4).

WM : Molecular weights for the reactants and products in the Average Stoichiometry Model.

WM(1): Molecular weight for H₂ [kg/gm-mol or lb/lbmol].

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WM(2): Molecular weight for H₂O [kg/gm-mol or lb/lbmol].
WM(3): Molecular weight for Fe [kg/gm-mol or lb/lbmol].
WM(4): Molecular weight for [C₆H₁₀O₅]/6 [kg/gm-mol or lb/lbmol].

Line 9.15 Descriptor. Reactant/product molecular weights, WM(5:10).

1

Line 9.16 (WM(I),I=5,10).

WM(5): Molecular weight for Fe(OH)₂ [kg/gm-mol or lb/lbmol].
WM(6): Molecular weight for FeS [kg/gm-mol or lb/lbmol].
WM(7): Molecular weight for MgO [kg/gm-mol or lb/lbmol].
WM(8): Molecular weight for Mg(OH)₂ [kg/gm-mol or lb/lbmol].
WM(9): Molecular weight for Hydromagnesite [kg/gm-mol or lb/lbmol].
WM(10): Molecular weight for MgCO₃ [kg/gm-mol or lb/lbmol].

Line 9.17 Descriptor. Stoichiometry Matrix.

The following line is repeated 8 times.

Line 9.18 S(I,J)

S(I,J): Stoichiometry coefficient matrix for the eight reactions currently considered in the average stoichiometry model [dimensionless]. The matrix is entered in rows and columns with I being the row and J being the column. The identity of each entry is described in Subsection 4.13.2, with the meaning of each row given in Table 1, and the meaning of each column given in Table 2. Guidance for the values of these coefficients is given in Subsections 4.13.3-4.13.5.

Currently lines 9.19-9.22 have to be entered even if IGASVAR = 0.

Line 9.19 Descriptor. Reactant/Product Densities DEN(1:4).

Line 9.20 (DEN(I),I=1,4) These are the densities listed in Table 3 for I = 1,4 in units of [kg/m³] or [lb/ft³]. The index and corresponding identity are given in Table 3, and will not be repeated here.

Line 9.21 Descriptor. Reactant/Product Densities DEN(5:9)

Line 9.22 (DEN(I),I=5,9) These are the densities listed in Table 3 for I = 5,9 in units of [kg/m³] or [lb/ft³]. The index and corresponding identity are given in Table 3, and will not be repeated here.

Line 9.23. Descriptor. Additional reaction parameters.

Line 9.24. SATWICK, LARXN, LARXN2, ALPHARXN.

SATWICK: Term modifying the brine saturation to simulate the effect of wicking on the net reaction rate by increasing the inundated rate and decreasing the humid rate [dimensionless]. Valid range: 0.0-1.0. A value of 0.0 will turn this feature off. Instead of using

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the actual brine saturation, S_b , to calculate reaction rates, the effective saturation S_{eff} is used as described in Subsection 4.13.1.

LARXN: Logical flag indicating whether to smooth humid reaction rates (.TRUE.) using the factor ALPHARXN, or use unmodified, discontinuous humid rates (.FALSE.). Recommended value: T.

LARXN2: Logical flag indicating whether to use concentration smoothing (.TRUE.) using the factor ALPHARXN, or use discontinuous rates (.FALSE.) when reactants run out. See Subsection 4.13.6 for a discussion of this feature.

ALPHARXN: Term used in smoothing functions to eliminate a discontinuity at brine saturation, $S_b = 0$, as described in Subsection 4.13.1. Always used in expression to obtain S_{eff} when wicking is modeled (i. e., when SATWICK > 0.). When LARXN = T, ALPHARXN (or α) is used in the smoothing function for all humid rates:

$$r_{h,eff} = r_h \left(1 - e^{\alpha S_{eff}}\right)$$

where:

$$\begin{aligned} r_h &= \text{humid rate} \\ &= \text{HF}(1) \times \text{RK}(1), \text{ or } \text{HF}(2) \times \text{RK}(2); \\ r_{h,eff} &= \text{effective (smoothed) humid rate.} \end{aligned}$$

If LARXN = F, then ALPHARXN is not used for the humid corrosion and biodegradation rates, and $r_{h,eff} = r_h$. The full rate is given by [where r_i is the inundated rate]:

$$\begin{aligned} r &= S_{eff} r_i + (1 - S_{eff}) r_{h,eff}, & S_{eff} > 0 \\ &= 0, & S_{eff} = 0 \end{aligned}$$

so, unless $r_{h,eff} = 0$, r will be discontinuous at $S_{eff} = 0$. This discontinuity tends to cause numerical problems. Generally, BRAGFLO will run better when LARXN = T, although exceptions to this rule have been encountered. ALPHARXN must be a negative value; if a positive value is input, BRAGFLO will convert the input value to a negative value before using it. Recommended value: -1000. A large negative value for ALPHARXN will approximate more closely the discontinuous function originally intended for r while remaining smooth enough to ease the numerical difficulties. Small negative values of ALPHARXN will result in values of $r_{h,eff}$ that are significantly different from r_h , and a value of zero will cause $r_{h,eff}$ to be zero.

If the Reaction Path Model is not used then skip to Section 7.2.11.

The parameters on the following lines of input are only needed if the Reaction Path Model is specified, i.e. IGASVAR = 2. THE REACTION PATH MODEL IS NOT USED IN WIPP COMPLIANCE CALCULATIONS.

The following section of the input file and corresponding features are not QA'd and we make no claims that the following documentation is accurate. We leave it here for future use.

Line 9.25 Descriptor. Reactant/product molecular weights, WMRXN(1:MSPEC).

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Line 9.26 (WMRXN(I),I=1,MSPEC).

WMRXN : Molecular weights for the reactants and products in the Reaction Path Model. MSPEC values are required. MSPEC is defined in the BRAGFLO PARAMETER INCLUDE STATEMENT and is assigned a value of 23.

WMRXN(1): Molecular weight for H₂ [kg/gm-mol or lb/lbmol].

WMRXN(2): Molecular weight for CO₂ [kg/gm-mol or lb/lbmol].

WMRXN(3): Molecular weight for CH₄ [kg/gm-mol or lb/lbmol].

WMRXN(4): Molecular weight for N₂ [kg/gm-mol or lb/lbmol].

WMRXN(5): Molecular weight for H₂S [kg/gm-mol or lb/lbmol].

WMRXN(6): Molecular weight for O₂ [kg/gm-mol or lb/lbmol].

WMRXN(7): Molecular weight for H₂O [kg/gm-mol or lb/lbmol].

WMRXN(8): Molecular weight for H₂SO₄ [kg/gm-mol or lb/lbmol].

WMRXN(9): Molecular weight for HNO₃ [kg/gm-mol or lb/lbmol].

WMRXN(10): Molecular weight for [C₆H₁₀O₅]/6 [kg/gm-mol or lb/lbmol].

WMRXN(11): Molecular weight for FE [kg/gm-mol or lb/lbmol].

WMRXN(12): Molecular weight for FES₂-F [kg/gm-mol or lb/lbmol].

WMRXN(13): Molecular weight for FES₂-O [kg/gm-mol or lb/lbmol].

WMRXN(14): Molecular weight for FECO₃ [kg/gm-mol or lb/lbmol].

WMRXN(15): Molecular weight for FECO₃-O [kg/gm-mol or lb/lbmol].

WMRXN(16): Molecular weight for FE(OH)₂ [kg/gm-mol or lb/lbmol].

WMRXN(17): Molecular weight for FEO(OH) [kg/gm-mol or lb/lbmol].

WMRXN(18): Molecular weight for FE₃O₄ [kg/gm-mol or lb/lbmol].

WMRXN(19): Molecular weight for FES [kg/gm-mol or lb/lbmol].

WMRXN(20): Molecular weight for CAO [kg/gm-mol or lb/lbmol].

WMRXN(21): Molecular weight for CA(OH)₂ [kg/gm-mol or lb/lbmol].

WMRXN(22): Molecular weight for CACO₃ [kg/gm-mol or lb/lbmol].

WMRXN(23): Molecular weight for H₂_RAD [kg/gm-mol or lb/lbmol].

7.2.11 Creep Closure Parameters

These parameters activate the creep closure sub-model. Using this model, the porosity of the Waste is calculated to simulate salt creep that, over time, closes in on the waste, compressing it. Four closure models, or "surfaces," are available, three that apply to waste and one for non-back-filled drifts. Two options are available for interpolating over the closure models. The porosity can be based on the quantity of gas present in the waste or on the pressure in the waste. The

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latter option is more current and conforms more closely to the theoretical basis on which creep closure is modeled.

Line 10.1. Descriptor. Creep closure control flag.

Line 10.2. CLOSURE.

CLOSURE: LOGICAL flag.

If CLOSURE = .TRUE., the porosity of the waste will be calculated using the creep closure model. If CLOSURE = .FALSE., the porosity of the waste will instead be calculated based simply on the compressibility of the waste, in the same manner as for all other materials.

If creep closure is selected, i.e. CLOSURE=.TRUE., then lines 10.3 to 10.10 are required.

Additionally an external file containing the closure look-up table data is also required. THIS INFORMATION IS ENTERED ON A SEPARATE INPUT DATA FILE AND THE BRAGFLO INPUT FILE. The description and format of this data is defined in Subsection 7.3.

If CLOSURE = .FALSE., no more closure data are input; go to Subsection 7.2.13.

Even if CLOSURE = .TRUE., the creep closure model is not used at any time prior to TIMEICRESET. The creep closure model is used only up to the maximum data time for each closure model, TIMEDATA_MAX (3.78716×10^{11} s, or 12,000 yr, in the current version of BRAGFLO. An upper limit of 12,000 yr, instead of 10,000 yr, is used to ensure that interpolation is done properly if a WIPP run goes slightly past 10,000 yr; for example, the completion time [FINISH] for a run is typically set at 3.1557×10^{11} s, which is 10,000.02 yr.); after that time, the porosity of the waste is computed from the compressibility. In order to preserve the waste porosity as a continuous function of time after TIMEDATA_MAX, BRAGFLO sets the reference pressure for porosity calculation, PREFROCK, equal to the current waste pressure, which is uniform throughout the waste in the creep closure model. In addition, the reference porosity, PORREFROCK, is set equal to the current waste porosity, which is also uniform throughout the waste.

Line 10.3. Descriptor. Creep closure parameters.

Line 10.4. NKLOS, KLOSINT, KLOSAVE.

NKLOS: Number of closure models to be used in this run. BRAGFLO currently has three closure surfaces from which to choose. NKLOS must be > 0 and \leq MKLOS, set in the PARAMETER statement; currently, MKLOS = 4.

KLOSINT: Flag indicating the basis on which interpolation on the creep closure data will be done. Recommended value: 1. KLOSINT = 0 was used exclusively in early versions of BRAGFLO that had closure surface capabilities, but is no longer considered reliable, especially with closure surfaces 1, 2, and 4 (surface 3 is the original closure surface). If KLOSAVE = 2 is used, KLOSINT = 0 may *not* be used.

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- = 0: Interpolation based on gas generation rate and quantity of gas present.
- = 1: Interpolation based on average waste pore pressure.

KLOSAVE: Flag indicating the scale over which properties are averaged for application of a closure model. Recommended value: 2.

= 1: Average brine pressures in all grid blocks using a given closure model to determine the porosity, which will be identical in all those grid blocks. This is done only when evaluating residuals; creep closure is not modeled when calculating the Jacobian. This averaging method was used exclusively in earlier versions of BRAGFLO. However, because creep closure effects cannot be accounted for in evaluating the Jacobian, convergence problems often arise. In general, this method should not be used except to replicate earlier results. On the other hand, in some instances solutions have been obtained using KLOSAVE = 1 where using KLOSAVE = 2 causes the run to fail.

= 2: Do no averaging; use only the brine pressure in individual grid blocks to obtain porosity from a closure surface, both for evaluating residuals and for evaluating the Jacobian. Because creep closure effects are properly accounted for in the Jacobian, convergence behavior should be superior to using KLOSAVE = 1. If KLOSINT = 0, BRAGFLO will abort with a message warning that KLOSINT must be 1 when KLOSAVE = 2.

Line 10.5. Descriptor. Creep closure parameters.

The following line is repeated NKLOS times:

Line 10.6. I, PLITHO(I), TIME_CLOSOFF(I), MODPERM(I),
INCR_PORO(I),LSOLPROD(I).

I: Closure surface or model number (1, 2, 3, or 4).

PLITHO(I): Maximum pressure allowed for closure to continue. If waste brine pressure exceeds PLITHO(I), closure is tuned off permanently. The user is informed if and when this happens by a warning printed to the screen and to the .SUM file, if it is used. If closure is turned off, the porosity of the waste may continue to vary with pressure depending on the value of compressibility of the waste, as specified in Line 7.45. For this purpose, the reference porosity and reference pressure are the values that exist in the closure region (if KLOSAVE = 1) or in the grid block undergoing closure (if KLOSAVE = 2) at the time when closure is turned off.

TIME_CLOSOFF(I): Time limit for creep closure to be active [s]. As an example, creep closure modeling may be turned off when a human intrusion occurs, since the closure surface is no longer valid under those circumstances. If there is no time limit on creep closure, a value equal to or greater than TIMEDATA_MAX(I) or FINISH (Line 1.7, end time for the run) can be input.

MODPERM(I): Model to use for determining changes in permeability with changes in porosity for regions that experience closure. Flag is new in BRAGFLO Version 6.0

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= 1: Use model of the form $k = a\phi^\eta$, where a and η are constants set by CLOSPERMFACT(I) and CLOSPERMEXP(I) described below in Line 10.8, k is the intrinsic permeability [m^2], and ϕ is the porosity in each region undergoing dynamic creep closure [m^2]. This model was the original model in BRAGFLO Version 5.0.

= 2: Use a Koseny-Carman like model (new in BRAGFLO Version 6.0)

$$k = k_{inp} \text{ for } \phi \geq \phi_{HIGH} \quad (177)$$

$$k = a \frac{\phi^3}{(1-\phi)^2} \text{ for } \phi_{LOW} \leq \phi < \phi_{HIGH} , \quad (178)$$

$$k = a \frac{\phi_{LOW}^3}{(1-\phi_{LOW})^2} \text{ for } \phi \leq \phi_{LOW} \quad (179)$$

where k_{inp} is the initial intrinsic permeability for the waste area given in Line 7.46, and the constant a is set in BRAGFLO Version 6.0 by matching the intrinsic permeability for the waste area at some porosity ϕ_{HIGH} (set by PHIUPPER given in Line 10.8 below) chosen by the user. These models are in the subroutine CONSOL1.

INCR_PORO(I): Flag to decide whether or not to allow the porosity to increase with time.

= True: Only allow porosity to decrease with time.

= False: Porosity can increase or decrease with time.

LSOLPROD(I): Flag to decide whether or not to use a model (i.e 1 or 2) for changes in permeability due to changes in porosity in regions that experience closure. Although these models have been tested we recommend that they not be used for compliance purposes, because correlations between permeability and porosity are difficult to technically defend.

= True: Use model given by MODPERM(I) to determine permeability in the waste area.

= False: Ignore effect of changes of porosity on permeability.

Note that lines 10.7 and 10.8 must be entered regardless of LSOLPROD(I)

Line 10.7 Descriptor. Parameters for the permeability versus porosity models.

The following line is repeated NKLOS times:

If MODPERM(I) = 1 then

Line 10.8 CLOSPERMFACT(I), CLOSPERMEXP(I)

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CLOSPERMFACT(I): Constant factor, a , in expression relating permeability, k , to porosity, ϕ , in each region undergoing dynamic creep closure [m^2] from model = 1 given above in Line 10.6. If the permeability of any region (KLOSAVE = 1) or grid block (KLOSAVE = 2) undergoing creep closure is to be constant, set CLOSPERMFACT(I) to the initial permeability for that material, XKX (Line 7.46). If KLOSAVE = 1, all grid blocks using the same closure surface will have the same porosity and, consequently, the same permeability.

CLOSPERMEXP(I): Exponent, η , in expression relating permeability, k , to porosity, ϕ , in each region undergoing dynamic creep closure [dimensionless]. If the permeability of any region or grid block is to be constant, set CLOSPERMEXP(I) to zero. Recommended value: 4.6.

IF MODPERM(I) = 2 then

Line 10.8 PHIUPPER(I), PHILOWER(I)

PHIUPPER(I) = ϕ_{HIGH} described above in Line 10.6. This value represents the upper porosity at which changes in permeability with porosity are no longer significant. It is also the value of porosity at which the model (described above in Line 10.6 for MODPERM = 2) sets the permeability equal to the initial intrinsic permeability of the material experiencing closure.

PHILOWER(I) = ϕ_{LOW} described above in Line 10.6. This value represents the lower porosity below which changes in permeability are not significant.

Line 10.9. Descriptor. Creep closure material control parameter.

Line 10.10. NMATCLOS.

NMATCLOS: Number of materials in which closure will take place. Each material that undergoes creep closure is referred to as a closure region. The number of closure regions cannot be greater than the number of materials. Thus, NMATCLOS must \leq MMAT (set in the PARAMETER statement) and must be ≥ 0 . (Inputting a value of 0 is pointless, but otherwise harmless, so it is permitted.)

If NMATCLOS = 0, no more closure data are input; go to Subsection 7.2.12.

Line 10.11. Descriptor. Creep closure parameters associating a material number with a creep closure model number.

The following line is repeated NMATCLOS times:

Line 10.12. I, MATCLOS(I), MODEL CLOS(I).

I: Closure region number. I must be > 0 and \leq MMAT (set in the PARAMETER statement).

MATCLOS(I): Material type number from the material map that will be a closure region. MATCLOS(I) must be > 0 and \leq MMAT (set in the PARAMETER statement). It is permissible for a material number not to be used in any material map, but there is no

check to be sure that material MATCLOS(I) is used in any map. For example, if an input file has one material map with two materials, numbered, say, 1 and 14 (and 14 sets of material properties are input in Section 8), one may input a value of, say, MATCLOS(I) = 5 here, which does not refer to any material actually used in the run. Creep closure will be calculated for material 5 even though it does not exist. This may have no effect on the run, but it may cause the run to abort (after it has reached TIMEICRESET) when the creep closure model tries to interpolate on the closure surface using brine pressures of 0.0, which is the default value when a material has not been defined. Thus, it is up to the user to ensure that valid material numbers are used as closure regions.

MODEL CLOS(I): Creep closure surface or model number used by closure region MATCLOS(I). MODEL CLOS(I) must be >0 and \leq MKLOS (set in PARAMETER statement; currently, MKLOS = 4). The available options are:

- 1: Waste without backfill. Used during 1995, this model is no longer considered the best available for application to waste, but is retained in BRAGFLO to enable earlier calculations to be reproduced.
- 2: Drift without backfill. This model was applied to access drifts ("North End") and the Experimental Region excavations during 1995. It is no longer recommended for application to WIPP, but is retained in BRAGFLO to enable earlier calculations to be reproduced.
- 3: Waste with backfill. This model was used in the 1992 Preliminary Performance Assessment and in subsequent calculations, until early 1995. Although the waste configuration is no longer considered likely, this model is retained in BRAGFLO to enable earlier calculations to be reproduced.
- 4: Waste without backfill. This model is used in the 1996 Compliance Certification Application (CCA) calculations (Stone, 1995).

7.2.12 Radionuclide Transport and Decay Parameters

RADIONUCLIDE TRANSPORT AND DECAY IN BRAGFLO IS NOT QUALIFIED FOR USE IN WIPP COMPLIANCE CALCULATIONS AND WILL NOT BE USED IN WIPP COMPLIANCE CALCUALTIONS.

The "transport" model currently implemented in BRAGFLO is really just a simple particle-tracking model. Radionuclides originating in waste blocks are carried to other grid blocks by simple advection. The only processes that take place other than advection are dissolution and precipitation and radionuclide decay. Diffusion, adsorption, and any other reactions are not included in the present model. The current implementation of transport is inefficient and computationally intensive, so it should be used with discretion. In particular, the number of radionuclides that are tracked has a strong effect on the amount of computing time required. The transport model is solved explicitly and can become unstable. If this happens, transport is turned off. A warning flag is printed to the screen and to the .SUM file both at the time when this occurs and again at the end of the run, and radionuclide concentrations and masses remain unchanged for the duration of the run.

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Because of stability limitations and potentially extreme run times associated with the current implementation of transport and radionuclide decay, this sub-model of BRAGFLO is of limited use and is being phased out. It has been replaced by a separate code, NUTS (Nuclide Transport Simulator), that uses a BRAGFLO flow field, but calculates transport and radionuclide decay implicitly, allowing for much faster and more efficient transport calculations than can be done within BRAGFLO. For now, the transport model remains coded in BRAGFLO, but its use is prohibited because of possible conflicts with the radiolysis model. Radiolysis can also be modeled in BRAGFLO.

Line 11.1. Descriptor. On/off flag for radionuclide decay, either during radiolysis or transport, or both.

Line 11.2. LRADDK.

LRADDK: Logical flag indicating whether radionuclide decay will be calculated.

If LRADDK = .TRUE., additional input is required.

Line 11.3. Descriptor. On/off flag for transport.

Line 11.4. LTRANS.

LTRANS: Logical flag indicating whether transport will be calculated.

If LTRANS = .TRUE., additional input is required. Transport may be turned off automatically if it becomes unstable.

Note: Transport is currently disabled. If LTRANS = .TRUE. on input, it will be set to .FALSE. If transport parameters that are not also needed for radiolysis are in the input file, and radiolysis is not being modeled (LRADDK = .FALSE.), the run will abort trying to read the rest of the input file.

Line 11.5. Descriptor. On/off flag for radiolysis.

Line 11.6. LRADLSIS.

LRADLSIS: Logical flag indicating whether radiolysis will be calculated.

If LRADLSIS = .FALSE. and LTRANS = .FALSE., then BRAGFLO sets LRADDK to .FALSE. even if it was input as .TRUE., and no additional radionuclide decay parameters are input; go to Subsection 7.2.13.

The following section of the input file and corresponding features are not QA'd and we make no claims that the following documentation is accurate. We leave it here for future use.

Line 11.7. Descriptor. Number of radionuclides.

Line 11.8. NRAD.

NRAD: Number of radionuclide species to be tracked in the transport and decay models.

NRAD must be greater than zero and less than or equal to MRAD, which is set in the PARAMETER statement. Otherwise, BRAGFLO will abort with the message:

*** Aborted in READRAD: Invalid NRAD value input.

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Note: None of the rest of the input is checked for validity or consistency.

The following two lines (11.9 and 11.10) are read in only if LRADDK = .TRUE.:

Line 11.9. Descriptor. Transport and decay control parameters.

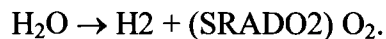
Line 11.10. XLIM, HALFMAX, T_SCALE, SRADO2, GH2AVG.

XLIM: Minimum decay factor; decay factor is set to zero when it is below XLIM [dimensionless]. Recommended value: 1.0×10^{-7} .

HALFMAX: Maximum number of half-lives during which decay will be calculated. Recommended value: 50.

T_SCALE: Time above which half-life is too large to bother calculating decay; used to shorten the decay chain [s]. Recommended value: 3.1557×10^7 s (1.0 yr).

SRADO2: Stoichiometric coefficient for O2 from radiolysis [gm-mol O₂/gm-mol H₂):



The value of SRADO2 should be between 0.0 and 0.5:

0.0 if O₂ is assumed to react immediately with other materials;

0.5 if O₂ is assumed to be inert.

Note that BRAGFLO, as used in WIPP PA calculations, assumes all gas to be H₂. The mass of gas produced by radiolysis as O₂ is:

$$M_{w,O_2} \cdot \text{SRADO2} = 31.988 \times 10^{-3} \text{SRADO2} [\text{kg O}_2 / \text{gm-mol H}_2],$$

where:

$$M_{w,O_2} = \text{molecular weight of O}_2 [\text{kg O}_2 / \text{gm-mol O}_2],$$

$$M_{w,H_2} = \text{molecular weight of H}_2 [\text{kg H}_2 / \text{gm-mol H}_2],$$

When this mass is treated as an equal mass of H₂, it is equivalent to:

$$\frac{M_{w,O_2} \cdot \text{SRADO2}}{M_{w,H_2}} = \frac{31.9988 \times 10^{-3} \text{SRADO2} \left[\frac{\text{kgH}_2 (= \text{kgO}_2)}{\text{gm - molH}_2} \right]}{2.01588 \times 10^{-3} \left[\frac{\text{kgH}_2}{\text{gm - molH}_2} \right]}$$

$$= 15.8734 \cdot \text{SRADO2} [\text{gm-mol H}_2 / \text{gm-mol H}_2]$$

$$= 7.93668 [\text{gm-mol H}_2/\text{gm-mol H}_2]$$

when SRADO2 = 0.5, which results in a far greater volume of gas (as H₂) than is realistically produced. It may be more realistic in BRAGFLO to consider radiolysis as producing 1/2 moles of H₂ (assuming the gas to be inert) (i. e., H₂O → H₂ + 1/2H₂), rather than M_{w,O₂} · SRADO2 kg of H₂.

Then the value SRADO2 should have in order to produce 0.5 gm-mol H₂ can be calculated from:

$$\frac{1}{2} \left[\text{mol H}_2 / \text{mol H}_2 \right] = \frac{M_{w,O_2} \cdot \text{SRADO2}}{M_{w,H_2}},$$

or,

$$\text{SRADO2} = \frac{\frac{1}{2} M_{w,H_2}}{M_{w,O_2}}$$

$$= \frac{\left(\frac{1}{2}\right) 2.01588 \times 10^{-3}}{31.9988 \times 10^{-3}}$$

$$= 0.314993.$$

GH2AVG: Average "G" value for H₂ [molecules/disintegration]. Recommended value: 0.0125.

Line 11.11. Descriptor. Isotope names.

Line 11.12. (IDION(I),I=1,NRAD).

IDION: Name of parent isotope. This is a CHARACTER*8 variable, read in free format, so it must be enclosed in tick marks. The name should be the element symbol followed by the atomic number (*e. g.*, 'Pu238') with no spaces or other punctuation between the element symbol and the atomic number. The element symbol can be either all upper case or upper and lower case. Trailing blanks are optional.

Line 11.13. Descriptor. Daughter names.

Line 11.14. (IDAUG(I),I=1,NRAD).

IDAUG: Name of immediate daughter isotope from the decay of isotope IDION(I). Same input rules as for the parent isotopes. If there is no daughter, use a blank: one to eight spaces between tick marks.

Line 11.15. Descriptor. Element indexes.

Line 11.16. (IELE(I),I=1,NRAD).

IELE: Element index for each isotope; must range from 1 to a maximum of NRAD, depending on how many elements there are. Applies to IDION only. Thus, all IDION isotopes of Pu, for example, will have the same IELE index, and all isotopes of Th will have another IELE index, all the same, but different from the index used for Pu. These are used to calculate the solubility when more than one isotope of an element is present, since the input solubility is of an element, not an isotope.

Line 11.17. Descriptor. Half lives.

Line 11.18. (THALF(I),I=1,NRAD).

THALF: Half-life of isotope IDION [s or yr].

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Line 11.19. Descriptor. Atomic weights.

Line 11.20. (AWT(I),I=1,NRAD).

AWT: Atomic weight of isotope IDION [kg/gm-mol or lb/lbmol].

Line 11.21. Descriptor. Solubilities.

Line 11.22. (SOLB_LIM(I),I=1,NRAD).

SOLB_LIM: Solubility limit of element in brine [gm-mol/m³ or lbmol/ft³]. Same value should be input for each isotope IDION of the element; *i. e.*, all IDION with the same IELE should have the same SOLB_LIM.

Line 11.23. Descriptor. Disintegration energy.

Line 11.24. (EVDP(I),I=1,NRAD).

EVDP: Disintegration energy if isotope IDION [MeV/disintegration]. Note that input units are MeV/dis; BRAGFLO converts to eV/dis.

*The following two lines (11.25 and 11.26) are repeated NRAD times,
once for each radionuclide:*

Line 11.25. Descriptor. Initial inventory.

Line 11.26. RADINIT(I).

RADINIT(I): Initial total mass of radionuclide IDION(I) in waste [kg or lb]. Assumed to exist initially in solid phase only; BRAGFLO will then calculate how much is dissolved in brine as part of transport and decay calculation, based on input solubilities. This initial inventory is distributed to all grid blocks having initial material type index MAT_WASTEI (Line 7.12) in proportion to the volume of each grid block relative to the total waste volume.

The following two lines are input only if LTRANS = .TRUE.:

Line 11.27. Descriptor. Transport and decay control parameters.

Line 11.28. SOLB_MULT, Q_BVOL_RATIO, TSUB_MAX.

SOLB_MULT: Multiplier on SOLB_LIM (solubility limit of radionuclide species in brine, Line 11.22) to avoid unrealistic precipitation of radionuclide outside of the waste regions [dimensionless]. Recommended value: 1.0×10^5 .

Q_BVOL_RATIO: Maximum inter-block flow allowed during transport calculation [fraction of grid block volume]. Recommended value: 0.10.

TSUB_MAX: Maximum number of times that BRAGFLO time step DELT is subdivided to keep the transport solution stable. Larger values may actually be needed, but the calculation may then require excessive computing time, so it is best to set some reasonable limit and hope it remains stable. Recommended value: 100 - 200. If the solution becomes unstable, TSUB_MAX should be increased. Q_BVOL_RATIO can be in-

creased, but should remain below 1.0. Increasing either of these will increase the computational effort.

7.2.13 Multi-Component Gas Transport Parameters

MULTI-COMPONENT GAS TRANSPORT IN BRAGFLO IS NOT QUALIFIED FOR USE IN WIPP COMPLIANCE CALCULATIONS AND WILL NOT BE USED IN WIPP COMPLIANCE CALCUALTIONS.

The current version of BRAGFLO has the capability to track multiple components of the gas phase as they are produced, consumed, and transported. This transport model accounts only for advective flow; diffusion and retardation are not considered. This feature is intended to supplement the reaction path gas generation model and gas dissolution model. Because the reaction path model has not yet been implemented, the gas transport model has not yet been tested or even debugged, so it should not be used except for testing purposes.

Line 12.1. Descriptor. Gas transport control flag.

Line 12.2. LRXGAST.

LRXGAST: Logical flag (.TRUE. or .FALSE.) indicating whether gas component transport will be used.

If LRXGAST = .FALSE., this is the end of the BRAGFLO input.

The following section of the input file and corresponding features are not QA'd and we make no claims that the following documentation is accurate. We leave it here for future use.

The next two lines are repeated MGAS times, where MGAS is the number of gas components, set in the PARAMETER statement.

Line 12.3. Descriptor. Initial gas component concentration.

Line 12.4. (((AFTER(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

AFTER: Initial mole fraction of each gas component [mol fraction].

THIS IS THE END OF THE BRAGFLO VERSION 6.02 INPUT, QUALIFIED FOR USE IN WIPP PA COMPLIANCE CALCULATIONS.

7.2.14 Restart Capability

THE RESTART FEATURE IN BRAGFLO IS NOT QUALIFIED FOR USE IN WIPP COMPLIANCE CALCULATIONS AND WILL NOT BE USED IN WIPP

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COMPLIANCE CALCUALTIONS. THE RESTART FEATURE IS NOT QUALIFIED.

The following section corresponding features are not QA'd and we make no claims that the following documentation is accurate. We leave it here for future use.

The restart capability in BRAGFLO enables runs to be restarted from any point specified in the input file and from the end of a run. The restarted run will continue exactly as it would have if the run had been done from the beginning without interruption. This capability is most useful for debugging, but also allows troublesome runs to be stopped and analyzed before wasting computing time. Occasionally, control parameters can be changed part way through a run, enabling a run to finish when it would otherwise remain stuck.

Some basic information on how to use the restart capability was presented earlier under "Files used by BRAGFLO." Initially, the input file must specify that a restart output file is to be written. This is indicated by setting the logical flag, LWRST, on Line 1.3 to T (.TRUE.). If LWRST is .FALSE., no restart output will be written, and the run cannot be restarted. If LWRST is .TRUE., a restart record will be written as specified in Section 2. Restart records, like ASCII and binary output, can be written at specified times, at specified time intervals, or at a specified time step frequency. If LWRST is .TRUE., a restart record will automatically be written at the end of a run, regardless of how they are specified to be written during a run. The restart record contains all the information needed to resume from the last converged time step before the restart record is written. Although there is no limit to the number of restart records that can be written during a run, the number of restart records needed is generally very small, at most a couple, or perhaps every 500 years in a 10,000-year run. The user has to know when the restart records are written in order to do a restart. This information is written to the screen or log file, to the ASCII output file [if one is being written (LWASC is .TRUE. on Line 1.3)], and to the .SUM file [if one is being written (LWSUM is .TRUE. on Line 1.3)] each time a restart record is written.

The procedure for restarting a BRAGFLO run is as follows:

1. Copy the restart output file [.ROT] into a restart input file [.RIN]. The name of the restart input file does not have to be the same as the restart output file, but it does have to be the same (except for the .RIN extension) as the ASCII input file that will be used for the restart.
2. Edit the ASCII input [.INP] file used in the initial run. If the flag LRRST in Line 1.3 is F, it must be changed to T, indicating that a restart input file will be read. The flag LWRST in Line 1.3 had to have been T in the initial run; it can (and probably should) be left as T, or can be changed to F for the restart, depending on whether the user wished to write any more restart output records during the restart run. If the initial run completed the maximum number of time steps allowed, then MAXITF (Line 1.7) must be increased, or the restart run will stop immediately, having already completed MAXITF steps. If the run is being restarted simply because MAXITF was too small in the initial run, or if the restart is a debugging run, these are the only changes needed. Almost anything in the ASCII input file can be changed for the restart run, with the exception of the dimensions of the problem (NX, NY, NZ, Line 1.5). If these are changed, the restart run will abort. Any parameter specifying the number of some-

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thing, such as the number of wells, the number of material types, or the number of history variables, can be changed, but should not be changed because it will likely confuse both the user and BRAGFLO and probably eventually abort. Print flags should not be changed because post-processing will be messed up. Grid block sizes and initial conditions should not be changed. Logically, the only changes that should be considered, other than file specifications, time or time step limits, and output times or frequencies, are numerical control parameters. In rare in-stances, one might want to modify material properties. Keep in mind that any changes to the input file that are in effect only at times earlier than the time of the restart, and are no longer in effect at the restart time, will not have any effect on the restart run. For example, if the restart is at 1000 years, and the input file is changed to request additional ASCII output at 500 years, the output at 500 years will not be written. The .INP file name can be changed from the initial run, but the name has to be the same as the restart input file name, except for the .INP extension.

3. Run BRAGFLO. As usual, BRAGFLO prompts for the name of the .INP file. Then it requests the number of the restart record from the restart input .RIN file. If the user wished to start the run from the beginning again (having made changes to the input file), a zero can be entered here. If a number greater than the number of restart records in the .RIN file is entered, the run will abort trying to read past the end of the .RIN file.
4. Post-processing. The binary file from the restart run will have the same structure as the initial run, but start from the restart time. Before post-processing in the CAMCON system using POSTBRAG, it is necessary first to run a utility, BINCOMBO, which merges the two binary files into a single binary file.

7.3 External Input File Containing Closure Look-up Table Data

This data is only required if creep closure has been selected, i.e. CLOSURE=.TRUE.. For each included Look-up Table, The data consists of two dependent variables, porosity and pressure as a function of two independent variables, an F Factor (related to gas generation rate) and time. This data has been generated external to BRAGFLO by a rock mechanics code. Since the rock mechanics codes uses a different definition or basis for determining porosity than does BRAGFLO, the rock-mechanics code porosity values were converted to those consistent with BRAGFLO's usage.

The dimensions of the data are defined on BRAGFLO's Parameter Include file. The defining dimensions are

- 1) MKLOS, the number of Look-up" Tables included on the file. Currently 4.

- 1: Porosity Surface #1, for Waste w/o Backfill. First used in SPM2 in January 1995. Raw data were SANCHO porosities, based on current time-dependent room volume; these were converted to initial room volume basis before inserting into BRAGFLO.

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- 2: Porosity Surface #2, for North End w/o Backfill. First used in SPM2 in January 1995. Raw data were SANCHO current time-dependent room volumes (SANCHO porosities are always 1.0); these were converted to porosities based on initial room volume before inserting in BRAGFLO.
- 3: Porosity Surface #3, the Original porosity surface used before SPM2 in January 1995. Raw data were SANCHO porosities, based on current time-dependent room volume; these were converted to initial room volume basis before inserting into BRAGFLO.
- 4: Porosity Surface #4, for Waste w/o Backfill, an improved version of Surface #1, installed 01/21/96. This is surface that was used in the 1996 CCA, 1997 PAVT PA, and the CRA-2004 and CRA-2004 PABC.

- 2) NSDATA, then number of F Factors considered in the table.
- 3) NTDATA, the number of times at which data is defined in the table.

The data arrays are sized according to the largest set of data. MKLOS =4, NSDATA =13, NTDATA = 214. For each of the MKLOS data sets there must be entries for each of the NSDAT x NTDATA points. Since the dependent variable arrays are sized according to the largest set of data, a given table may not have sufficient calculated entries. In these cases the remaining portion of the table is zero filled. Similarly, the independent variable arrays are sized according to the largest set of data, in the event that there are not NSDATA F Factors defining the table, the remaining portion of the F Factor array is zero filled. In the event that there are not NTDATA times corresponding to data in the table, the remaining portion of the time array is zero filled. This will become clearer below. Because of the large amount of data on the closure data input file, a generous number of "descriptor lines" are include and required to help the user clearly delineate the data being entered.

Line 1.0 Descriptor. Minimum porosity value for each look-up table (surface)

Line 2.0 (PHIMIN_BRAG(I),I=1,MKLOS)

Line 3.0 Descriptor. Maximum porosity value for each look-up table (surface)

Line 4.0 (PHIMAX_BRAG(I),I=1,MKLOS)

Line 5.0 Descriptor. Maximum time of data for each look-up table (surface)

Line 6.0 (TIME_DATA_MAX (I),I=1,MKLOS)

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Line 7.0 Descriptor. F Factor Data

Repeat Line 8.0 and 9.0 MKLOS times

Line 8.0 Descriptor. F Factor Data for Look-up Table J, J=1 to MKLOS.

Line 9.0 (FDATA(I,J),I=1,NSDATA)

FDATA: Fraction of base gas generation rate [dimensionless]. MKLOS values are required. If there are not MKLOS values then fill the remaining entries with 0.

Line 10.0 Descriptor. Time data.

Line 11.0 Descriptor. TDATA(1:NTDATA)

Line 12.0 (TDATA(I),I=1,NTDATA)

TDATA: Time corresponding to data entry [sec or day]. NTDATA values are required. All the look-up tables in use have the same number and times at which data is entered. Therefore TDATA is only a one-dimensional array.

Repeat Line 13.0 to 21.0, K=1 to MKLOS times

Line 13.0 Descriptor. Description of Look-up Table K, K=1 to MKLOS.

Line 14.0 Descriptor. PDATA and SDATA.

Line 15.0 Descriptor. For Look-up Table K data for xxx F Factors are used.

Repeat Line 16.0 to 21.0 J=1 to NSDATA times

Line 16.0 Descriptor. PDATA For Look-Up Table K, and F Factor (J).

Line 17.0 Descriptor. (PDATA(J,I,K) ,I=1,NTDATA)

Line 18.0 (PDATA(J,I,K) ,I=1,NTDATA)

PDATA(J,I,K): Time varying pressure data for Kth look-up table and Jth F Factor [Pa or psi]. NTDATA values are required. If there are not NTDATA values, the remaining entries should be zero filled.

Line 19.0 Descriptor. SDATA For Look-Up Table K, and F Factor (J).

Line 20.0 Descriptor. (SDATA(J,I,K) ,I=1,NTDATA)

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Line 21.0 (SDATA(J,I,K),I=1,NTDATA)

SDATA(J,I,K): time varying porosity data for Kth look-up table and Jth F factor [Pa or psi]. NTDATA values are required. If there are not NTDATA values, the remaining entries should be zero filled.

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8.0 Error Messages

BRAGFLO outputs a number of error messages and aborts execution when it detects invalid input parameters. The following list of error messages are common and discussed in Section 7.0. However nearly every line in the input file has a corresponding error message if it detects something wrong or inconsistent. We refer the user to the source code in the event that such an error message appears.

7.2.2 Line 1.5

```
*** MODTYPE Error in READSTARTUP ***  
The ASCII output file provides additional information:  
  
**FATAL ERROR in Input:  MODTYPE = <input value>  
  
**MODTYPE must be 1, 2, or 3.
```

.....

7.2.2 Line 1.5

```
*** Size error in READSTARTUP; invalid NX, NY, or NZ  
The ASCII output file provides additional information:  
  
** FATAL ERROR in Input:      NX,NY,NZ = <input values>  
  
** Maximum values dimensioned:  MX,MY,MZ = <values set in PARAMETER  
statement>  
  
** Minimum values allowed:     MX,MY,MZ =      1      1      1
```

.....

7.2.2 Line 1.11

```
*** ERROR in READSTARTUP:  NDTFIXMAX needs to be larger;  
  
    NDTFIX = <input value>  
  
*** NDTFIX error in READSTARTUP ***
```

.....

7.2.3 Line 2.20

```
*** ERROR:  Too many Monitor Blocks in Input:  
Specified:  NMON = <NMON input value>  
Maximum:    MMON = <MMON value set in PARAMETER statement>
```

*** Monitor error in READPRTYPE ***

7.2.4 Line 3.2

Number of FATAL errors in READMESH = <number of errors>

*** FATAL geometry input errors in READMESH ***

7.2.5 Line 4.2

In READWELL, NWTIME needs to be larger. NWELLTIMES = <NWELLTIMES input value>

*** Well time errors in READWELL ***

7.2.8 Line 7.24

ICWASTE must be 0 when TIMEICRESET = START.

*** ICWASTE error in READMAT.

9.0 Description of Output Files

There can be up to 4 output files created by BRAGFLO. They are as follows:

- The BRAGFLO binary output (.BIN). This file is the primary results file that is converted by POSTBRAG into CAMDAT Database (.CDB) format.
 - The BRAGFLO ASCII output (.OUT). This file echoes input and provides user-readable output and QA information.
 - The BRAGFLO summary (.SUM). This file contains a limited amount of summary information on results at each time step for monitoring progress of the solution over time.
- The BRAGFLO restart output (.ROT). Enough information is stored in this binary file to permit restarting BRAGFLO if execution is halted.

9.1 Binary Output (.BIN) File

This file is the primary results file that is converted by POSTBRAG (Figure 29) into standard .CDB format. This file contains output in a more compact form than is possible in an ASCII output file. Most results of interest printed typically every 20 or so time steps and a more limited amount of information printed every time step. The beginning of the file contains QA information, as in the ASCII file (Subsection 9.2). It also contains an output variable glossary. Enough information is stored to enable a postprocessor, POSTBRAG to read the file and place the results into a CAMDAT data base for additional post-processing and analysis by the downstream codes. The structure of this file is described below. Although it does not contain all the information used in a BRAGFLO run (for example, material properties are absent), it can contain all the results needed for a complete analysis of the results, so it should not be necessary to modify the code or to write additional output files for further post-processing.

A FORTRAN program that will read the binary output file is listed on the following page to illustrate the structure of the file. In this program, the header information is read and saved as variables whose values are not changed later. The information at each time step is read and stored in local variables that are over-written at the next time step, so this information must be written to the output file at each time step as needed for subsequent analysis and post-processing. Although the code BINREAD dates from 1996, the source code has been visually checked to ensure that it accurately represents the .BIN output format for BRAGFLO Version 6.02. Additional comments have been added for clarity. The grid dimensions in the parameter statement in the program BINREAD do not reflect the current WIPP PA grid for BRAGFLO.

PROGRAM BINREAD

```
C
C   Translates BRAGFLO binary file into ASCII file.
C   J. Schreiber, SAIC, 03/08/96
C   Additional comments added by M. Nemer 3/4/07

C   Nemer: Ignore the fact that the dimensions below do not reflect current
C   WIPP PA grid. Not relevant for understanding BRAGFLO BIN output format
C
C   PARAMETER (MX=50,MY=40,MZ=10,NVPR=107,MXHIV=15000,
1   MVHIV=MX*MY*MZ,MGVAR=10)

C
CHARACTER*8   RTIME(2),PNAME(2),VRSION(2),UNITS,REVDATE(2)
CHARACTER*8   NAMVAREL(NVPR),NAMVARHI(MXHIV),NAMVARGL(MGVAR)
CHARACTER*50  LABEL(L(NVPR),LABELHI(MXHIV),LABELGL(MGVAR)
CHARACTER*20  LABUNTEL(NVPR),LABUNTHI(MXHIV),LABUNTGL(MGVAR)
CHARACTER*9   DATE(2)
CHARACTER*32  CPUNAME
CHARACTER*1   FILTYP
CHARACTER*80  FILNAM(6),BRAGNAM
CHARACTER*132 TITLE
DIMENSION IIVHIV(MVHIV,NVPR),JJHIV(MVHIV,NVPR),KKHIV(MVHIV,NVPR)
DIMENSION UNTCNVEL(NVPR),UNTCNVHI(MXHIV),UNTCNVGL(MGVAR)
DIMENSION DXGRID(MX,MY,MZ),DYGRID(MX,MY,MZ),DZGRID(MX,MY,MZ)
DIMENSION GRIDVOL(MX,MY,MZ),LHI(NVPR),LE(NVPR),LH(MXHIV),LG(MGVAR)
DIMENSION HVAR(MXHIV),YY(MX,MY,MZ),NGBHIV(NVPR)
REAL IBBALMX,JBBALMX,KBBALMX,IGBALMX,JGBALMX,KGBALMX

C
C
WRITE (*,*) 'Enter name of BRAGFLO binary file.'
READ (*,'(A)') BRAGNAM

C
OPEN (8,FILE=BRAGNAM,STATUS='OLD',FORM='UNFORMATTED')
OPEN (9,FILE='ASCII.OUT',STATUS='NEW')

C
C   Read header section with QA info, vbl glossary, grid dimensions:
C   Note: If first record is 'PREBRAG', then the file starts with
C   PREBRAG QA info; otherwise, there is no PREBRAG info, and
C   the file starts with BRAGFLO QA info.
C   PNAME(1) = Preprocessor name (PREBRAG).
C   VRSION(1) = PREBRAG version number.
C   REVDATE(1) = PREBRAG revision date.
C   DATE(1) = PREBRAG run date.
C   RTIME(1) = PREBRAG run time.
C   DATE(2) = BRAGFLO run date.
C   RTIME(2) = BRAGFLO run time.
C   PNAME(2) = Program name (BRAGFLO).
C   VRSION(2) = BRAGFLO version number.
C   REVDATE(2) = BRAGFLO revision date.
C   CPUNAME = Name of machine on which BRAGFLO was run.
C   FILTYP = Type of file ('B'=binary).
C   NUMFIL = Number of files used in the BRAGFLO run.
C   FILNAM = Names of NUMFIL files used by BRAGFLO.
C   TITLE = Title of run.
C   NX,NY,NZ = Dimensions of problem run.
C   UNITSO = Units system used for output ('SI' or 'ENGLISH').
C   NVAREL = Number of element variables.
C   MHIVM = Number of time- & performance-related history vbls.
C   MHIV = Total no. of element vbl-based history vbls printed
C   at each time step.
C   NHIV = No. of element vbls that are printed as history vbls.
C   NGVAR = Number of global variables.
```

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```
      READ (8) PNAME(1)
      IF (PNAME(1)(1:7) .EQ. 'PREBRAG') THEN
        READ (8) VRSION(1)
        READ (8) REVDATE(1)
        READ (8) DATE(1)
        READ (8) RTIME(1)
        READ (8) DATE(2)
      ELSE
        DATE(2) = PNAME(1)
      END IF
C
      READ (8) RTIME(2)
      READ (8) PNAME(2)
      READ (8) VRSION(2)
      READ (8) REVDATE(2)
      READ (8) CPUNAME
      READ (8) FILTYP
      READ (8) NUMFIL
      DO 10 I=1,NUMFIL
        READ (8) FILNAM(I)
10 CONTINUE
      READ (8) TITLE
      READ (8) NX,NY,NZ
      READ (8) UNITS
      READ (8) NVAREL,MHIVM,MHIV,NHIV,NGVAR
      MHIVT = MHIVM + MHIV
C
C      Read glossary of variables:
C      LHI      = Element vbl no. from User Manual Table 7 for this
C              history vbl.
C      NGBHIV   = No. of grid blocks to be printed as history vbl for
C              variable LHI.
C      IIHIV    = I-index of grid block for this history variable.
C      JJHIV    = J-index of grid block for this history variable.
C      KKHIV    = K-index of grid block for this history variable.
C      LE       = Number of the element variable.
C      NAMVAREL = Variable name to be used in POSTBRAG.
C      LABELEL  = Description of this variable.
C      LABUNTEL = Units label for this variable (e.g., Pa).
C      UNTCNVEL = Factor to convert from UNITSO to SI units.
C      LH       = Number of the history variable.
C      NAMVARHI = Variable name to be used in POSTBRAG.
C      LABELHI  = Description of this variable.
C      LABUNTHI = Units label for this variable (e.g., Pa).
C      UNTCNVHI = Factor to convert from UNITSO to SI units.
C      LG       = Number of the global variable.
C      NAMVARGL = Variable name to be used in POSTBRAG.
C      LABELGL  = Description of this variable.
C      LABUNTGL = Units label for this variable (e.g., kg).
C      UNTCNVGL = Factor to convert from UNITSO to SI units.
C
      DO 20 I=1,NHIV
        READ (8) LHI(I),NGBHIV(I), (IIHIV(J,I),JJHIV(J,I),KKHIV(J,I),
1        J=1,NGBHIV(I))
20 CONTINUE
      DO 30 I=1,NVAREL
        READ (8) LE(I),NAMVAREL(I),LABELEL(I),LABUNTEL(I),UNTCNVEL(I)
30 CONTINUE
      DO 40 I=1,MHIVT
        READ (8) LH(I),NAMVARHI(I),LABELHI(I),LABUNTHI(I),UNTCNVHI(I)
40 CONTINUE
      DO 50 I=1,NGVAR
        READ (8) LG(I),NAMVARGL(I),LABELGL(I),LABUNTGL(I),UNTCNVGL(I)
```

50 CONTINUE

C
C
C

Mesh dimensions and grid block volumes.

```
READ (8) (((DXGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
READ (8) (((DYGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
READ (8) (((DZGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
READ (8) (((GRIDVOL(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
```

C
C
C
C

*** End of header section (READ) ***

```
IF (PNAME(1)(1:7) .EQ. 'PREBRAG') THEN
  WRITE (9,*) '** PREBRAG Program Name **'
  WRITE (9,*) PNAME(1)
  WRITE (9,*) '** PREBRAG Version Number **'
  WRITE (9,*) VRSION(1)
  WRITE (9,*) '** PREBRAG Revision Date **'
  WRITE (9,*) REVDATE(1)
  WRITE (9,*) '** PREBRAG Run Date **'
  WRITE (9,*) DATE(1)
  WRITE (9,*) '** PREBRAG Run Time **'
  WRITE (9,*) RTIME(1)
END IF
```

C

```
WRITE (9,*) '** BRAGFLO Run Date **'
WRITE (9,*) DATE(2)
WRITE (9,*) '** BRAGFLO Run Time **'
WRITE (9,*) RTIME(2)
WRITE (9,*) '** BRAGFLO Program Name **'
WRITE (9,*) PNAME(2)
WRITE (9,*) '** BRAGFLO Version Number **'
WRITE (9,*) VRSION(2)
WRITE (9,*) '** BRAGFLO Revision Date **'
WRITE (9,*) REVDATE(2)
```

C

```
WRITE (9,*) '** Computer Name **'
WRITE (9,*) CPUNAME
WRITE (9,*) '** Output File Type **'
WRITE (9,*) FILTYP
WRITE (9,*) '** Number of Files Used **'
WRITE (9,*) NUMFIL
WRITE (9,*) '** Names of Files Used **'
DO 60 I=1,NUMFIL
  WRITE (9,*) FILNAM(I)
```

60 CONTINUE

C

```
WRITE (9,*) '** Title of Run **'
WRITE (9,*(A)) TITLE
WRITE (9,*) '** NX, NY, NZ **'
WRITE (9,*) NX,NY,NZ
WRITE (9,*) '** Output Units **'
WRITE (9,*) UNITS
```

C

```
WRITE (9,*) '** NVAREL, MHIVM, MHIV, NHIV, MGVAR **'
WRITE (9,*) NVAREL,MHIVM,MHIV,NHIV,NGVAR
WRITE (9,*)
WRITE (9,*) '** History Vbl Locations **'
DO 70 I=1,NHIV
  WRITE (9,*(2I5,10(3X,3I3))) LHI(I),NGBHIV(I),
1 (IIHIV(J,I),JJHIV(J,I),KKHIV(J,I),J=1,NGBHIV(I))
```

70 CONTINUE

```
WRITE (9,*)
```

```

      WRITE (9,*) '** Element Vbl Labels **'
      DO 80 I=1,NVAREL
        WRITE (9, '(I4,2X,A,2X,A,2X,A,1PE16.6)') LE(I),NAMVAREL(I),
1      LABELLEL(I),LABUNTEL(I),UNTCNVEL(I)
80 CONTINUE
      WRITE (9,*)
      WRITE (9,*) '** History Vbl Labels **'
      DO 90 I=1,MHIVT
        WRITE (9, '(I4,2X,A,2X,A,2X,A,1PE16.6)') LH(I),NAMVARHI(I),
1      LABELHI(I),LABUNTHI(I),UNTCNVHI(I)
90 CONTINUE
      WRITE (9,*)
      WRITE (9,*) '** Global Vbl Labels **'
      DO 100 I=1,NGVAR
        WRITE (9, '(I4,2X,A,2X,A,2X,A,1PE16.6)') LG(I),NAMVARGL(I),
1      LABELGL(I),LABUNTGL(I),UNTCNVGL(I)
100 CONTINUE
C
      WRITE (9,*)
      WRITE (9,*) '** Mesh Sizes: DXGRID **'
      WRITE (9,*) (((DXGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      WRITE (9,*)
      WRITE (9,*) '** Mesh Sizes: DYGRID **'
      WRITE (9,*) (((DYGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      WRITE (9,*)
      WRITE (9,*) '** Mesh Sizes: DZGRID **'
      WRITE (9,*) (((DZGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      WRITE (9,*)
      WRITE (9,*) '** Mesh Sizes: GRIDVOL **'
      WRITE (9,*) (((GRIDVOL(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
C
C      *** End of header section (WRITE) ***
C
C
C      *** Cycle through time steps ***
C
C      First read time, time step, CPU time, performance measures:
C      TIME      = Elapsed simulation time [s].
C      TIMED     = Elapsed simulation time [days].
C      TIMEYR    = Elapsed simulation time [yr].
C      DELT     = Time step [s].
C      DELTD    = Time step [days].
C      DELTYR   = Time step [yr].
C      AVGITER  = Average Newton-Raphson iterations per time step.
C      CPUS     = CPU time used for this time step [s].
C      CPUHR    = Total CPU time used so far in the run [hr].
C      RNSTEP   = Time step number (REAL).
C      RITERTOT = Total Newton-Raphson iterations so far (REAL).
C      KBIN     = Flag indicating:
C                =0: only history vbl output will follow.
C                =1: history vbals and global and element vbals output
C                    will follow at this time step.
C
      NPO = 0
110 READ (8,END=130) TIME,TIMED,TIMEYR,DELT,DELTD,DELTYP,AVGITER,
1      CPUS,CPUHR,RNSTEP,RITERTOT,KBIN
C
C      Read history variables, if there are any.
C
      IF (MHIV .GT. 0) READ (8,END=130) (HVAR(I),I=1,MHIV)
C
      WRITE (9,*)
      WRITE (9,*)

```

```

WRITE (9,*) '** TIME (s,d,y), DELT (s,d,y), IterAvg, CPU (s,hr),'
1  //' Step No., IterTot, KBIN'
WRITE (9,*) TIME,TIMED,TIMEYR,DELT,DELTD,DELTyr,AVGITER,
1  CPUS,CPUHR,RNSTEP,RITERTOT,KBIN
WRITE (9,*)
WRITE (9,*) '** History Vbls at Time Step',RNSTEP
IF (MHIV.LE. 0) THEN
  WRITE (9,*) ' (no element-variable-based history variables)'
ELSE
  WRITE (9,*) (HVAR(I),I=1,MHIV)
END IF

C
C (History vbls only, if KBIN=0)
C
IF (KBIN.EQ. 1) THEN
C
C Global vbls (mass balance info at current step) are read next:
C   BBALC = Brine mass balance error over entire mesh [kg].
C   GBALC = Gas mass balance error over entire mesh [kg].
C   BBALMX = Max relative brine mass bal error in any grid block.
C   GBALMX = Max relative gas mass bal error in any grid block.
C   IBBALMX = I-index of grid block with BBALMX \
C   JBBALMX = J-index of grid block with BBALMX | These are
C   KBBALMX = K-index of grid block with BBALMX | saved as
C   IGBALMX = I-index of grid block with GBALMX | REAL vbls
C   JGBALMX = J-index of grid block with GBALMX |
C   KGBALMX = K-index of grid block with GBALMX /
C
  READ (8,END=130) BBALC,GBALC,BBALMX,GBALMX,
1  IBBALMX,JBBALMX,KBBALMX,IGBALMX,JGBALMX,KGBALMX
C
  NPO = NPO + 1
  WRITE (9,*)
  WRITE (9,*) '** Mass Balances (Global Vbls) Printout No.',NPO
  WRITE (9,*) BBALC,GBALC,BBALMX,GBALMX
  WRITE (9,*) IBBALMX,JBBALMX,KBBALMX,IGBALMX,JGBALMX,KGBALMX
C
C The Element vbl distributions are read next.
C
  DO 120 L=1,NVAREL
    READ (8,END=130) (((YY(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
    WRITE (9,*)
    WRITE (9, '(A,I3,3X,A,F10.1)') '** Element Vbl: (No., Name,'
1  //'Time Step No.) =',L,NAMVAREL(L),RNSTEP
    WRITE (9,*) (((YY(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
120  CONTINUE
  END IF
C
C Continue to next time step.
C
  GO TO 110
C
130 CLOSE (8)
  CLOSE (9)
  STOP '** Normal Completion **'
C
  END

```

9.2 ASCII Output (.OUT) File

This file echoes input and provides user-readable output and QA information. It has a "standard" text file format. It starts with QA information, including a time-and-date-of-run stamp, BRAGFLO version number, and revision date. It then echoes the input, but with more information and annotation than found (or allowed) in the input file. Therefore, when problems are encountered with the input, this file should be checked first to be sure that the input was read as intended. Some processed input is then printed out, including information on grid sizes and volumes of each grid block, since this is not necessarily input directly. Then initial conditions are printed, with the amount of information specified by the user. Results specified by the user are printed periodically, at times or frequencies specified by the user. Results at the end of the run are also printed, the amount of information printed being specified by the user. Finally an ending time-and-date stamp is printed. Use of this file is optional when BRAGFLO is run, but is strongly recommended because it always contains an echo of the input, the initial conditions, and results at the end of the run, which makes it useful for debugging input. Additional results are at the discretion of the user and depend on user input. A sample output file is provided in Subsection 11.3 (Appendix C).

9.3 Summary (.SUM) File

A limited amount of summary information is written at each time step to the screen (when BRAGFLO is run interactively) or to a log file (when run in background). The same information is written to this summary file so that a detailed time step summary is available later if BRAGFLO is run interactively. This information is often useful for diagnostic purposes when problems occur.

A typical summary output at one time step appears as follows:

1		3.376E-03	8.043E-08	8.951E-01	6.868E-02				
2		15 12 1	2 20 1	11 27 1	1 20 1				
3	1146	1.226E+03	1.101E+03	3 3.31	9.96E-03	10 14	1 3.50E+04	19 8 1	
4		-8.44E-05	15 12 1	3.16E-08	11 9 1	8.48E-14	3.21E-18	LU	
5	** Monitor Block Arrays:	PO,	PG,	SO,	SOEFC				
6		PERMGX,	QR(1),	PHI,	PORSOLID				
7		QOBLOCKI,	QOBLOCKJ,	QGBLOCKI,	QGBLOCKJ				
8		CONCFE,	CONCBIO,	CONCMGO,	CONCHYDRO				
9	Monitor Block # 1:	(26, 12, 1)							
10		3.9152210460E+06	3.9152210460E+06	1.5000093210E-02	9.3769648059E-08				
11		2.4032401063E-13	4.3464428375E-17	7.0246988282E-02	1.8071445869E-02				
12		0.0000000000E+00	0.0000000000E+00	8.4023003688E-07	-1.4217272580E-11				
13		1.1738049324E+02	1.8251680998E+01	6.7933538603E+01	2.0502677594E-02				
14	Monitor Block # 2:	(32, 12, 1)							
15		2.6628900596E+06	2.6628900596E+06	1.5000107635E-02	1.0838170744E-07				
16		2.4048109254E-13	5.0244935991E-17	5.5314077124E-02	1.7453495760E-02				
17		2.0895341248E-12	0.0000000000E+00	1.2491024208E-07	-9.9230520030E-07				
18		1.1738069953E+02	1.8251873662E+01	6.9367286781E+01	2.0008960985E-02				
19	Monitor Block # 3:	(36, 12, 1)							
20		1.7762631345E+06	1.7762631345E+06	1.5000196086E-02	1.9856475257E-07				
21		2.4072622281E-13	9.2045625566E-17	4.8978107400E-02	1.7674502997E-02				
22		1.5659264471E-11	0.0000000000E+00	0.0000000000E+00	-5.5313414058E-07				
23		1.1738062711E+02	1.8251804889E+01	6.8854557479E+01	2.0282501408E-02				

Lines 1-2 contain information on how well the variable change or mass balance meets or does not meet the convergence criteria specified in the input. The variables that are written are as follows:

Line 1: EPSMAX(1), EPSMAX(2), FTOLMAX(1), FTOLMAX(2)

Line 2: IEPS(1), JEPS(1), KEPS(1), IEPS(2), JEPS(2), KEPS(2), IFTOL(1), JFTOL(1), KFTOL(1), IFTOL(2), JFTOL(2), KFTOL(2)

where

$$\text{EPSMAX}(1) = \max(\Delta S_g \times 10^{\epsilon_1}),$$

$$\text{EPSMAX}(2) = \max\left(\frac{\Delta P_b}{P_b \epsilon_2}\right).$$

ΔS_g = change in gas saturation in a grid block since last iteration,
 ΔP_b = change in brine pressure in a grid block since last iteration,
 P_b = brine pressure at end of current iteration.

$$\text{FTOLMAX}(1) = \begin{cases} \max\left(\frac{F_1 / T_{3g}}{f_1}\right), & T_{3g} \geq T_{3o} \text{ and } F_1 > f_1, \\ \max\left(\frac{F_1}{f_1}\right), & T_{3g} \geq T_{3o} \text{ and } F_1 \leq f_1, \\ 0., & T_{3g} < T_{3o} \end{cases}$$

$$\text{FTOLMAX}(2) = \begin{cases} \max\left(\frac{F_2 / T_{3b}}{f_2}\right), & T_{3b} \geq T_{3o} \text{ and } F_2 > f_2, \\ \max\left(\frac{F_2}{f_2}\right), & T_{3b} \geq T_{3o} \text{ and } F_2 \leq f_2, \\ 0., & T_{3b} < T_{3o} \end{cases}$$

F_1 = discretized gas mass balance equation (see equation (92)),
 F_2 = discretized brine mass balance equation,

and the grid block locations where these occur are, respectively:

[IEPS(1),JEPS(1),KEPS(1)],
 [IEPS(2),JEPS(2),KEPS(2)],

[IFTOL(1),JFTOL(1),KFTOL(1)],
[IFTOL(2),JFTOL(2),KFTOL(2)].

T_{3g} and T_{3b} are, respectively, the mass of gas and mass of brine in a grid block in [(kg phase)/(m³ grid block)]. T_{3o} is a small number, set at 1.0×10^{-15} kg/m³, intended to prevent division by zero and to de-emphasize minute amounts of phase that may be nothing more than round-off.

The maxima are taken over the entire grid for the Newton-Raphson iteration just completed.

The convergence limits are specified in the input [Lines 6.10 and 6.14 in Subsection 7.2.7]:

$\epsilon_1 = \text{EPSNORM}(1)$ = required number of digits of accuracy to the right of the decimal in the change in gas saturation from the last time step.

$\epsilon_2 = \text{EPSNORM}(2)$ = maximum relative change allowed in brine pressure over a time step.

$f_1 = \text{FTOLNORM}(1)$ = maximum allowable residual for the gas mass balance, normalized by the amount of gas present in the grid block.

$f_2 = \text{FTOLNORM}(2)$ = maximum allowable residual for the brine mass balance, normalized by the amount of brine present in the grid block.

Thus, $\text{EPSMAX}(1)$ is the maximum fraction of the total allowable change in the gas saturation. It should have a value less than 1.0 when the solution has converged at each time step if ICONVTEST [Line 6.8 in Subsection 7.2.7] has a value of 1. If $\text{ICONVTEST} = 0$, $\text{EPSMAX}(1)$ may be greater than 1.0 when the solution has converged. (In this case, at least two of the values on Line 1 above must be less than or equal to 1.0.)

$\text{EPSMAX}(2)$ is the maximum fraction of the allowable change in the brine pressure over an iteration that was obtained in the time step just completed. It should have a value less than 1.0 if $\text{ICONVTEST} = 1$. If $\text{ICONVTEST} = 0$, $\text{EPSMAX}(2)$ may be greater than 1.0 when the solution has converged (but at least two other values on Line 1 will be less than 1.0).

$\text{FTOLMAX}(1)$ is the maximum fraction of the allowable normalized residual in the gas mass balance that was obtained in the time step just completed. It should have a value less than 1.0 if $\text{ICONVTEST} = 1$, but may be greater than 1.0 if $\text{ICONVTEST} = 0$.

$\text{FTOLMAX}(2)$ is the maximum fraction of the allowable normalized residual in the brine mass balance that was obtained in the time step just completed. It should have a value less than 1.0 if $\text{ICONVTEST} = 1$, but may be greater than 1.0 if $\text{ICONVTEST} = 0$.

Occasionally, BRAGFLO encounters difficulty in converging to a solution. If a solution has not been obtained at a particular time step after numerous (30-50) time step reductions, it is quite likely that further time step reductions will not improve the solution suf-

ficiently to satisfy the normal convergence criteria, EPSNORM(1) and EPSNORM(2) and FTOLNORM(1) and FTOLNORM(2). One option at this point is for BRAGFLO to abort. The user would then rerun the problem after adjusting one or more of the control parameters and hope for better results. However, it is often the case that BRAGFLO's difficulties are temporary, and that if it can get past the trouble spot, it will complete the run without further major difficulties. Thus, a second option has been built into BRAGFLO to handle those occasions when repeated time step reductions fail to provide convergence: The convergence criteria are temporarily relaxed. These relaxed criteria are applied after user-specified IJACSWITCH time step reductions have occurred, and they continue to be applied only until convergence is obtained at that time step. After IJACRESET time steps, and at all subsequent time steps, the normal convergence criteria are used. This capability makes BRAGFLO a little more robust, enabling it to complete runs that would otherwise abort and require input modifications before rerunning, at only a minor cost in overall accuracy. This feature becomes important when carrying out large number of runs in automated batch systems. It can be turned off by setting all input values of the loosened criteria equal to the normal criteria. Caution is advised when using this feature because large mass balance errors can be introduced which may not be apparent in a cursory examination of the results. The following BRAGFLO Input control file parameters define the looser convergence criteria:

EPSLOOSE(1): Same meaning as EPSNORM(1); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1 to 4 with a best estimate of 2.

EPSLOOSE(2): Same meaning as EPSNORM(2); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1.0×10^{-1} to 1.0×10^{-4} with a best estimate of 1.0×10^{-2} .

FTOLLOOSE(1): Relaxed value of normalized residual for gas saturation below which convergence is accepted regardless of EPSLOOSE(1); used after IJACSWITCH time step reductions have occurred [kg gas in residual/kg gas in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1} .

FTOLLOOSE(2): Relaxed value of normalized residual for brine pressure below which convergence is accepted regardless of EPSLOOSE(2); used after IJACSWITCH time step reductions have occurred [kg brine in residual/kg brine in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1} .

When convergence is *not* obtained within ITMAX [Line 6.22 in Subsection 7.2.7] iterations, lines 1 and 2 are still printed out, providing valuable information as to the magnitude of the convergence problems and where those problems are occurring.

Lines 3 and 4 include time information and global mass balance results, along with grid block locations where maximum mass balance errors occur:

Line 3: IPRINT, TIME*SECYR, DELT/DAYSEC, ITER, CPU, DELTASATMAX, IDEPMAX(1), JDEPMAX(1), KDEPMAX(1), DELTAPRESMAX, IDEPMAX(2), JDEPMAX(2), KDEPMAX(2),

Information Only

Line 4: GASBALMAX, IGBALMX, JGBALMX, KGBALMX, BRNBALMAX, IBBALMX, JBBALMX, KBBALMX, GASBALCUM, BRNBALCUM, CHSOLVER.

where:

IPRINT	= time step number;
TIME*SECYR	= elapsed simulation time since start of run [yr];
DELT/DAYSEC	= time step size [days];
ITER	= number of Newton-Raphson iterations to reach convergence;
CPU	= CPU time to complete this time step [s];
DELTASATMAX	= maximum saturation change since last time step anywhere in the grid;
IDEPMAX(1)	= I-index of grid block where DELTASATMAX occurred;
JDEPMAX(1)	= J-index of grid block where DELTASATMAX occurred;
KDEPMAX(1)	= K-index of grid block where DELTASATMAX occurred;
DELTAPRESMAX	= maximum brine pressure change since last time step anywhere in the grid [Pa];
IDEPMAX(2)	= I-index of grid block where DELTAPRESMAX occurred;
JDEPMAX(2)	= J-index of grid block where DELTAPRESMAX occurred;
KDEPMAX(2)	= K-index of grid block where DELTAPRESMAX occurred;
GASBALMAX	= maximum gas mass balance error relative to mass of gas present in a grid block [kg gas (error)/kg gas in grid block];
IGBALMX	= I-index of grid block where GASBALMAX occurred;
JGBALMX	= J-index of grid block where GASBALMAX occurred;
KGBALMX	= K-index of grid block where GASBALMAX occurred;
BRNBALMAX	= maximum brine mass balance error relative to mass of brine present in a grid block [kg brine (error)/kg brine in grid block];
IBBALMX	= I-index of grid block where BRNBALMAX occurred;
JBBALMX	= J-index of grid block where BRNBALMAX occurred;
KBBALMX	= K-index of grid block where BRNBALMAX occurred;
GASBALCUM	= sum of gas mass balance errors over all grid blocks for this time step normalized by the mass of gas in the entire mesh [kg gas(error)/kg gas total grid].
BRNBALCUM	= sum of brine mass balance errors over all grid blocks for this time step, normalized by the mass of brine in the entire mesh [kg brine (error)/kg brine total grid].
CHSOLVER	= linear equation solver being used [input on Line 6.20 in Subsection 7.2.7].

GASBALMAX and BRNBALMAX are computed as follows:

$$\begin{aligned} \text{GASBALMAX} &= \max(F_1). \\ \text{BRNBALMAX} &= \max(F_2). \end{aligned}$$

These mass balance measures are closely related to FTOLMAX(1) and FTOLMAX(2), respectively, the latter being normalized by $T_{3x}f_1$ or $T_{3y}f_2$ in the denominator.

Information Only

Lines 5 through 8 indicate which arrays are being monitored (see discussion of Monitor Blocks, Lines 2.17 - 2.22, in Section 7.2.3). In this example, three grid blocks are being monitored; the grid block locations are indicated on lines 9, 14, and 19. For each monitored grid block, the 16 array values being monitored are listed on the four lines that follow the grid block location.

In BRAGFLO, the following sixteen variables are printed at the monitor grid blocks: PO (brine pressure, Pa), PG (gas pressure, Pa), SO (brine saturation), SOEFC (effective brine saturation), PERMGX (permeability to gas in the x -direction, m^2), QR(1) [H_2 generation rate, $kg/(s\ m^3)$], PHI (porosity), PORSOLID (volume change due to chemistry m^3/m^3), QOBLOCKI (inter-block brine flow in x -direction, m^3/s at reference conditions), QOBLOCKJ (inter-block brine flow in y -direction, m^3/s at reference conditions), QGBLOCKI (inter-block gas flow in x -direction, m^3/s at reference conditions), QGBLOCKJ (inter-block gas flow in y -direction, m^3/s at reference conditions), CONCFE (iron concentration, kg/m^3), CONCBIO (cellulosics concentration, kg/m^3), CONCMGO (MgO concentration, kg/m^3), CONCHYDRO (hydromagnesite concentration, kg/m^3).

9.4 Restart Output (.ROT) File

THE RESTART FEATURE IS NOT QUALIFIED FOR USE IN WIPP COMPLIANCE CALCULATIONS AND WILL NOT BE USED IN WIPP COMPLIANCE CALCULATIONS. This binary file is written, if requested in the input, at specified times during a run. It is always written at the end of a run if the restart write flag has been set in the input. Enough information is saved to enable BRAGFLO to pick up from where it left off. Each batch of information written is referred to as a restart record. It is up to the user to keep track of when each restart record is written so that if a restart run is needed, the point where BRAGFLO is to resume can be indicated by the number of the restart record. Periodic writing of restart records is strongly recommended in calculations that are anticipated to be lengthy as a precaution against computer or power failures or unforeseen input errors that do not go into effect until late in the calculation. A message is written to the screen and to the summary file (if one is being written) when a restart record is written to assist the user in keeping track of when and how many restart records were written.

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11.0 Appendices

11.1 Appendix A: Sample BRAGFLO Input Control File

Below we list a Sample BRAGFLO input control file. This file is given here for illustrative purposes only. Its contents are not necessarily those that would be run for a WIPP compliance PA. Parts of this file have been added/changed for illustrating the new features in BRAGFLO Version 6.02.

```
**QA**           = PREBRAG QA RECORDS (Line 0.1)
PREBRAG         = PROGRAM NAME (Line 0.2)
8.00           = PROGRAM VERSION (Line 0.3)
03/08/07       = PROGRAM REVISION DATE (Line 0.4)
03/09/07       = PROGRAM RUN DATE (Line 0.5)
11:16:45       = PROGRAM RUN TIME (Line 0.6)
1996 BRAGFLO CASE 2: MEDIAN UNDISTURBED NO MIGRATION VARIANCE PETITION CALCULATION (Line 1.1)
FILE FLAGS...ASCII, BINARY, SUMMARY, RESTART OUT, RESTART INPUT (Line 1.2)
T T T T F (Line 1.3)
MODEL TYPE AND NUMBER OF GRID BLOCKS IN X, Y, AND Z (line 1.4)
  2  33  31  1 (Line 1.5)
TSTART,  TMAX,  MAXSTEPS (Line 1.6)
-1.5779E+08  3.1557E+11  10000 (Line 1.7)
DT_INIT,  DT_MIN,  DT_MAX,  DT_INCR,  IAUTODT,  TSWITCH (Line 1.8)
  8.6400E+00  8.6400E-04  1.7280E+09  1.2500E+00  1  1.0000E+00 (Line 1.9)
TIME-STEP CHANGES: NUMBER OF CHANGES, TIME OF CHANGE, DELT USED (Line 1.10)
  7 (Line 1.11)
  0.0000E+00  8.6400E+02 (Line 1.12)
  3.1557E+08  8.6400E+02
  7.8892E+08  8.6400E+02
  1.5778E+09  8.6400E+02
  3.1557E+09  8.6400E+02
  6.3114E+09  8.6400E+02
  1.2623E+10  8.6400E+02
IPRTYPEASC IPRTYPEBIN IPRTYPERST UNITSI UNITSO (Line 2.1)
  2  0  2  'SI'  'SI' (Line 2.2)
ASCII PRINTOUT CONTROLLED BY USER SPECIFIED TIMES (line 2.3)
  2 (Line 2.4)
```

Information Only

USER REQUESTED PRINTOUT TIMES

(Line

2.4.1)

0.0000E+00 3.1557E+11

(Line

2.4.2)

BINARY PRINTOUT CONTROLLED BY STEP INTERVAL, IPRNTBIN

(Line 2.5)

20

(Line 2.6)

RESTART PRINTOUT CONTROLLED BY USER SPECIFIED TIMES

(Line 2.7)

1

(Line 2.8)

USER REQUESTED RESTART TIMES

(Line

2.8.1)

3.1557E+11

(Line

2.8.2)

ASCII PRINT FLAGS

(Line 2.9)

1 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0
0 1 1 0 0
0
0
0 0 0 0 0 0

(Line 2.10)

0 0

0 0

0 0

BINARY PRINT FLAGS

(Line 2.11)

1 1 0 0 0 1 0 0 0 1 1 0 0 1 0 1 0 0 0 0 0 0 0 0 0
0 0 0 0 0 1 1 0 1 1 0 0 0 0 0 0 0 0 0 1 0 0 1 1 0 0
0
0
0 0 0 0 0 0

(Line 2.12)

0 0

0 0

0 0

HISTORY VARIABLE OUTPUT

(Line 2.13)

6

(Line 2.14)

1 31 NAME=BRINE PRESSURE

(Line 2.15)

9 8 1 10 8 1 11 8 1 12 8 1 13 8 1 14 8 1
15 8 1 9 9 1 10 9 1 11 9 1 12 9 1 13 9 1
14 9 1 15 9 1 9 10 1 10 10 1 11 10 1 12 10 1
13 10 1 14 10 1 15 10 1 17 8 1 18 8 1 19 8 1
17 9 1 18 9 1 19 9 1 17 10 1 18 10 1 19 10 1
12 1 1

18 30 NAME=GAS SATURATION

(Line 2.15)

9 8 1 10 8 1 11 8 1 12 8 1 13 8 1 14 8 1

Information Only

```
15 8 1 9 9 1 10 9 1 11 9 1 12 9 1 13 9 1
14 9 1 15 9 1 9 10 1 10 10 1 11 10 1 12 10 1
13 10 1 14 10 1 15 10 1 17 8 1 18 8 1 19 8 1
17 9 1 18 9 1 19 9 1 17 10 1 18 10 1 19 10 1
31 94 NAME=TIME-AVERAGE INTERBLOCK BRINE FLOW, X-DIRECTION
3 6 1 3 12 1 3 15 1 3 23 1 3 24 1 3 25 1
3 26 1 3 27 1 3 28 1 3 29 1 3 30 1 3 31 1
32 6 1 32 12 1 32 15 1 32 23 1 32 24 1 32 25 1
32 26 1 32 27 1 32 28 1 32 29 1 32 30 1 32 31 1
9 6 1 9 12 1 9 15 1 26 6 1 26 12 1 26 15 1
17 8 1 17 9 1 17 10 1 20 8 1 20 9 1 20 10 1
9 8 1 9 9 1 9 10 1 16 8 1 16 9 1 16 10 1
23 6 1 23 7 1 23 8 1 23 9 1 23 10 1 23 11 1
23 12 1 23 13 1 23 14 1 23 15 1 23 16 1 23 17 1
23 18 1 23 19 1 23 20 1 23 21 1 23 22 1 23 23 1
23 24 1 23 25 1 23 26 1 23 27 1 23 28 1 23 29 1
23 30 1 23 31 1 24 6 1 24 7 1 24 8 1 24 9 1
24 10 1 24 11 1 24 12 1 24 13 1 24 14 1 24 15 1
24 16 1 24 17 1 24 18 1 24 19 1 24 20 1 24 21 1
24 22 1 24 23 1 24 24 1 24 25 1 24 26 1 24 27 1
24 28 1 24 29 1 24 30 1 24 31 1
32 46 NAME=TIME-AVERAGE INTERBLOCK BRINE FLOW, Y-DIRECTION
9 11 1 10 11 1 11 11 1 12 11 1 13 11 1 14 11 1
15 11 1 9 8 1 10 8 1 11 8 1 12 8 1 13 8 1
14 8 1 15 8 1 17 11 1 18 11 1 19 11 1 17 8 1
18 8 1 19 8 1 23 6 1 23 7 1 23 8 1 23 9 1
23 10 1 23 11 1 23 12 1 23 13 1 23 14 1 23 15 1
23 16 1 23 17 1 23 18 1 23 19 1 23 20 1 23 21 1
23 22 1 23 23 1 23 24 1 23 25 1 23 26 1 23 27 1
23 28 1 23 29 1 23 30 1 23 31 1
34 94 NAME=TIME-AVERAGE INTERBLOCK GAS FLOW, X-DIRECTION
3 6 1 3 12 1 3 15 1 3 23 1 3 24 1 3 25 1
3 26 1 3 27 1 3 28 1 3 29 1 3 30 1 3 31 1
32 6 1 32 12 1 32 15 1 32 23 1 32 24 1 32 25 1
32 26 1 32 27 1 32 28 1 32 29 1 32 30 1 32 31 1
9 6 1 9 12 1 9 15 1 26 6 1 26 12 1 26 15 1
17 8 1 17 9 1 17 10 1 20 8 1 20 9 1 20 10 1
9 8 1 9 9 1 9 10 1 16 8 1 16 9 1 16 10 1
23 6 1 23 7 1 23 8 1 23 9 1 23 10 1 23 11 1
23 12 1 23 13 1 23 14 1 23 15 1 23 16 1 23 17 1
23 18 1 23 19 1 23 20 1 23 21 1 23 22 1 23 23 1
```

(Line 2.15)

(Line 2.15)

(Line 2.15)

Information Only

23 24 1 23 25 1 23 26 1 23 27 1 23 28 1 23 29 1
23 30 1 23 31 1 24 6 1 24 7 1 24 8 1 24 9 1
24 10 1 24 11 1 24 12 1 24 13 1 24 14 1 24 15 1
24 16 1 24 17 1 24 18 1 24 19 1 24 20 1 24 21 1
24 22 1 24 23 1 24 24 1 24 25 1 24 26 1 24 27 1
24 28 1 24 29 1 24 30 1 24 31 1

35 46 NAME=TIME-AVERAGE INTERBLOCK GAS FLOW, Y-DIRECTION

(Line 2.15)

9 11 1 10 11 1 11 11 1 12 11 1 13 11 1 14 11 1
15 11 1 9 8 1 10 8 1 11 8 1 12 8 1 13 8 1
14 8 1 15 8 1 17 11 1 18 11 1 19 11 1 17 8 1
18 8 1 19 8 1 23 6 1 23 7 1 23 8 1 23 9 1
23 10 1 23 11 1 23 12 1 23 13 1 23 14 1 23 15 1
23 16 1 23 17 1 23 18 1 23 19 1 23 20 1 23 21 1
23 22 1 23 23 1 23 24 1 23 25 1 23 26 1 23 27 1
23 28 1 23 29 1 23 30 1 23 31 1

MONITOR PARAMETER VALUES AT GRIDBLOCK(S)

(Line 2.17)

T

(Line 2.18)

NUMBER OF MONITOR BLOCKS

(Line 2.19)

3

(Line 2.20)

MONITOR BLOCKS (I, J, K)

(Line 2.21)

12 10 1

(Line 2.22)

18 10 1

26 12 1

GRID DATA FLAGS: IDXFLAG, IDYFLAG, IDZFLAG, IDEPTHFLAG

(Line 3.1)

1 2 1 7

(Line 3.2)

GRID DATA CARDS: GRID BLOCK DX'S

(Line 3.3)

1.500000E+04 5.000000E+03 1.000000E+03 7.500000E+02 5.000000E+02 1.000000E+02
4.000000E+01 1.000000E+01 4.380000E+01 1.000000E+01 2.000000E+00 4.000000E-01
2.000000E+00 1.000000E+01 4.380000E+01 4.000000E+01 1.000000E+02 4.950000E+02
1.000000E+02 8.000000E+01 2.830000E+02 5.000000E+01 1.000000E+01 6.000000E+01
5.000000E+02 1.000000E+01 4.000000E+01 1.000000E+02 5.000000E+02 7.500000E+02
1.000000E+03 5.000000E+03 1.500000E+04

(Line 3.4)

GRID DATA CARDS: GRID BLOCK DY'S

(Line 3.5)

2.728000E+00 4.737200E+01 1.391600E+02 5.000000E+01 1.100000E+01 8.500000E-01
1.380000E+00 1.320800E+00 1.320800E+00 1.320800E+00 2.617600E+00 2.700000E-01
4.610000E+00 4.450000E+00 1.800000E-01 2.390000E+01 5.242000E+01 5.242000E+01
8.588000E+01 8.588000E+01 4.534000E+01 3.728000E+01 3.600000E+01 7.700000E+00
2.480000E+01 8.500000E+00 1.730000E+01 1.060000E+02 4.330000E+01 1.566000E+01
1.000000E-01

(Line 3.6)

GRID DATA CARDS: GRID BLOCK DZ'S

(Line 3.7)

6.131430E+04 2.131430E+04 8.748800E+03 6.561600E+03 3.314300E+03 2.114300E+03

(Line 3.8)

Information Only

1.834300E+03	1.734300E+03	1.262000E+02	2.880000E+01	4.800000E+00	4.000000E-01
4.800000E+00	2.880000E+01	1.262000E+02	1.000000E+01	1.323000E+02	1.435000E+02
1.416000E+02	1.890000E+01	1.890000E+01	1.890000E+01	9.500000E+00	2.050000E+01
5.310000E+01	1.258900E+03	1.458900E+03	2.018900E+03	3.928000E+03	6.910600E+03
9.214100E+03	2.172690E+04	6.172690E+04			

GRID BLOCK ELEVATIONS

33*01.293640E+02

33*01.544140E+02

1*03.441824E+01	1*01.401058E+02	1*01.924630E+02	1*02.077339E+02
1*02.186417E+02	1*02.238774E+02	1*02.250991E+02	1*02.255354E+02
1*02.260048E+02	1*02.264743E+02	1*02.265790E+02	1*02.266000E+02
1*02.266209E+02	1*02.267256E+02	1*02.271951E+02	1*02.279264E+02
1*02.291480E+02	1*02.343401E+02	1*02.395322E+02	1*02.411029E+02
1*02.442706E+02	1*02.471764E+02	1*02.477000E+02	1*02.483108E+02
1*02.531975E+02	1*02.576478E+02	1*02.580841E+02	1*02.593058E+02
1*02.645415E+02	1*02.754493E+02	1*02.907201E+02	1*03.430774E+02
1*05.176014E+02			
1*06.014737E+01	1*02.346714E+02	1*02.870287E+02	1*03.022995E+02
1*03.132073E+02	1*03.184430E+02	1*03.196646E+02	1*03.201010E+02
1*03.205704E+02	1*03.210399E+02	1*03.211446E+02	1*03.211656E+02
1*03.211865E+02	1*03.212912E+02	1*03.217607E+02	1*03.224920E+02
1*03.237137E+02	1*03.289057E+02	1*03.340978E+02	1*03.356685E+02
1*03.388362E+02	1*03.417420E+02	1*03.422656E+02	1*03.428764E+02
1*03.477631E+02	1*03.522134E+02	1*03.526497E+02	1*03.538714E+02
1*03.591071E+02	1*03.700149E+02	1*03.852857E+02	1*04.376429E+02
1*06.121671E+02			
1*09.064270E+01	1*02.651668E+02	1*03.175240E+02	1*03.327949E+02
1*03.437026E+02	1*03.489384E+02	1*03.501600E+02	1*03.505963E+02
1*03.510658E+02	1*03.515353E+02	1*03.516400E+02	1*03.516609E+02
1*03.516819E+02	1*03.517866E+02	1*03.522561E+02	1*03.529873E+02
1*03.542090E+02	1*03.594011E+02	1*03.645932E+02	1*03.661639E+02
1*03.693315E+02	1*03.722373E+02	1*03.727609E+02	1*03.733717E+02
1*03.782584E+02	1*03.827088E+02	1*03.831451E+02	1*03.843668E+02
1*03.896025E+02	1*04.005103E+02	1*04.157811E+02	1*04.681383E+02
1*06.426624E+02			
1*09.656680E+01	1*02.710909E+02	1*03.234481E+02	1*03.387190E+02
1*03.496267E+02	1*03.548625E+02	1*03.560841E+02	1*03.565204E+02
1*03.569899E+02	1*03.574594E+02	1*03.575641E+02	1*03.575851E+02
1*03.576060E+02	1*03.577107E+02	1*03.581802E+02	1*03.589114E+02
1*03.601331E+02	1*03.653252E+02	1*03.705173E+02	1*03.720880E+02
1*03.752556E+02	1*03.781614E+02	1*03.786850E+02	1*03.792958E+02

(Line 3.9)

(Line 3.10)

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1*03.841825E+02	1*03.886329E+02	1*03.890692E+02	1*03.902909E+02
1*03.955266E+02	1*04.064343E+02	1*04.217052E+02	1*04.740624E+02
1*06.485865E+02			
1*09.768167E+01	1*02.722057E+02	1*03.245630E+02	1*03.398338E+02
1*03.507415E+02	1*03.559773E+02	1*03.571989E+02	1*03.576353E+02
1*03.581047E+02	1*03.585742E+02	1*03.586789E+02	1*03.586999E+02
1*03.587208E+02	1*03.588255E+02	1*03.592950E+02	1*03.600263E+02
1*03.612480E+02	1*03.664400E+02	1*03.716321E+02	1*03.732029E+02
1*03.763705E+02	1*03.792763E+02	1*03.797998E+02	1*03.804107E+02
1*03.852974E+02	1*03.897477E+02	1*03.901840E+02	1*03.914057E+02
1*03.966414E+02	1*04.075492E+02	1*04.228200E+02	1*04.751772E+02
1*06.497014E+02			
1*09.903186E+01	1*02.735559E+02	1*03.259131E+02	1*03.411840E+02
1*03.520918E+02	1*03.573275E+02	1*03.585491E+02	1*03.589854E+02
1*03.594549E+02	1*03.599244E+02	1*03.600291E+02	1*03.600501E+02
1*03.600710E+02	1*03.601757E+02	1*03.606452E+02	1*03.613765E+02
1*03.625981E+02	1*03.677902E+02	1*03.729823E+02	1*03.745530E+02
1*03.777206E+02	1*03.806265E+02	1*03.811501E+02	1*03.817609E+02
1*03.866476E+02	1*03.910979E+02	1*03.915342E+02	1*03.927559E+02
1*03.979916E+02	1*04.088994E+02	1*04.241702E+02	1*04.765274E+02
1*06.510515E+02			
1*01.003524E+02	1*02.748765E+02	1*03.272337E+02	1*03.425046E+02
1*03.534124E+02	1*03.586481E+02	1*03.598698E+02	1*03.603061E+02
1*03.607755E+02	1*03.612450E+02	1*03.613497E+02	1*03.613707E+02
1*03.613916E+02	1*03.614963E+02	1*03.619658E+02	1*03.626971E+02
1*03.639187E+02	1*03.691108E+02	1*03.743029E+02	1*03.758736E+02
1*03.790413E+02	1*03.819471E+02	1*03.824706E+02	1*03.830815E+02
1*03.879681E+02	1*03.924185E+02	1*03.928548E+02	1*03.940765E+02
1*03.993122E+02	1*04.102200E+02	1*04.254908E+02	1*04.778481E+02
1*06.523721E+02			
1*01.016731E+02	1*02.761971E+02	1*03.285544E+02	1*03.438252E+02
1*03.547329E+02	1*03.599687E+02	1*03.611903E+02	1*03.616266E+02
1*03.620961E+02	1*03.625656E+02	1*03.626703E+02	1*03.626913E+02
1*03.627122E+02	1*03.628169E+02	1*03.632864E+02	1*03.640177E+02
1*03.652393E+02	1*03.704314E+02	1*03.756235E+02	1*03.771942E+02
1*03.803618E+02	1*03.832677E+02	1*03.837913E+02	1*03.844021E+02
1*03.892888E+02	1*03.937391E+02	1*03.941754E+02	1*03.953971E+02
1*04.006328E+02	1*04.115406E+02	1*04.268114E+02	1*04.791686E+02
1*06.536927E+02			
1*01.036419E+02	1*02.781660E+02	1*03.305233E+02	1*03.457941E+02
1*03.567019E+02	1*03.619376E+02	1*03.631592E+02	1*03.635956E+02

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1*03.640650E+02	1*03.645345E+02	1*03.646392E+02	1*03.646602E+02
1*03.646811E+02	1*03.647858E+02	1*03.652553E+02	1*03.659866E+02
1*03.672083E+02	1*03.724003E+02	1*03.775924E+02	1*03.791631E+02
1*03.823307E+02	1*03.852366E+02	1*03.857602E+02	1*03.863710E+02
1*03.912577E+02	1*03.957080E+02	1*03.961443E+02	1*03.973660E+02
1*04.026017E+02	1*04.135095E+02	1*04.287803E+02	1*04.811375E+02
1*06.556616E+02			
1*01.050855E+02	1*02.796096E+02	1*03.319668E+02	1*03.472377E+02
1*03.581454E+02	1*03.633812E+02	1*03.646028E+02	1*03.650392E+02
1*03.655086E+02	1*03.659781E+02	1*03.660828E+02	1*03.661038E+02
1*03.661247E+02	1*03.662294E+02	1*03.666989E+02	1*03.674301E+02
1*03.686518E+02	1*03.738439E+02	1*03.790360E+02	1*03.806067E+02
1*03.837743E+02	1*03.866802E+02	1*03.872037E+02	1*03.878146E+02
1*03.927012E+02	1*03.971516E+02	1*03.975879E+02	1*03.988096E+02
1*04.040453E+02	1*04.149531E+02	1*04.302239E+02	1*04.825811E+02
1*06.571052E+02			
1*01.075252E+02	1*02.820492E+02	1*03.344065E+02	1*03.496773E+02
1*03.605851E+02	1*03.658208E+02	1*03.670424E+02	1*03.674788E+02
1*03.679482E+02	1*03.684177E+02	1*03.685224E+02	1*03.685434E+02
1*03.685643E+02	1*03.686690E+02	1*03.691385E+02	1*03.698698E+02
1*03.710914E+02	1*03.762835E+02	1*03.814756E+02	1*03.830464E+02
1*03.862140E+02	1*03.891198E+02	1*03.896433E+02	1*03.902542E+02
1*03.951409E+02	1*03.995912E+02	1*04.000275E+02	1*04.012492E+02
1*04.064849E+02	1*04.173927E+02	1*04.326635E+02	1*04.850208E+02
1*06.595449E+02			
1*01.120545E+02	1*02.865786E+02	1*03.389358E+02	1*03.542066E+02
1*03.651144E+02	1*03.703501E+02	1*03.715717E+02	1*03.720081E+02
1*03.724775E+02	1*03.729470E+02	1*03.730517E+02	1*03.730727E+02
1*03.730936E+02	1*03.731983E+02	1*03.736678E+02	1*03.743991E+02
1*03.756208E+02	1*03.808128E+02	1*03.860049E+02	1*03.875757E+02
1*03.907433E+02	1*03.936491E+02	1*03.941727E+02	1*03.947835E+02
1*03.996702E+02	1*04.041205E+02	1*04.045569E+02	1*04.057785E+02
1*04.110142E+02	1*04.219220E+02	1*04.371928E+02	1*04.895500E+02
1*06.640742E+02			
1*01.143691E+02	1*02.888932E+02	1*03.412504E+02	1*03.565213E+02
1*03.674290E+02	1*03.726647E+02	1*03.738864E+02	1*03.743227E+02
1*03.747922E+02	1*03.752617E+02	1*03.753664E+02	1*03.753873E+02
1*03.754083E+02	1*03.755130E+02	1*03.759825E+02	1*03.767137E+02
1*03.779354E+02	1*03.831275E+02	1*03.883196E+02	1*03.898903E+02
1*03.930579E+02	1*03.959637E+02	1*03.964873E+02	1*03.970981E+02
1*04.019848E+02	1*04.064352E+02	1*04.068715E+02	1*04.080932E+02

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1*04.133289E+02	1*04.242366E+02	1*04.395075E+02	1*04.918647E+02
1*06.663888E+02			
1*01.264073E+02	1*03.009314E+02	1*03.532886E+02	1*03.685594E+02
1*03.794672E+02	1*03.847029E+02	1*03.859246E+02	1*03.863609E+02
1*03.868304E+02	1*03.872998E+02	1*03.874045E+02	1*03.874255E+02
1*03.874464E+02	1*03.875511E+02	1*03.880206E+02	1*03.887519E+02
1*03.899736E+02	1*03.951656E+02	1*04.003578E+02	1*04.019285E+02
1*04.050961E+02	1*04.080019E+02	1*04.085255E+02	1*04.091363E+02
1*04.140230E+02	1*04.184733E+02	1*04.189096E+02	1*04.201313E+02
1*04.253670E+02	1*04.362748E+02	1*04.515457E+02	1*05.039029E+02
1*06.784269E+02			
1*01.645615E+02	1*03.390855E+02	1*03.914427E+02	1*04.067136E+02
1*04.176214E+02	1*04.228571E+02	1*04.240788E+02	1*04.245151E+02
1*04.249846E+02	1*04.254540E+02	1*04.255587E+02	1*04.255797E+02
1*04.256006E+02	1*04.257054E+02	1*04.261748E+02	1*04.269061E+02
1*04.281277E+02	1*04.333199E+02	1*04.385119E+02	1*04.400826E+02
1*04.432503E+02	1*04.461561E+02	1*04.466797E+02	1*04.472905E+02
1*04.521772E+02	1*04.566275E+02	1*04.570638E+02	1*04.582855E+02
1*04.635212E+02	1*04.744290E+02	1*04.896999E+02	1*05.420571E+02
1*07.165811E+02			
1*02.169735E+02	1*03.914976E+02	1*04.438548E+02	1*04.591256E+02
1*04.700334E+02	1*04.752691E+02	1*04.764908E+02	1*04.769271E+02
1*04.773966E+02	1*04.778661E+02	1*04.779708E+02	1*04.779917E+02
1*04.780127E+02	1*04.781174E+02	1*04.785869E+02	1*04.793181E+02
1*04.805398E+02	1*04.857319E+02	1*04.909240E+02	1*04.924947E+02
1*04.956623E+02	1*04.985681E+02	1*04.990917E+02	1*04.997025E+02
1*05.045892E+02	1*05.090396E+02	1*05.094759E+02	1*05.106975E+02
1*05.159333E+02	1*05.268410E+02	1*05.421119E+02	1*05.944691E+02
1*07.689932E+02			
1*02.861129E+02	1*04.606370E+02	1*05.129943E+02	1*05.282651E+02
1*05.391729E+02	1*05.444086E+02	1*05.456302E+02	1*05.460666E+02
1*05.465360E+02	1*05.470055E+02	1*05.471102E+02	1*05.471312E+02
1*05.471521E+02	1*05.472568E+02	1*05.477263E+02	1*05.484576E+02
1*05.496793E+02	1*05.548713E+02	1*05.600634E+02	1*05.616342E+02
1*05.648018E+02	1*05.677076E+02	1*05.682311E+02	1*05.688420E+02
1*05.737287E+02	1*05.781790E+02	1*05.786154E+02	1*05.798370E+02
1*05.850727E+02	1*05.959805E+02	1*06.112513E+02	1*06.636086E+02
1*08.381326E+02			
1*03.719799E+02	1*05.465040E+02	1*05.988612E+02	1*06.141321E+02
1*06.250398E+02	1*06.302755E+02	1*06.314972E+02	1*06.319335E+02
1*06.324030E+02	1*06.328724E+02	1*06.329772E+02	1*06.329981E+02

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1*06.330190E+02	1*06.331238E+02	1*06.335933E+02	1*06.343245E+02
1*06.355461E+02	1*06.407383E+02	1*06.459304E+02	1*06.475011E+02
1*06.506687E+02	1*06.535745E+02	1*06.540981E+02	1*06.547089E+02
1*06.595956E+02	1*06.640460E+02	1*06.644822E+02	1*06.657039E+02
1*06.709396E+02	1*06.818474E+02	1*06.971183E+02	1*07.494755E+02
1*09.239996E+02			
1*04.375799E+02	1*06.121040E+02	1*06.644612E+02	1*06.797321E+02
1*06.906398E+02	1*06.958755E+02	1*06.970972E+02	1*06.975335E+02
1*06.980030E+02	1*06.984725E+02	1*06.985772E+02	1*06.985981E+02
1*06.986191E+02	1*06.987238E+02	1*06.991933E+02	1*06.999246E+02
1*07.011462E+02	1*07.063383E+02	1*07.115304E+02	1*07.131011E+02
1*07.162687E+02	1*07.191746E+02	1*07.196981E+02	1*07.203090E+02
1*07.251956E+02	1*07.296460E+02	1*07.300823E+02	1*07.313040E+02
1*07.365397E+02	1*07.474474E+02	1*07.627183E+02	1*08.150755E+02
1*09.895996E+02			
1*04.788837E+02	1*06.534077E+02	1*07.057650E+02	1*07.210358E+02
1*07.319436E+02	1*07.371793E+02	1*07.384010E+02	1*07.388373E+02
1*07.393068E+02	1*07.397762E+02	1*07.398810E+02	1*07.399019E+02
1*07.399228E+02	1*07.400275E+02	1*07.404970E+02	1*07.412283E+02
1*07.424500E+02	1*07.476420E+02	1*07.528342E+02	1*07.544048E+02
1*07.575725E+02	1*07.604783E+02	1*07.610018E+02	1*07.616127E+02
1*07.664994E+02	1*07.709497E+02	1*07.713860E+02	1*07.726077E+02
1*07.778434E+02	1*07.887512E+02	1*08.040220E+02	1*08.563793E+02
1*01.030903E+03			
33*07.977001E+02			
33*08.195501E+02			
33*08.358001E+02			
33*08.524501E+02			
33*08.653501E+02			
33*09.270001E+02			
33*01.001650E+03			
33*01.031130E+03			
33*01.039010E+03			

WELL DATA

0

DIRICHLET CONDITIONS

T 37

1	24	1	T	F	8.520000E+05	0.000000E+00
33	24	1	T	F	8.520000E+05	0.000000E+00
1	26	1	T	F	9.000000E+05	0.000000E+00
33	26	1	T	F	9.000000E+05	0.000000E+00

(Line 4.1)

(Line 4.2)

(Line 4.7)

(Line 4.8)

(Line 4.9)

Information Only

1	31	1	T	T	1.013250E+05	2.000000E-01
2	31	1	T	T	1.013250E+05	2.000000E-01
3	31	1	T	T	1.013250E+05	2.000000E-01
4	31	1	T	T	1.013250E+05	2.000000E-01
5	31	1	T	T	1.013250E+05	2.000000E-01
6	31	1	T	T	1.013250E+05	2.000000E-01
7	31	1	T	T	1.013250E+05	2.000000E-01
8	31	1	T	T	1.013250E+05	2.000000E-01
9	31	1	T	T	1.013250E+05	2.000000E-01
10	31	1	T	T	1.013250E+05	2.000000E-01
11	31	1	T	T	1.013250E+05	2.000000E-01
12	31	1	T	T	1.013250E+05	2.000000E-01
13	31	1	T	T	1.013250E+05	2.000000E-01
14	31	1	T	T	1.013250E+05	2.000000E-01
15	31	1	T	T	1.013250E+05	2.000000E-01
16	31	1	T	T	1.013250E+05	2.000000E-01
17	31	1	T	T	1.013250E+05	2.000000E-01
18	31	1	T	T	1.013250E+05	2.000000E-01
19	31	1	T	T	1.013250E+05	2.000000E-01
20	31	1	T	T	1.013250E+05	2.000000E-01
21	31	1	T	T	1.013250E+05	2.000000E-01
22	31	1	T	T	1.013250E+05	2.000000E-01
23	31	1	T	T	1.013250E+05	8.000000E-01
24	31	1	T	T	1.013250E+05	2.000000E-01
25	31	1	T	T	1.013250E+05	2.000000E-01
26	31	1	T	T	1.013250E+05	2.000000E-01
27	31	1	T	T	1.013250E+05	2.000000E-01
28	31	1	T	T	1.013250E+05	2.000000E-01
29	31	1	T	T	1.013250E+05	2.000000E-01
30	31	1	T	T	1.013250E+05	2.000000E-01
31	31	1	T	T	1.013250E+05	2.000000E-01
32	31	1	T	T	1.013250E+05	2.000000E-01
33	31	1	T	T	1.013250E+05	2.000000E-01

GRID BLOCK BRINE PRESSURE INITIAL CONDITIONS

2*01.550225E+07	29*01.270000E+07	2*01.550225E+07	
33*01.520060E+07			
1*01.747447E+07	1*01.537290E+07	1*01.474243E+07	1*01.455854E+07
1*01.442719E+07	1*01.436415E+07	1*01.434944E+07	1*01.434418E+07
1*01.433853E+07	1*01.433288E+07	1*01.433161E+07	1*01.433136E+07
1*01.433111E+07	1*01.432985E+07	1*01.432420E+07	1*01.431539E+07
1*01.430068E+07	1*01.423816E+07	1*01.417564E+07	1*01.415672E+07

(Line 5.1)
(Line 5.2)

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1*01.411858E+07	1*01.408359E+07	1*01.407728E+07	1*01.406993E+07
1*01.401108E+07	1*01.395749E+07	1*01.395224E+07	1*01.393753E+07
1*01.387448E+07	1*01.374313E+07	1*01.355925E+07	1*01.292878E+07
1*01.082721E+07			
1*01.633574E+07	1*01.423417E+07	1*01.360370E+07	1*01.341981E+07
1*01.328846E+07	1*01.322542E+07	1*01.321071E+07	1*01.320545E+07
1*01.319980E+07	1*01.319415E+07	1*01.319289E+07	1*01.319263E+07
1*01.319238E+07	1*01.319112E+07	1*01.318547E+07	1*01.317666E+07
1*01.316195E+07	1*01.309943E+07	1*01.303691E+07	1*01.301799E+07
1*01.297985E+07	1*01.294486E+07	1*01.293855E+07	1*01.293120E+07
1*01.287235E+07	1*01.281876E+07	1*01.281351E+07	1*01.279880E+07
1*01.273575E+07	1*01.260440E+07	1*01.242052E+07	1*01.179005E+07
1*09.688480E+06			
1*01.596852E+07	1*01.386695E+07	1*01.323648E+07	1*01.305260E+07
1*01.292125E+07	1*01.285820E+07	1*01.284349E+07	1*01.283824E+07
1*01.283258E+07	1*01.282693E+07	1*01.282567E+07	1*01.282542E+07
1*01.282516E+07	1*01.282390E+07	1*01.281825E+07	1*01.280945E+07
1*01.279473E+07	1*01.273221E+07	1*01.266969E+07	1*01.265078E+07
1*01.261263E+07	1*01.257764E+07	1*01.257134E+07	1*01.256398E+07
1*01.250514E+07	1*01.245155E+07	1*01.244629E+07	1*01.243158E+07
1*01.236854E+07	1*01.223719E+07	1*01.205330E+07	1*01.142283E+07
1*09.321264E+06			
1*01.589718E+07	1*01.379562E+07	1*01.316515E+07	1*01.298126E+07
1*01.284991E+07	1*01.278687E+07	1*01.277215E+07	1*01.276690E+07
1*01.276125E+07	1*01.275559E+07	1*01.275433E+07	1*01.275408E+07
1*01.275383E+07	1*01.275257E+07	1*01.274691E+07	1*01.273811E+07
1*01.272340E+07	1*01.266088E+07	1*01.259835E+07	1*01.257944E+07
1*01.254130E+07	1*01.250631E+07	1*01.013250E+05	1*01.249265E+07
1*01.243380E+07	1*01.238021E+07	1*01.237496E+07	1*01.236025E+07
1*01.229720E+07	1*01.216585E+07	1*01.198196E+07	1*01.135150E+07
1*09.249928E+06			
1*01.588376E+07	1*01.378219E+07	1*01.315172E+07	1*01.296784E+07
1*01.283649E+07	1*01.277344E+07	1*01.275873E+07	1*01.275348E+07
1*01.274782E+07	1*01.274217E+07	1*01.274091E+07	1*01.274066E+07
1*01.274040E+07	1*01.273914E+07	1*01.273349E+07	1*01.272468E+07
1*01.270997E+07	1*01.264745E+07	1*01.258493E+07	1*01.256602E+07
1*01.252787E+07	1*01.249288E+07	1*01.013250E+05	1*01.247922E+07
1*01.242038E+07	1*01.236679E+07	1*01.236153E+07	1*01.234682E+07
1*01.228378E+07	1*01.215243E+07	1*01.196854E+07	1*01.133807E+07
1*09.236503E+06			
1*01.586750E+07	1*01.376594E+07	1*01.313546E+07	1*01.295158E+07

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1*01.282023E+07	1*01.275718E+07	1*01.274247E+07	1*01.273722E+07
17*01.013250E+05	1*01.235053E+07	1*01.234528E+07	1*01.233056E+07
1*01.226752E+07	1*01.213617E+07	1*01.195228E+07	1*01.132181E+07
1*09.220245E+06			
1*01.585160E+07	1*01.375003E+07	1*01.311956E+07	1*01.293567E+07
1*01.280433E+07	1*01.274128E+07	1*01.272657E+07	1*01.272132E+07
17*01.013250E+05	1*01.233463E+07	1*01.232937E+07	1*01.231466E+07
1*01.225161E+07	1*01.212027E+07	1*01.193638E+07	1*01.130591E+07
1*09.204342E+06			
1*01.583570E+07	1*01.373413E+07	1*01.310366E+07	1*01.291977E+07
1*01.278843E+07	1*01.272538E+07	1*01.271067E+07	1*01.270541E+07
17*01.013250E+05	1*01.231872E+07	1*01.231347E+07	1*01.229876E+07
1*01.223571E+07	1*01.210437E+07	1*01.192048E+07	1*01.129001E+07
1*09.188441E+06			
1*01.581199E+07	1*01.371042E+07	1*01.307995E+07	1*01.289606E+07
1*01.276472E+07	1*01.270167E+07	1*01.268696E+07	1*01.268170E+07
1*01.267605E+07	1*01.267040E+07	1*01.266914E+07	1*01.266888E+07
1*01.266863E+07	1*01.266737E+07	1*01.266172E+07	1*01.265291E+07
1*01.263820E+07	1*01.257568E+07	1*01.251316E+07	1*01.249424E+07
1*01.245610E+07	1*01.242111E+07	1*01.013250E+05	1*01.240745E+07
1*01.234860E+07	1*01.229502E+07	1*01.228976E+07	1*01.227505E+07
1*01.221200E+07	1*01.208066E+07	1*01.189677E+07	1*01.126630E+07
1*09.164732E+06			
1*01.579460E+07	1*01.369304E+07	1*01.306257E+07	1*01.287868E+07
1*01.274733E+07	1*01.268429E+07	1*01.266957E+07	1*01.266432E+07
1*01.265867E+07	1*01.265301E+07	1*01.265175E+07	1*01.265150E+07
1*01.265125E+07	1*01.264999E+07	1*01.264433E+07	1*01.263553E+07
1*01.262082E+07	1*01.255830E+07	1*01.249577E+07	1*01.247686E+07
1*01.243872E+07	1*01.240373E+07	1*01.013250E+05	1*01.239007E+07
1*01.233122E+07	1*01.227763E+07	1*01.227238E+07	1*01.225767E+07
1*01.219462E+07	1*01.206327E+07	1*01.187938E+07	1*01.124892E+07
1*09.147348E+06			
1*01.576523E+07	1*01.366366E+07	1*01.303319E+07	1*01.284930E+07
1*01.271796E+07	1*01.265491E+07	1*01.264020E+07	1*01.263494E+07
1*01.262929E+07	1*01.262364E+07	1*01.262238E+07	1*01.262212E+07
1*01.262187E+07	1*01.262061E+07	1*01.261496E+07	1*01.260615E+07
1*01.259144E+07	1*01.252892E+07	1*01.246640E+07	1*01.244748E+07
1*01.240934E+07	1*01.237435E+07	1*01.013250E+05	1*01.236069E+07
1*01.230184E+07	1*01.224825E+07	1*01.224300E+07	1*01.222829E+07
1*01.216524E+07	1*01.203390E+07	1*01.185001E+07	1*01.121954E+07
1*09.117971E+06			

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1*01.571069E+07	1*01.360912E+07	1*01.297865E+07	1*01.279476E+07
1*01.266342E+07	1*01.260037E+07	1*01.258566E+07	1*01.258040E+07
1*01.257475E+07	1*01.256910E+07	1*01.256783E+07	1*01.256758E+07
1*01.256733E+07	1*01.256607E+07	1*01.256042E+07	1*01.255161E+07
1*01.253690E+07	1*01.247438E+07	1*01.241186E+07	1*01.239294E+07
1*01.235480E+07	1*01.231981E+07	1*01.013250E+05	1*01.230615E+07
1*01.224730E+07	1*01.219371E+07	1*01.218846E+07	1*01.217375E+07
1*01.211070E+07	1*01.197936E+07	1*01.179547E+07	1*01.116500E+07
1*09.063431E+06			
1*01.568281E+07	1*01.358125E+07	1*01.295078E+07	1*01.276689E+07
1*01.263554E+07	1*01.257250E+07	1*01.255778E+07	1*01.255253E+07
1*01.254688E+07	1*01.254122E+07	1*01.253996E+07	1*01.253971E+07
1*01.253946E+07	1*01.253820E+07	1*01.253254E+07	1*01.252374E+07
1*01.250903E+07	1*01.244651E+07	1*01.238398E+07	1*01.236507E+07
1*01.232693E+07	1*01.229194E+07	1*01.013250E+05	1*01.227828E+07
1*01.221943E+07	1*01.216584E+07	1*01.216059E+07	1*01.214588E+07
1*01.208283E+07	1*01.195148E+07	1*01.176759E+07	1*01.113713E+07
1*09.035558E+06			
1*01.553785E+07	1*01.343629E+07	1*01.280582E+07	1*01.262193E+07
1*01.249058E+07	1*01.242754E+07	1*01.241282E+07	1*01.240757E+07
1*01.240192E+07	1*01.239626E+07	1*01.239500E+07	1*01.239475E+07
1*01.239450E+07	1*01.239324E+07	1*01.238758E+07	1*01.237878E+07
1*01.236407E+07	1*01.230155E+07	1*01.223902E+07	1*01.222011E+07
1*01.218197E+07	1*01.214698E+07	1*01.013250E+05	1*01.213332E+07
1*01.207447E+07	1*01.202088E+07	1*01.201563E+07	1*01.200092E+07
1*01.193787E+07	1*01.180652E+07	1*01.162264E+07	1*01.099217E+07
1*08.890598E+06			
1*01.507841E+07	1*01.297685E+07	1*01.234638E+07	1*01.216249E+07
1*01.203114E+07	1*01.196809E+07	1*01.195338E+07	1*01.194813E+07
1*01.194248E+07	1*01.193682E+07	1*01.193556E+07	1*01.193531E+07
1*01.193506E+07	1*01.193380E+07	1*01.192814E+07	1*01.191934E+07
1*01.190463E+07	1*01.184210E+07	1*01.177958E+07	1*01.176067E+07
1*01.172253E+07	1*01.168753E+07	1*01.013250E+05	1*01.167388E+07
1*01.161503E+07	1*01.156144E+07	1*01.155619E+07	1*01.154148E+07
1*01.147843E+07	1*01.134708E+07	1*01.116319E+07	1*01.053272E+07
1*08.431157E+06			
1*01.444728E+07	1*01.234572E+07	1*01.171525E+07	1*01.153136E+07
1*01.140001E+07	1*01.133696E+07	1*01.132225E+07	1*01.131700E+07
1*01.131135E+07	1*01.130569E+07	1*01.130443E+07	1*01.130418E+07
1*01.130393E+07	1*01.130267E+07	1*01.129701E+07	1*01.128821E+07
1*01.127350E+07	1*01.121098E+07	1*01.114845E+07	1*01.112954E+07

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1*01.109140E+07	1*01.105641E+07	1*01.013250E+05	1*01.104274E+07
1*01.098390E+07	1*01.093031E+07	1*01.092506E+07	1*01.091035E+07
1*01.084730E+07	1*01.071595E+07	1*01.053206E+07	1*09.901595E+06
1*07.800027E+06			
1*01.361473E+07	1*01.151316E+07	1*01.088269E+07	1*01.069880E+07
1*01.056745E+07	1*01.050441E+07	1*01.048970E+07	1*01.048444E+07
1*01.047879E+07	1*01.047314E+07	1*01.047188E+07	1*01.047162E+07
1*01.047137E+07	1*01.047011E+07	1*01.046446E+07	1*01.045565E+07
1*01.044094E+07	1*01.037842E+07	1*01.031590E+07	1*01.029698E+07
1*01.025884E+07	1*01.022385E+07	1*01.013250E+05	1*01.021019E+07
1*01.015134E+07	1*01.009775E+07	1*01.009250E+07	1*01.007779E+07
1*01.001474E+07	1*09.883394E+06	1*09.699507E+06	1*09.069037E+06
1*06.967471E+06			
1*01.258074E+07	1*01.047918E+07	1*09.848706E+06	1*09.664818E+06
1*09.533470E+06	1*09.470423E+06	1*09.455712E+06	1*09.450458E+06
1*09.444806E+06	1*09.439152E+06	1*09.437891E+06	1*09.437639E+06
1*09.437386E+06	1*09.436126E+06	1*09.430472E+06	1*09.421667E+06
1*09.406956E+06	1*09.344434E+06	1*09.281913E+06	1*09.262998E+06
1*09.224856E+06	1*09.189865E+06	1*01.013250E+05	1*09.176204E+06
1*09.117360E+06	1*09.063770E+06	1*09.058516E+06	1*09.043805E+06
1*08.980758E+06	1*08.849410E+06	1*08.665523E+06	1*08.035053E+06
1*05.933486E+06			
1*01.179081E+07	1*09.689240E+06	1*09.058770E+06	1*08.874882E+06
1*08.743534E+06	1*08.680487E+06	1*08.665777E+06	1*08.660523E+06
1*08.654869E+06	1*08.649216E+06	1*08.647955E+06	1*08.647703E+06
1*08.647450E+06	1*08.646190E+06	1*08.640537E+06	1*08.631731E+06
1*08.617020E+06	1*08.554498E+06	1*08.491977E+06	1*08.473063E+06
1*08.434919E+06	1*08.399928E+06	1*01.013250E+05	1*08.386268E+06
1*08.327424E+06	1*08.273834E+06	1*08.268580E+06	1*08.253869E+06
1*08.190822E+06	1*08.059474E+06	1*07.875587E+06	1*07.245117E+06
1*05.143550E+06			
1*01.129344E+07	1*09.191873E+06	1*08.561402E+06	1*08.377515E+06
1*08.246167E+06	1*08.183120E+06	1*08.168410E+06	1*08.163155E+06
1*08.157502E+06	1*08.151849E+06	1*08.150588E+06	1*08.150335E+06
1*08.150083E+06	1*08.148823E+06	1*08.143169E+06	1*08.134364E+06
1*08.119653E+06	1*08.057131E+06	1*07.994610E+06	1*07.975695E+06
1*07.937552E+06	1*07.902561E+06	1*01.013250E+05	1*07.888901E+06
1*07.830057E+06	1*07.776467E+06	1*07.771213E+06	1*07.756502E+06
1*07.693455E+06	1*07.562107E+06	1*07.378220E+06	1*06.747750E+06
1*04.646184E+06			
22*02.296527E+06	1*01.013250E+05	10*02.296527E+06	

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33*00.000000E+00
 33*00.000000E+00
 33*00.000000E+00
 33*00.000000E+00
 8*00.000000E+00 7*09.244771E+01 1*00.000000E+00 3*09.244771E+01
 14*00.000000E+00
 8*00.000000E+00 7*09.244771E+01 1*00.000000E+00 3*09.244771E+01
 14*00.000000E+00
 8*00.000000E+00 7*09.244771E+01 1*00.000000E+00 3*09.244771E+01
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GRID BLOCK MGO CONCENTRATION INITIAL CONDITIONS

33*00.000000E+00
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 33*00.000000E+00
 33*00.000000E+00
 33*00.000000E+00
 8*00.000000E+00 7*09.244771E+01 1*00.000000E+00 3*09.244771E+01
 14*00.000000E+00

(Line 5.9)
 (Line 5.10)

Information Only

8*00.000000E+00	7*09.244771E+01	1*00.000000E+00	3*09.244771E+01	
14*00.000000E+00				
8*00.000000E+00	7*09.244771E+01	1*00.000000E+00	3*09.244771E+01	
14*00.000000E+00				
33*00.000000E+00				
33*00.000000E+00				
33*00.000000E+00				
33*00.000000E+00				
33*00.000000E+00				
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33*00.000000E+00				
DSATLIM, DPRESLIM, SATLIMIT				(Line 6.1)
2.0000E-01 -1.0000E+08 1.0000E-03				(Line 6.2)
SATNORM, PRESNORM: NOMINAL CHANGE DEPENDENT VARIABLE				(Line 6.3)
3.0000E-01 5.0000E+05				(Line 6.4)
MAXIMUM ALLOWABLE VARIABLE CHANGES: DSAT_MAX DPRES_MAX				(Line 6.5)
1.0000E+00 1.0000E+07				(Line 6.6)
CONVERGENCE TEST FLAG: 0=OR/1=AND				(Line 6.7)
1				(Line 6.8)
EPS_SAT, EPS_PRES: NORMAL CONVERGENCE CRITERIA				(Line 6.9)
3.0000E+00 1.0000E-02				(Line 6.10)
EPS_SAT, EPS_PRES: RELAXED CONVERGENCE CRITERIA				(Line 6.11)
3.0000E+00 1.0000E-02				(Line 6.12)
FTOL_SAT FTOL_PRES: NORMAL RESIDUAL' TOLERANCE				(Line 6.13)
1.0000E-02 1.0000E-02				(Line 6.14)
FTOL_SAT FTOL_PRES: RELAXED RESIDUAL' TOLERANCE				(Line 6.15)
1.0000E-02 1.0000E-02				(Line 6.16)

Information Only

GAS TRANSPORT TOLERANCES	(Line 6.17)
1.0000E-05 1.0000E-05 1.0000E-05 1.0000E-05	(Line 6.18)
LINEAR EQUATION SOLVER TYPE	(Line 6.19)
LU	(Line 6.20)
ITMAX, IRESETMAX, IJACINT, LSCALE, P_SCALE, LVARSWITCH	(Line 6.21)
8 40 1 T 1.0000E+07 F	(Line 6.22)
IUPRPFLAG, IUPMFLAG, DT_REDU, ITRAVE, IMFRAVE	(Line 6.23)
9 9 5.0000E-01 1 0	(Line 6.24)
IJACSWITCH, IJACMIN, IJACRESET, IUPRPLOOSE, IUPMFLOOSE	(Line 6.25)
41 1 5 9 9	
DHSAT_REL, DHPRES_REL: REL. CHANGE FOR JACOBIAN ELEMENT CALCS	(Line 6.27)
1.0000E-08 1.0000E-08	(Line 6.28)
DHSAT_MIN, DHPRES_MIN: MIN. CHANGE ALLOWED FOR JACOBIAN CALCS	(Line 6.29)
1.0000E-10 1.0000E-02	(Line 6.30)
NUMBER OF TIMES FOR SPECIFYING MATERIAL MAP	(Line 7.1)
8	(Line 7.2)
START TIME FOR MAP 1	(Line 7.3)
-1.5779E+08	(Line 7.4)
MATERIAL TYPE GRID MAP	(Line 7.5)
2*010 29*011 2*010	
33*010	
33*001	
33*001	
33*001	
8*003 14*002 1*009 2*002 8*003	
8*001 14*002 1*009 2*002 8*001	
8*001 7*006 1*009 3*007 1*009 2*008 1*009 2*008 8*001	
8*001 7*006 1*009 3*007 1*009 2*008 1*009 2*008 8*001	
8*001 7*006 1*009 3*007 1*009 2*008 1*009 2*008 8*001	
8*001 14*002 1*009 2*002 8*001	
8*004 14*002 1*009 2*002 8*004	
8*001 14*002 1*009 2*002 8*001	
8*001 14*002 1*009 2*002 8*001	
22*005 1*009 10*005	
22*001 1*009 10*001	
22*001 1*009 10*001	
22*001 1*009 10*001	
22*001 1*009 10*001	
22*001 1*009 10*001	
22*001 1*009 10*001	
22*001 1*009 10*001	

Information Only

22*010 1*009 10*010
22*010 1*009 10*010
22*010 1*009 10*010
22*010 1*009 10*010
22*010 1*009 10*010
22*010 1*009 10*010
22*010 1*009 10*010
22*010 1*009 10*010
22*010 1*009 10*010

START TIME FOR MAP 2

0.0000E+00

MATERIAL TYPE GRID MAP

2*010 29*011 2*010

33*010

33*001

33*001

33*001

8*003 14*002 1*027 2*002 8*003

8*001 14*002 1*027 2*002 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 14*002 1*027 2*002 8*001

8*004 14*002 1*027 2*002 8*004

8*001 14*002 1*027 2*002 8*001

8*001 14*002 1*041 2*002 8*001

22*005 1*041 10*005

22*001 1*033 10*001

22*001 1*028 10*001

22*001 1*028 10*001

22*001 1*036 10*001

22*001 1*036 10*001

22*001 1*026 10*001

22*001 1*025 10*001

22*014 1*024 10*014

22*015 1*024 10*015

22*016 1*024 10*016

22*017 1*024 10*017

22*018 1*024 10*018

22*019 1*023 10*019

22*019 1*023 10*019

(Line 7.3)

(Line 7.4)

(Line 7.5)

(Line 7.6)

Information Only

22*020 1*023 10*020

22*020 1*023 10*020

START TIME FOR MAP 3

3.1557E+08

MATERIAL TYPE GRID MAP

2*010 29*011 2*010

33*010

33*001

33*001

33*001

8*003 14*002 1*027 2*002 8*003

8*001 14*002 1*027 2*002 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 14*002 1*027 2*002 8*001

8*004 14*002 1*027 2*002 8*004

8*001 14*002 1*027 2*002 8*001

8*001 14*002 1*041 2*002 8*001

22*005 1*041 10*005

22*001 1*034 10*001

22*001 1*029 10*001

22*001 1*029 10*001

22*001 1*036 10*001

22*001 1*036 10*001

22*001 1*026 10*001

22*001 1*025 10*001

22*014 1*024 10*014

22*015 1*024 10*015

22*016 1*024 10*016

22*017 1*024 10*017

22*018 1*024 10*018

22*019 1*023 10*019

22*019 1*023 10*019

22*020 1*023 10*020

22*020 1*023 10*020

START TIME FOR MAP 4

7.8892E+08

MATERIAL TYPE GRID MAP

2*010 29*011 2*010

33*010

(Line 7.3)

(Line 7.4)

(Line 7.5)

(Line 7.6)

(Line 7.3)

(Line 7.4)

(Line 7.5)

(Line 7.6)

Information Only

```
33*001
33*001
33*001
 8*003 14*002 1*027 2*002 8*003
 8*001 14*002 1*027 2*002 8*001
 8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001
 8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001
 8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001
 8*001 14*002 1*027 2*002 8*001
 8*004 14*002 1*027 2*002 8*004
 8*001 14*002 1*027 2*002 8*001
 8*001 14*002 1*041 2*002 8*001
22*005 1*041 10*005
22*001 1*035 10*001
22*001 1*030 10*001
22*001 1*030 10*001
22*001 1*036 10*001
22*001 1*036 10*001
22*001 1*026 10*001
22*001 1*025 10*001
22*014 1*024 10*014
22*015 1*024 10*015
22*016 1*024 10*016
22*017 1*024 10*017
22*018 1*024 10*018
22*019 1*023 10*019
22*019 1*023 10*019
22*020 1*023 10*020
22*020 1*023 10*020
START TIME FOR MAP 5
1.5578E+09
MATERIAL TYPE GRID MAP
 2*010 29*011 2*010
33*010
33*001
33*001
33*001
 8*003 14*002 1*027 2*002 8*003
 8*001 14*002 1*027 2*002 8*001
 8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001
 8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001
```

(Line 7.3)
(Line 7.4)
(Line 7.5)
(Line 7.6)

Information Only

8*001	7*012	1*042	3*013	1*042	2*021	1*027	2*022	8*001
8*001	14*002	1*027	2*002	8*001				
8*004	14*002	1*027	2*002	8*004				
8*001	14*002	1*027	2*002	8*001				
8*001	14*002	1*041	2*002	8*001				
22*005	1*041	10*005						
22*001	1*035	10*001						
22*001	1*031	10*001						
22*001	1*031	10*001						
22*001	1*037	10*001						
22*001	1*037	10*001						
22*001	1*026	10*001						
22*001	1*025	10*001						
22*014	1*024	10*014						
22*015	1*024	10*015						
22*016	1*024	10*016						
22*017	1*024	10*017						
22*018	1*024	10*018						
22*019	1*023	10*019						
22*019	1*023	10*019						
22*020	1*023	10*020						
22*020	1*023	10*020						
START TIME FOR MAP 6								
3.1557E+09								
MATERIAL TYPE GRID MAP								
2*010	29*011	2*010						
33*010								
33*001								
33*001								
33*001								
8*003	14*002	1*027	2*002	8*003				
8*001	14*002	1*027	2*002	8*001				
8*001	7*012	1*042	3*013	1*042	2*021	1*027	2*022	8*001
8*001	7*012	1*042	3*013	1*042	2*021	1*027	2*022	8*001
8*001	7*012	1*042	3*013	1*042	2*021	1*027	2*022	8*001
8*001	14*002	1*027	2*002	8*001				
8*004	14*002	1*027	2*002	8*004				
8*001	14*002	1*027	2*002	8*001				
8*001	14*002	1*041	2*002	8*001				
22*005	1*041	10*005						
22*001	1*035	10*001						

(Line 7.3)
(Line 7.4)
(Line 7.5)
(Line 7.6)

Information Only

22*001 1*032 10*001
22*001 1*032 10*001
22*001 1*038 10*001
22*001 1*038 10*001
22*001 1*027 10*001
22*001 1*025 10*001
22*014 1*024 10*014
22*015 1*024 10*015
22*016 1*024 10*016
22*017 1*024 10*017
22*018 1*024 10*018
22*019 1*023 10*019
22*019 1*023 10*019
22*020 1*023 10*020
22*020 1*023 10*020

START TIME FOR MAP 7

6.3114E+09

MATERIAL TYPE GRID MAP

2*010 29*011 2*010

33*010

33*001

33*001

33*001

8*003 14*002 1*027 2*002 8*003

8*001 14*002 1*027 2*002 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 14*002 1*027 2*002 8*001

8*004 14*002 1*027 2*002 8*004

8*001 14*002 1*027 2*002 8*001

8*001 14*002 1*041 2*002 8*001

22*005 1*041 10*005

22*001 1*035 10*001

22*001 1*032 10*001

22*001 1*032 10*001

22*001 1*039 10*001

22*001 1*039 10*001

22*001 1*027 10*001

22*001 1*025 10*001

22*014 1*024 10*014

(Line 7.3)

(Line 7.4)

(Line 7.5)

(Line 7.6)

Information Only

22*015 1*024 10*015
22*016 1*024 10*016
22*017 1*024 10*017
22*018 1*024 10*018
22*019 1*023 10*019
22*019 1*023 10*019
22*020 1*023 10*020
22*020 1*023 10*020

START TIME FOR MAP 8

1.2623E+10

MATERIAL TYPE GRID MAP

2*010 29*011 2*010

33*010

33*001

33*001

33*001

8*003 14*002 1*027 2*002 8*003

8*001 14*002 1*027 2*002 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 7*012 1*042 3*013 1*042 2*021 1*027 2*022 8*001

8*001 14*002 1*027 2*002 8*001

8*004 14*002 1*027 2*002 8*004

8*001 14*002 1*027 2*002 8*001

8*001 14*002 1*041 2*002 8*001

22*005 1*041 10*005

22*001 1*035 10*001

22*001 1*032 10*001

22*001 1*032 10*001

22*001 1*040 10*001

22*001 1*040 10*001

22*001 1*027 10*001

22*001 1*025 10*001

22*014 1*024 10*014

22*015 1*024 10*015

22*016 1*024 10*016

22*017 1*024 10*017

22*018 1*024 10*018

22*019 1*023 10*019

22*019 1*023 10*019

22*020 1*023 10*020

(Line 7.3)

(Line 7.4)

(Line 7.5)

(Line 7.6)

Information Only

22*020 1*023 10*020

#	NAME
1	S_HALITE
2	DRZ_0
3	S_MB139
4	S_ANH_AB
5	S_MB138
6	CAVITY_1
7	CAVITY_2
8	CAVITY_3
9	CAVITY_4
10	IMPERM_Z
11	CASTILER
12	WAS_AREA
13	REPOSIT
14	UNNAMED
15	CULEBRA
16	TAMARISK
17	MAGENTA
18	FORTYNIN
19	DEWYLAKE
20	SANTAROS
21	BACKFILL
22	EXP_AREA
23	EARTH
24	CLAY
25	ASPHALT
26	CONC_T1
27	CONC_T2
28	CL_M_T1
29	CL_M_T2
30	CL_M_T3
31	CL_M_T4
32	CL_M_T5
33	CL_L_T1
34	CL_L_T2
35	CL_L_T3
36	SALT_T1
37	SALT_T2
38	SALT_T3
39	SALT_T4

(Line 7.7)

Information Only

40	SALT_T5				
41	CLAY_BOT				
42	PAN_S_1				
NWST					
2					(Line 7.10)
MAT_WASTE1		MAT_WASTE			(Line 7.11)
6	7				(Line 7.12)
12	13				
NDRZ					
0					(Line 7.13)
NMATRESET					
4					(Line 7.14)
MATRESET					
6	7	8	9		(Line 7.17)
BORE HOLE MATERIAL NUMBER					
0					(Line 7.18)
RESET TIME,		ICWASTE			(Line 7.19)
0.0000E+00	1				(Line 7.20)
POWASTEIC					
1.013250E+05					(Line 7.21)
1.013250E+05					(Line 7.22)
SOWASTEIC					
0.000000E+00					(Line 7.23)
0.000000E+00					(Line 7.24)
PRESDRZ					
					(Line 7.25)
					(Line 7.26)
NBORERESET					
1					(Line 7.27)
NBORETIME, NMATBORE, MATBORE (NMATBORE)					
4	2	12	13		(Line 7.28)
PORESET					
1.013250E+05					(Line 7.29)
SORESET					
0.999999E+00					(Line 7.30)
ICHEM					
1					(Line 7.31)
#	LAMBDA	SOR	SGR		(Line 7.32)
1	7.000000E-01	3.000000E-01	2.000000E-01		(Line 7.33)
2	7.000000E-01	0.000000E+00	0.000000E+00		(Line 7.34)
3	7.000000E-01	2.000000E-01	1.650000E-01		(Line 7.35)
4	7.000000E-01	2.000000E-01	1.650000E-01		(Line 7.36)

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5 7.000000E-01 2.000000E-01 1.650000E-01
6 7.000000E-01 0.000000E+00 0.000000E+00
7 7.000000E-01 0.000000E+00 0.000000E+00
8 7.000000E-01 0.000000E+00 0.000000E+00
9 7.000000E-01 0.000000E+00 0.000000E+00
10 1.000000E+00 0.000000E+00 0.000000E+00
11 7.000000E-01 2.000000E-01 2.000000E-01
12 7.000000E-01 2.000000E-01 2.000000E-01
13 7.000000E-01 2.000000E-01 2.000000E-01
14 7.000000E-01 2.000000E-01 2.000000E-01
15 7.000000E-01 2.000000E-01 2.000000E-01
16 7.000000E-01 2.000000E-01 2.000000E-01
17 7.000000E-01 2.000000E-01 2.000000E-01
18 7.000000E-01 2.000000E-01 2.000000E-01
19 7.000000E-01 2.000000E-01 2.000000E-01
20 7.000000E-01 2.000000E-01 2.000000E-01
21 7.000000E-01 0.000000E+00 0.000000E+00
22 7.000000E-01 0.000000E+00 0.000000E+00
23 1.700000E+00 2.210000E-01 2.000000E-01
24 1.900000E-01 2.240000E-02 2.240000E-02
25 7.000000E-01 0.000000E+00 0.000000E+00
26 7.000000E-01 2.000000E-01 2.000000E-01
27 7.000000E-01 2.000000E-01 2.000000E-01
28 1.900000E-01 2.240000E-02 2.240000E-02
29 1.900000E-01 2.240000E-02 2.240000E-02
30 1.900000E-01 2.240000E-02 2.240000E-02
31 1.900000E-01 2.240000E-02 2.240000E-02
32 1.900000E-01 2.240000E-02 2.240000E-02
33 1.900000E-01 2.240000E-02 2.240000E-02
34 1.900000E-01 2.240000E-02 2.240000E-02
35 1.900000E-01 2.240000E-02 2.240000E-02
36 7.000000E-01 2.000000E-01 2.000000E-01
37 7.000000E-01 2.000000E-01 2.000000E-01
38 7.000000E-01 2.000000E-01 2.000000E-01
39 7.000000E-01 2.000000E-01 2.000000E-01
40 7.000000E-01 2.000000E-01 2.000000E-01
41 1.900000E-01 2.240000E-02 2.240000E-02
42 7.000000E-01 2.000000E-01 2.000000E-01

#	SBMIN	PBMIN	PCMAX	PCT_A	PCT_EXP	KRP	KPC	KTP
1	3.150000E-01	1.013250E+05	1.000000E+08	9.000000E+06	0.000000E+00	4	2	0
2	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0

(Line 7.43)

(Line 7.44)

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3	2.100000E-01	1.013250E+05	1.000000E+08	2.630268E-02	-3.460000E-01	4	2	0
4	2.100000E-01	1.013250E+05	1.000000E+08	2.630268E-02	-3.460000E-01	4	2	0
5	2.100000E-01	1.013250E+05	1.000000E+08	2.630268E-02	-3.460000E-01	4	2	0
6	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
7	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
8	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
9	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
10	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
11	2.100000E-01	1.013250E+05	1.000000E+08	5.600000E-01	-3.460000E-01	4	2	0
12	2.100000E-01	1.013250E+05	1.000000E+08	5.600000E-01	-3.460000E-01	4	4	0
13	2.100000E-01	1.013250E+05	1.000000E+08	5.600000E-01	-3.460000E-01	4	4	0
14	2.100000E-01	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
15	2.100000E-01	1.013250E+05	1.000000E+08	5.600000E-01	-3.460000E-01	4	2	0
16	2.100000E-01	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
17	2.100000E-01	1.013250E+05	1.000000E+08	5.600000E-01	-3.460000E-01	4	2	0
18	2.100000E-01	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
19	2.100000E-01	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
20	2.100000E-01	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
21	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
22	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
23	2.320500E-01	1.013250E+05	1.000000E+08	1.422000E+04	0.000000E+00	4	2	0
24	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
25	0.000000E+00	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0
26	2.100000E-01	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
27	2.100000E-01	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
28	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
29	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
30	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
31	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
32	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
33	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
34	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
35	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
36	2.100000E-01	1.013250E+05	1.000000E+08	3.900000E+04	0.000000E+00	4	2	0
37	2.100000E-01	1.013250E+05	1.000000E+08	2.180000E+05	0.000000E+00	4	2	0
38	2.100000E-01	1.013250E+05	1.000000E+08	9.470000E+05	0.000000E+00	4	2	0
39	2.100000E-01	1.013250E+05	1.000000E+08	4.700000E+06	0.000000E+00	4	2	0
40	2.100000E-01	1.013250E+05	1.000000E+08	4.700000E+06	0.000000E+00	4	2	0
41	2.352000E-02	1.013250E+05	1.000000E+08	1.500000E+06	0.000000E+00	4	2	0
42	2.100000E-01	1.013250E+05	1.000000E+08	0.000000E+00	0.000000E+00	4	1	0

PERMX PERMY PERMZ POROSITY COMPRES

(Line 7.45)

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1	1.000000E-21	1.000000E-21	1.000000E-21	1.000000E-02	8.054475E-09
2	1.000000E-15	1.000000E-15	1.000000E-15	1.000000E-02	8.279475E-08
3	2.511884E-19	2.511884E-19	2.511884E-19	1.900000E-02	4.120777E-09
4	2.511884E-19	2.511884E-19	2.511884E-19	1.900000E-02	4.120777E-09
5	2.511884E-19	2.511884E-19	2.511884E-19	1.900000E-02	4.120777E-09
6	1.000000E-10	1.000000E-10	1.000000E-10	1.000000E+00	0.000000E+00
7	1.000000E-10	1.000000E-10	1.000000E-10	1.000000E+00	0.000000E+00
8	1.000000E-10	1.000000E-10	1.000000E-10	1.000000E+00	0.000000E+00
9	1.000000E-10	1.000000E-10	1.000000E-10	1.000000E+00	0.000000E+00
10	1.000000E-35	1.000000E-35	1.000000E-35	5.000000E-03	0.000000E+00
11	1.330453E-11	1.330453E-11	1.330453E-11	5.200000E-03	1.923077E-07
12	5.584699E-12	5.584699E-12	5.584699E-12	8.810350E-01	1.203130E-09
13	5.584699E-12	5.584699E-12	5.584699E-12	8.810350E-01	1.203130E-09
14	1.000000E-35	1.000000E-35	1.000000E-35	2.000000E-01	0.000000E+00
15	2.648502E-13	2.648502E-13	2.648502E-13	1.460000E-01	1.417160E-09
16	1.000000E-35	1.000000E-35	1.000000E-35	2.000000E-01	0.000000E+00
17	1.096478E-16	1.096478E-16	1.096478E-16	9.000000E-02	2.199962E-09
18	1.000000E-35	1.000000E-35	1.000000E-35	2.000000E-01	0.000000E+00
19	9.332549E-16	9.332549E-16	9.332549E-16	1.500000E-01	6.666667E-08
20	1.000000E-10	1.000000E-10	1.000000E-10	1.750000E-01	5.714286E-08
21	1.000000E-11	1.000000E-11	1.000000E-11	1.000000E+00	0.000000E+00
22	1.000000E-11	1.000000E-11	1.000000E-11	1.000000E+00	0.000000E+00
23	1.000000E-14	1.000000E-14	1.000000E-14	2.500000E-01	0.000000E+00
24	9.999999E-19	9.999999E-19	9.999999E-19	2.500000E-01	0.000000E+00
25	3.311315E-17	3.311315E-17	3.311315E-17	1.000000E-02	0.000000E+00
26	5.000338E-19	5.000338E-19	5.000338E-19	7.500000E-02	0.000000E+00
27	1.000000E-14	1.000000E-14	1.000000E-14	7.500000E-02	0.000000E+00
28	3.837069E-17	3.837069E-17	3.837069E-17	7.500000E-02	0.000000E+00
29	2.529297E-17	2.529297E-17	2.529297E-17	7.500000E-02	0.000000E+00
30	1.581246E-17	1.581246E-17	1.581246E-17	7.500000E-02	0.000000E+00
31	6.531313E-18	6.531313E-18	6.531313E-18	7.500000E-02	0.000000E+00
32	9.999999E-19	9.999999E-19	9.999999E-19	7.500000E-02	0.000000E+00
33	4.677352E-17	4.677352E-17	4.677352E-17	7.500000E-02	0.000000E+00
34	9.078209E-18	9.078209E-18	9.078209E-18	7.500000E-02	0.000000E+00
35	9.999999E-19	9.999999E-19	9.999999E-19	7.500000E-02	0.000000E+00
36	1.000000E-14	1.000000E-14	1.000000E-14	4.000000E-02	0.000000E+00
37	6.998409E-17	6.998409E-17	6.998409E-17	4.000000E-02	0.000000E+00
38	9.999999E-19	9.999999E-19	9.999999E-19	4.000000E-02	0.000000E+00
39	3.303688E-21	3.303688E-21	3.303688E-21	4.000000E-02	0.000000E+00
40	1.000000E-21	1.000000E-21	1.000000E-21	4.000000E-02	0.000000E+00
41	9.999999E-19	9.999999E-19	9.999999E-19	7.500000E-02	0.000000E+00

(Line 7.46)

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42 1.000000E-12 1.000000E-12 1.000000E-12 7.500000E-02 1.333333E-08
TOL AND SOCEFFMIN FOR PERMEABILITY MODELS 11 & 12 (Line 7.47)
1.000000E-02 1.000000E-03 (Line 7.48)
NMATSP, FOR SMOOTH PERMEABILITY TRANSITION MODEL (Line 7.49)
1 (Line 7.50)
MATSP, MATSPF, TEND, TCHANGE (Line 7.51)
2 1 6.3114E+09 6.3114E+09 (Line 7.52)
NSMPRMC, SMPRMC (Line 7.53)
6 0.000000E+00 1.000000E+00 0.000000E+00 0.000000E+00 0.000000E+01 0.000000E+00 (Line 7.54)
FRACTURE MODEL DATA TO FOLLOW :T OR F (Line 7.55)
T (Line 7.56)
NFRAC (Line 7.57)
3 (Line 7.58)
DELTA_PI DELTA_PF FRAC_PHI FRAC_EXP IFRX IFRY IFRZ LFPC (Line 7.59)
3 1.800000E+06 2.500000E+06 2.900000E-02 5.320828E+01 1 1 0 F (Line 7.60)
4 1.800000E+06 2.500000E+06 2.900000E-02 5.320828E+01 1 1 0 F
5 1.800000E+06 2.500000E+06 2.900000E-02 5.320828E+01 1 1 0 F
KLINKENBERG EFFECT TO BE USED? True or False (Line 7.61)
T (Line 7.62)
BKLINK EXPKLINK
9.80000E-01 -3.30000E-01
GRAVITY CONSTANT (GSTD) AND GAS CONSTANT R (Line 8.0)
9.79D+00 8.314510D+00 (Line 8.1)
REFERENCE TEMPERATURE AND PRESSURE FOR DENSITY CALCULATIONS (Line 8.2)
3.00150E+02 1.01325E+05 (Line 8.3)
SALT(WT.%) DEN_BR KGSAT IDGAS COMPR_BR WMSALT WMH2O (Line 8.4)
2.9600E+01 1.2300E+03 1 0 2.5000E-10 58.442468D-03 18.01528D-03 (Line 8.5)
VISC_BR VISC_GAS (Line 8.6)
1.80000E-03 8.92000E-06 (Line 8.6)
GAS DENSITY DATA: =0 OR -2 COMPUTE USING RKS OR IDEAL GAS; =1 OR -1 INTERPOLATE (Line 8.8)
1 (Line 8.9)
GAS MOLE FRACTIONS FOR H2, CO2, CH4, N2, H2S, AND O2 (Line 8.10)
1.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 (Line 8.11)
GAS MOLE CULAR WIEGHTS FOR H2, CO2, CH4, N2, H2S, AND O2 (Line 8.12)
2.01588D-03 44.0098D-03 16.04276D-03 28.01348D-03 34.08188D-03 31.9988D-03 (Line 8.13)
NUMBER OF GAS COMPONENTS ACTUALL USED (NGAS) AND COMPONET NUMBER (N1GAS) (Line 8.16)
1 1 (Line 8.17)
RKS SPECIFIED: TC FOR H2, CO2, CH4, N2, H2S, AND O2 (Line 8.18)
43.60D+00 304.15D+00 190.63D+00 126.15D+00 373.55D+00 154.77D+00 (Line 8.19)
RKS SPECIFIED: PC FOR H2, CO2, CH4, N2, H2S, AND O2 (Line 8.20)
20.47D+05 73.76D+05 46.17D+05 33.94D+05 90.07D+05 50.80D+05 (Line 8.21)

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RKS SPECIFIED: ACEN FOR H2, CO2, CH4, N2, H2S, AND O2 (Line 8.22)
0.00D+00 0.231D+00 0.010D+00 0.045D+00 0.100D+00 0.019D+00 (Line 8.23)
RKS SPECIFIED: SPECIAL PROPERTIES FOR H2- TCH2, PCH2, WMH2 (Line 8.24)
43.6D+00 20.47D+05 2.01588D-03 (Line 8.25)
RKS SPECIFIED: CONSTANTS OMEGAA AND OMEGAB (Line 8.26)
0.42747D+00 0.08664D+00 (Line 8.27)
RKS SPECIFIED: BINARY INTERACTION PARAMETERS, AKIJ(1-MGAS, 1-MGAS) (Line 8.28)
BINARY INTERACTION PARAMETERS FOR H2 (Line 8.29.1)
+0.0000D+00 -0.3426D+00 -0.0222D+00 +0.0978D+00 0.0000D+00 +0.0000D+00 (Line 8.29.2)
BINARY INTERACTION PARAMETERS FOR CO2 (Line 8.29.3)
-0.3426D+00 +0.0000D+00 +0.0933D+00 -0.0315D+00 +0.0989D+00 +0.0000D+00 (Line 8.29.4)
BINARY INTERACTION PARAMETERS FOR CH4 (Line 8.29.5)
-0.0222D+00 +0.0933D+00 +0.0000D+00 +0.0278D+00 +0.0850D+00 +0.0000D+00 (Line 8.29.6)
BINARY INTERACTION PARAMETERS FOR N2 (Line 8.29.7)
+0.0978D+00 -0.0315D+00 +0.0278D+00 +0.0000D+00 +0.1696D+00 -0.0078D+00 (Line 8.29.8)
BINARY INTERACTION PARAMETERS FOR H2S (Line 8.29.9)
+0.0000D+00 +0.0989D+00 +0.0850D+00 +0.1696D+00 +0.0000D+00 +0.0000D+00 (Line 8.29.10)
BINARY INTERACTION PARAMETERS FOR O2 (Line 8.29.11)
+0.0000D+00 +0.0000D+00 +0.0000D+00 -0.0078D+00 +0.000D+00 +0.0000D+00 (Line 8.29.12)
IGASVAR (2= REACTION PATH, 1= USING AVG. STOICH. , 0= USING WELLS) (Line 9.1)
1 (Line 9.2)
RATE CONSTANTS: CORROSION (RKCOR) AND BIODEGRADATION (RKBIO) (Line 9.3)
3.0437E-08 2.6642E-07 (Line 9.4)
HUMIDITY FACTORS: HUMFAC_COR, HUMFAC_BIO (Line 9.5)
0.0000E+00 1.0000E-01 (Line 9.6)
RATE CONSTANTS: BRUCITEI, BRUCITEH and HYMAGCON (Line 9.7)
7.2000E-06 7.2000E-06 3.8000E-11 (Line 9.8)
RATE COEFFICIENTS FOR EACH WASTE AREA: GAS AND CO2 (Line 9.9)
4.8575E-01 1.0000E+00 (Line 9.10)
4.8575E-01 1.0000E+00
CHEMISTRY CUTOFF SATURATION: SOCMIN (Line 9.11)
0.0150E+00 (Line 9.12)
REACTANT/PRODUCT MOLECULAR WEIGHTS (H2, H2O, FE, [C6-H10-O5])/6 (Line 9.13)
2.01588D-03 18.01528D-03 55.847D-03 27.023D-03 (Line 9.14)
REACTANT/PRODUCT MOLECULAR WEIGHTS (Fe(OH)2, FeS, MgO, Mg(OH)2, Hydro, MgCO3) (Line 9.15)
8.98617E-02 8.79000E-02 4.03044E-02 5.83196E-02 4.64740E-01 8.43142E-02 (Line 9.16)
S_H2, S_H2O, S_Fe, S_Bio, S_FeOH2, S_FeS, S_MgO, S_MgOH2, S_Hydro, S_MgCO3 (Line 9.17)
1.0E+00 -2.0E+00 -1.0E+00 0.0E+00 1.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 (Line 9.18)
0.0E+00 8.3E-01 0.0E+00 -1.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00
-1.0E+00 2.0E+00 0.0E+00 0.0E+00 -1.0E+00 1.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00
0.0E+00 0.0E+00 -1.0E+00 0.0E+00 0.0E+00 1.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00

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0.0E+00 -1.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 -1.0E+00 1.0E+00 0.0E+00 0.0E+00	
0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 -1.25E+00 0.25E+00 0.0E+00	
0.0E+00 4.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 1.0E+00 -1.0E+00 4.0E+00	
REACTANT/PRODUCT DENSITIES (Fe, Fe(OH)2, FeS, Bio)	(Line 9.19)
7.8700E+03 3.40000E+03 4.70000E+03 1.10000E+03	(Line 9.20)
REACTANT/PRODUCT DENSITIES (MgO, Mg(OH)2, Hydro, MgCO3, SALT)	(Line 9.21)
3.6000E+03 2.37000E+03 2.18000E+03 3.05000E+03 2.17000E+03	(Line 9.22)
WICKING SATURATION, HUMID RATE SMOOTHING ALPHARXN	(Line 9.23)
5.0000E-01 T 1.0000E+03	(Line 9.24)
CREEP CLOSURE? IF TRUE THEN AN EXTERNAL FILE OF CLOSURE DATA IS ALSO EXPECTED	(Line 10.1)
T	(Line 10.2)
NKLOS, KLOSINT (0=MOLES,1=PRESSURE) KLOSAVE (1=REGION AVE,2=CELL)	(Line 10.3)
1 1 2	(Line 10.4)
CLOSURE PARAMETERS: PRES_LITHO, TIME_OFF MODPERM(I), LSOLPROD(I)	(Line 10.5)
4 5.0000E+07 3.1557E+12 2 F T	(Line 10.6)
MODPERM PARAMETERS	(Line 10.7)
1.5000E-01 1.0000E-02	(Line 10.8)
NUMBER OF MATERIAL REGIONS FOR CLOSURE	(Line 10.9)
2	(Line
10.10)	
# MAT NO.MODEL 1= WASTE-NOBCKFIL, 2=DRIFT-NOBCKFIL, 3=WASTE-BCKFIL 4=JAN_96:WASTE-NOBCKFIL	(Line
10.11)	
1 12 4	(Line
10.12)	
2 13 4	
WILL RADIONUCLIDE DECAY BE CALCULATED? T or F	(Line 11.1)
F	(Line 11.2)
WILL TRANSPORT BE CALCULATED? T or F	(Line 11.3)
F	(Line 11.4)
WILL RADIOLYSIS BE CALCULATED? T or F	(Line 11.5)
F	(Line 11.6)
BRAGFLO GAS COMPONENT TRANSPORT MODEL	(Line 12.1)
F	(Line 12.2)

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11.2 Appendix B: Sample BRAGFLO Closure Look-Up Table Data Input File

Below is listed the closure file BF2_CRA1BC_CLOSURE.DAT which was used in the 1996 CCA, the 1997 PAVT PA, the CRA-2004 PA, and the CRA-2004 PABC. This file is located in the Code Management System library: LIBCRA1BC_BF.

```
PHIMIN_BRAG(1:MKLOS); MKLOS=4 (Line 1.0)
    4.626436E-02, 2.272370E-02, 9.461577E-02, 4.659957E-02 (Line 2.0)
PHIMAX_BRAG(1:MKLOS); MKLOS=4 (Line 3.0)
    4*1.0D0 (Line 4.0)
TIME_DATA_MAX(1:MKLOS); MKLOS=4 (Line 5.0)
    4*3.787160E+11 (Line 6.0)
F FACTOR DATA, FDATA (1:MKLOS,1:NSDATA); MKLOS=4, NSDATA=13. (Line 7.0)
FDATA(I,1),I=1,13, ALL 13 ARE USED. (Line 8.0)
    0.D0,      0.025D0,    0.05D0,      0.1D0,      0.2D0,
    0.4D0,      0.5D0,      0.6D0,      0.8D0,      1.0D0,
    1.2D0,      1.6D0,      2.0D0
FDATA(I,2),I=1,13, ONLY FIRST 7 ARE USED.
    0.D0,      0.01D0,    0.1D0,      0.2D0,      0.4D0,
    0.6D0,      1.0D0      6*0.0D0
FDATA(I,3),I=1,5, ONLY FIRST 5 ARE USED.
    0.D0,      0.2D0,      0.4D0,      0.6D0,      1.0D0
    8*0.0D0
FDATA(I,4),I=1,13, ALL 13 ARE USED.
    0.D0,      0.025D    0.05D0,      0.1D0,      0.2D0,
    0.4D0,      0.5D0,      0.6D0,      0.8D0,      1.0D0,
    1.2D0,      1.6D0,      2.0D0
Time data, TDATA (1:NTDATA); NTDATA=214 (Line 10.0)
TDATA(1:214) (Line 11.0)
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0.000000E+00,1.579360E+07,3.158860E+07,1.895220E+08,3.474430E+08,
5.053850E+08,6.633280E+08,8.212710E+08,9.792140E+08,1.137120E+09,
1.295070E+09,1.453010E+09,1.610950E+09,1.768860E+09,1.926810E+09,
2.084750E+09,2.242690E+09,2.400600E+09,2.558550E+09,2.716490E+09,
2.874430E+09,3.032340E+09,3.190410E+09,3.506300E+09,3.822180E+09,
4.137750E+09,4.453640E+09,4.769520E+09,5.085410E+09,5.401300E+09,
5.717180E+09,6.033070E+09,6.348950E+09,6.664840E+09,6.980720E+09,
7.296610E+09,7.612490E+09,7.928380E+09,8.244270E+09,8.560150E+09,
8.876040E+09,9.191920E+09,9.507810E+09,9.823690E+09,1.013960E+10,
1.045550E+10,1.077100E+10,1.108690E+10,1.140280E+10,1.171870E+10,
1.203460E+10,1.235050E+10,1.266630E+10,1.298220E+10,1.329810E+10,
1.361400E+10,1.392990E+10,1.424580E+10,1.456170E+10,1.487750E+10,
1.519340E+10,1.550930E+10,1.582520E+10,1.614110E+10,1.645700E+10,
1.677290E+10,1.708870E+10,1.740430E+10,1.772020E+10,1.803610E+10,
1.835200E+10,1.866790E+10,1.898370E+10,1.929960E+10,1.961550E+10,
1.993140E+10,2.024730E+10,2.056320E+10,2.087910E+10,2.119490E+10,
2.151080E+10,2.182670E+10,2.214260E+10,2.245850E+10,2.277440E+10,
2.309030E+10,2.340610E+10,2.372200E+10,2.403760E+10,2.435350E+10,
2.466940E+10,2.498530E+10,2.530110E+10,2.561700E+10,2.593290E+10,
2.624880E+10,2.656470E+10,2.688060E+10,2.719650E+10,2.751230E+10,
2.782820E+10,2.814410E+10,2.846000E+10,2.877590E+10,2.909180E+10,
2.940770E+10,2.972350E+10,3.003940E+10,3.035530E+10,3.067120E+10,
3.098680E+10,3.130260E+10,3.162010E+10,3.193570E+10,3.225130E+10,
3.256680E+10,3.288240E+10,3.319800E+10,3.351350E+10,3.382910E+10,
3.414470E+10,3.446020E+10,3.477580E+10,3.509450E+10,3.541010E+10,
3.572570E+10,3.604120E+10,3.635680E+10,3.667240E+10,3.698800E+10,
3.730350E+10,3.761910E+10,3.793470E+10,3.825340E+10,3.856900E+10,
3.888450E+10,3.920010E+10,3.951570E+10,3.983120E+10,4.014680E+10,
4.046240E+10,4.077800E+10,4.109350E+10,4.140910E+10,4.172780E+10,
4.204340E+10,4.235900E+10,4.267450E+10,4.299010E+10,4.330570E+10,
4.362120E+10,4.393680E+10,4.425240E+10,4.456800E+10,4.488670E+10,
4.520220E+10,4.551780E+10,4.583340E+10,4.614900E+10,4.646450E+10,
4.678010E+10,4.709570E+10,4.741120E+10,4.772680E+10,4.804240E+10,
4.836110E+10,4.867670E+10,4.899220E+10,4.930780E+10,4.962340E+10,
4.993900E+10,5.025450E+10,5.057010E+10,5.088570E+10,5.120120E+10,
5.152000E+10,5.183550E+10,5.215110E+10,5.246670E+10,5.278220E+10,
5.309780E+10,5.341340E+10,5.372890E+10,5.404450E+10,5.436010E+10,
5.467570E+10,5.499440E+10,5.531000E+10,5.562550E+10,5.594110E+10,
5.625670E+10,5.657220E+10,5.688780E+10,5.720340E+10,5.751890E+10,
5.783450E+10,5.815320E+10,5.846880E+10,5.878440E+10,5.910000E+10,
5.941550E+10,5.973110E+10,6.004670E+10,6.036220E+10,6.067780E+10,

(Line 12.0)

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6.099340E+10,6.130890E+10,6.162770E+10,6.194320E+10,6.225880E+10,  
6.257440E+10,6.288990E+10,3.155600E+11,3.787160E+11  
POROSITY SURFACE #1, FOR WASTE w/o BACKFILL. FIRST USED IN SPM2 IN JANUARY 1995. (Line 13.0)  
PDATA(1:NSDATA,1:NTDATA,1:MKLOS); NSDATA=13, NTDATA=214, MKLOS=4 (Line 14.0)  
FOR POROSITY SURFACE 1 ALL NSDATA=13 GAS GENERATION RATES ARE USED. (Line 15.0)  
POROSITY SURFACE #1; GAS GENERATION RATE #1. (Line 16.0)  
PDATA(NSDATA =1,NTDATA=1:214,MKLOS =1) (Line 17.0)  
214*1.013250E+05 (Line 18.0)  
POROSITY SURFACE #1; GAS GENERATION RATE #1. (Line 19.0)  
SDATA(NSDATA =1,NTDATA=1:214,MKLOS =1) (Line 20.0)  
8.810350E-01,7.909613E-01,7.699415E-01,6.453196E-01,5.579810E-01, (Line 21.0)  
4.866897E-01,4.265381E-01,3.755593E-01,3.309335E-01,2.913361E-01,  
2.595732E-01,2.358209E-01,2.162501E-01,1.994990E-01,1.851858E-01,  
1.726563E-01,1.614584E-01,1.514950E-01,1.425229E-01,1.345649E-01,  
1.276992E-01,1.216721E-01,1.163047E-01,1.076678E-01,1.009734E-01,  
9.551831E-02,9.107586E-02,8.735865E-02,8.417166E-02,8.149481E-02,  
7.912877E-02,7.704604E-02,7.525639E-02,7.366161E-02,7.223621E-02,  
7.089778E-02,6.966358E-02,6.857235E-02,6.754140E-02,6.661480E-02,  
6.575147E-02,6.496387E-02,6.422624E-02,6.357566E-02,6.294840E-02,  
6.236779E-02,6.185073E-02,6.137885E-02,6.094715E-02,6.055912E-02,  
6.018355E-02,5.985228E-02,5.954783E-02,5.926633E-02,5.900282E-02,  
5.876056E-02,5.853290E-02,5.832731E-02,5.813213E-02,5.795657E-02,  
5.778482E-02,5.762698E-02,5.747973E-02,5.734067E-02,5.721126E-02,  
5.708883E-02,5.697286E-02,5.686177E-02,5.675687E-02,5.665609E-02,  
5.656113E-02,5.647026E-02,5.638501E-02,5.630387E-02,5.622649E-02,  
5.615193E-02,5.608442E-02,5.601713E-02,5.595489E-02,5.589122E-02,  
5.583263E-02,5.576873E-02,5.571390E-02,5.564831E-02,5.558945E-02,  
5.552706E-02,5.545690E-02,5.540540E-02,5.535025E-02,5.527718E-02,  
5.521085E-02,5.515222E-02,5.511455E-02,5.506625E-02,5.502141E-02,  
5.498708E-02,5.492466E-02,5.487102E-02,5.482500E-02,5.477400E-02,  
5.472510E-02,5.468725E-02,5.463648E-02,5.459473E-02,5.455007E-02,  
5.451035E-02,5.446816E-02,5.442653E-02,5.438810E-02,5.434694E-02,  
5.430385E-02,5.426159E-02,5.422026E-02,5.417703E-02,5.413686E-02,  
5.409108E-02,5.405105E-02,5.401858E-02,5.398791E-02,5.394840E-02,  
5.391139E-02,5.387466E-02,5.383576E-02,5.380633E-02,5.377182E-02,  
5.373050E-02,5.368623E-02,5.364412E-02,5.361052E-02,5.357119E-02,  
5.353217E-02,5.350279E-02,5.347263E-02,5.343913E-02,5.340780E-02,  
5.337415E-02,5.334398E-02,5.331050E-02,5.327755E-02,5.324477E-02,  
5.321542E-02,5.318796E-02,5.315666E-02,5.311928E-02,5.308886E-02,  
5.305849E-02,5.302211E-02,5.299333E-02,5.296538E-02,5.293484E-02,  
5.290299E-02,5.287226E-02,5.283883E-02,5.280245E-02,5.276829E-02,
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5.274186E-02, 5.271408E-02, 5.268065E-02, 5.265105E-02, 5.262190E-02,
5.258839E-02, 5.256448E-02, 5.253892E-02, 5.251020E-02, 5.248101E-02,
5.245431E-02, 5.242561E-02, 5.239886E-02, 5.236899E-02, 5.234378E-02,
5.231841E-02, 5.228456E-02, 5.225512E-02, 5.222511E-02, 5.220105E-02,
5.217583E-02, 5.214536E-02, 5.211682E-02, 5.209041E-02, 5.206093E-02,
5.203069E-02, 5.200773E-02, 5.198026E-02, 5.195722E-02, 5.193010E-02,
5.190480E-02, 5.187608E-02, 5.185134E-02, 5.182656E-02, 5.180279E-02,
5.178026E-02, 5.175327E-02, 5.172765E-02, 5.170392E-02, 5.168111E-02,
5.165425E-02, 5.162997E-02, 5.160804E-02, 5.157814E-02, 5.155257E-02,
5.152908E-02, 5.150847E-02, 5.148877E-02, 5.146525E-02, 5.144211E-02,
5.142215E-02, 5.139977E-02, 5.137468E-02, 5.135003E-02, 5.132905E-02,
5.130884E-02, 5.128795E-02, 4.626436E-02, 4.626436E-02

POROSITY SURFACE #1; GAS GENERATION RATE #2.

PDATA (NSDATA =2, NTDATA=1:214, MKLOS =1)

1.013250E+05, 1.015174E+05, 1.017112E+05, 1.036490E+05, 1.064923E+05,
1.100090E+05, 1.135256E+05, 1.179715E+05, 1.247003E+05, 1.314275E+05,
1.381696E+05, 1.476690E+05, 1.571683E+05, 1.666659E+05, 1.782637E+05,
1.906761E+05, 2.030886E+05, 2.168228E+05, 2.322767E+05, 2.477296E+05,
2.634673E+05, 2.808018E+05, 2.981539E+05, 3.335535E+05, 3.698959E+05,
4.072442E+05, 4.450862E+05, 4.839659E+05, 5.228656E+05, 5.617838E+05,
6.007690E+05, 6.398436E+05, 6.791887E+05, 7.186298E+05, 7.581384E+05,
7.976508E+05, 8.371044E+05, 8.764213E+05, 9.157769E+05, 9.551494E+05,
9.943030E+05, 1.033261E+06, 1.071886E+06, 1.110250E+06, 1.148454E+06,
1.185933E+06, 1.223204E+06, 1.260318E+06, 1.296839E+06, 1.333140E+06,
1.369057E+06, 1.404777E+06, 1.440299E+06, 1.475451E+06, 1.510445E+06,
1.545102E+06, 1.579591E+06, 1.613964E+06, 1.648173E+06, 1.682346E+06,
1.716495E+06, 1.750632E+06, 1.784764E+06, 1.818929E+06, 1.853087E+06,
1.887235E+06, 1.920918E+06, 1.952935E+06, 1.970266E+06, 1.987613E+06,
2.004982E+06, 2.022333E+06, 2.039685E+06, 2.057096E+06, 2.074492E+06,
2.091876E+06, 2.109277E+06, 2.126672E+06, 2.144045E+06, 2.161443E+06,
2.178865E+06, 2.196263E+06, 2.213666E+06, 2.231083E+06, 2.248457E+06,
2.265810E+06, 2.283175E+06, 2.300541E+06, 2.317880E+06, 2.335213E+06,
2.352537E+06, 2.369852E+06, 2.387167E+06, 2.404495E+06, 2.421820E+06,
2.439141E+06, 2.456440E+06, 2.473736E+06, 2.491031E+06, 2.508323E+06,
2.525617E+06, 2.542902E+06, 2.560191E+06, 2.577483E+06, 2.594765E+06,
2.612046E+06, 2.629320E+06, 2.646590E+06, 2.663855E+06, 2.681118E+06,
2.698367E+06, 2.715630E+06, 2.732967E+06, 2.750192E+06, 2.767404E+06,
2.784611E+06, 2.801823E+06, 2.810361E+06, 2.815902E+06, 2.816229E+06,
2.816547E+06, 2.816859E+06, 2.817173E+06, 2.817488E+06, 2.817794E+06,
2.818091E+06, 2.818382E+06, 2.818672E+06, 2.818964E+06, 2.819261E+06,
2.819556E+06, 2.819851E+06, 2.820150E+06, 2.820455E+06, 2.820760E+06,

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2.821060E+06,2.821361E+06,2.821668E+06,2.821971E+06,2.822269E+06,
2.822575E+06,2.822882E+06,2.823179E+06,2.823474E+06,2.823769E+06,
2.824067E+06,2.824365E+06,2.824666E+06,2.824965E+06,2.825262E+06,
2.825574E+06,2.825882E+06,2.826182E+06,2.826484E+06,2.826789E+06,
2.827082E+06,2.827373E+06,2.827660E+06,2.827947E+06,2.828233E+06,
2.828520E+06,2.828806E+06,2.829091E+06,2.829372E+06,2.829654E+06,
2.829948E+06,2.830293E+06,2.830680E+06,2.831081E+06,2.831494E+06,
2.831935E+06,2.832365E+06,2.832789E+06,2.833203E+06,2.833603E+06,
2.833980E+06,2.834368E+06,2.834761E+06,2.835108E+06,2.835455E+06,
2.835804E+06,2.836185E+06,2.836572E+06,2.836941E+06,2.837298E+06,
2.837641E+06,2.837968E+06,2.838304E+06,2.838699E+06,2.839080E+06,
2.839450E+06,2.839788E+06,2.840119E+06,2.840440E+06,2.840766E+06,
2.841095E+06,2.841423E+06,2.841761E+06,2.842122E+06,2.842484E+06,
2.842843E+06,2.843162E+06,2.843481E+06,2.843798E+06,2.844090E+06,
2.844375E+06,2.844661E+06,2.844939E+06,2.845205E+06,2.845476E+06,
2.845744E+06,2.845997E+06,2.910266E+06,2.910266E+06

POROSITY SURFACE #1; GAS GENERATION RATE #2.

SDATA(NSDATA =2,NTDATAB=1:214,MKLOS =1)

8.810350E-01,8.188063E-01,8.046822E-01,6.634560E-01,5.660348E-01,
5.011425E-01,4.362498E-01,3.787115E-01,3.392426E-01,2.997831E-01,
2.604075E-01,2.411708E-01,2.219341E-01,2.027010E-01,1.888255E-01,
1.770353E-01,1.652451E-01,1.550910E-01,1.470522E-01,1.390139E-01,
1.314060E-01,1.262166E-01,1.210220E-01,1.122410E-01,1.055497E-01,
1.004457E-01,9.592828E-02,9.241154E-02,8.937923E-02,8.681977E-02,
8.478336E-02,8.291220E-02,8.133219E-02,7.992029E-02,7.863041E-02,
7.755699E-02,7.655498E-02,7.568885E-02,7.490499E-02,7.416621E-02,
7.354797E-02,7.297393E-02,7.247556E-02,7.203903E-02,7.163397E-02,
7.131842E-02,7.102773E-02,7.076764E-02,7.056212E-02,7.037701E-02,
7.022778E-02,7.009558E-02,6.997947E-02,6.989089E-02,6.981271E-02,
6.975582E-02,6.970902E-02,6.966930E-02,6.963976E-02,6.961204E-02,
6.958710E-02,6.956373E-02,6.954117E-02,6.951880E-02,6.949719E-02,
6.947683E-02,6.945728E-02,6.943809E-02,6.941938E-02,6.940034E-02,
6.938092E-02,6.936266E-02,6.934436E-02,6.932439E-02,6.930528E-02,
6.928696E-02,6.926864E-02,6.925063E-02,6.923358E-02,6.921590E-02,
6.919777E-02,6.918103E-02,6.916425E-02,6.914723E-02,6.913190E-02,
6.911741E-02,6.910275E-02,6.908836E-02,6.907444E-02,6.906157E-02,
6.904914E-02,6.903719E-02,6.902526E-02,6.901332E-02,6.900168E-02,
6.899026E-02,6.897959E-02,6.896912E-02,6.895881E-02,6.894884E-02,
6.893899E-02,6.892941E-02,6.891994E-02,6.891053E-02,6.890166E-02,
6.889281E-02,6.888396E-02,6.887560E-02,6.886749E-02,6.885972E-02,
6.885189E-02,6.884395E-02,6.883665E-02,6.882967E-02,6.882318E-02,

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6.881678E-02, 6.881047E-02, 6.880416E-02, 6.879750E-02, 6.878920E-02,
6.878109E-02, 6.877317E-02, 6.876524E-02, 6.875727E-02, 6.874952E-02,
6.874200E-02, 6.873462E-02, 6.872723E-02, 6.871984E-02, 6.871246E-02,
6.870495E-02, 6.869739E-02, 6.868982E-02, 6.868219E-02, 6.867463E-02,
6.866707E-02, 6.865948E-02, 6.865174E-02, 6.864409E-02, 6.863653E-02,
6.862882E-02, 6.862112E-02, 6.861356E-02, 6.860610E-02, 6.859865E-02,
6.859111E-02, 6.858356E-02, 6.857601E-02, 6.856856E-02, 6.856118E-02,
6.855329E-02, 6.854550E-02, 6.853794E-02, 6.853039E-02, 6.852278E-02,
6.851541E-02, 6.850804E-02, 6.850067E-02, 6.849344E-02, 6.848625E-02,
6.847907E-02, 6.847188E-02, 6.846470E-02, 6.845766E-02, 6.845062E-02,
6.844337E-02, 6.843478E-02, 6.842508E-02, 6.841488E-02, 6.840445E-02,
6.839351E-02, 6.838279E-02, 6.837220E-02, 6.836179E-02, 6.835175E-02,
6.834233E-02, 6.833261E-02, 6.832282E-02, 6.831422E-02, 6.830554E-02,
6.829675E-02, 6.828727E-02, 6.827764E-02, 6.826832E-02, 6.825943E-02,
6.825100E-02, 6.824280E-02, 6.823436E-02, 6.822450E-02, 6.821505E-02,
6.820592E-02, 6.819744E-02, 6.818912E-02, 6.818106E-02, 6.817301E-02,
6.816495E-02, 6.815681E-02, 6.814837E-02, 6.813924E-02, 6.813023E-02,
6.812136E-02, 6.811348E-02, 6.810561E-02, 6.809774E-02, 6.809042E-02,
6.808329E-02, 6.807632E-02, 6.806945E-02, 6.806283E-02, 6.805606E-02,
6.804938E-02, 6.804313E-02, 6.648637E-02, 6.648637E-02

POROSITY SURFACE #1; GAS GENERATION RATE #3.

PDATA(NSDATA =3,NTDATA=1:214,MKLOS =1)

1.013250E+05, 1.016308E+05, 1.019518E+05, 1.056790E+05, 1.106154E+05,
1.168006E+05, 1.243913E+05, 1.336190E+05, 1.448739E+05, 1.586777E+05,
1.744537E+05, 1.913094E+05, 2.097839E+05, 2.300384E+05, 2.517451E+05,
2.750654E+05, 3.002028E+05, 3.268750E+05, 3.555871E+05, 3.856941E+05,
4.168713E+05, 4.485953E+05, 4.814415E+05, 5.485011E+05, 6.159141E+05,
6.848275E+05, 7.550881E+05, 8.263959E+05, 8.977026E+05, 9.687704E+05,
1.038944E+06, 1.109952E+06, 1.179958E+06, 1.250028E+06, 1.320080E+06,
1.389464E+06, 1.458387E+06, 1.527280E+06, 1.595285E+06, 1.663131E+06,
1.729934E+06, 1.796178E+06, 1.861647E+06, 1.926187E+06, 1.989762E+06,
2.052799E+06, 2.115038E+06, 2.176844E+06, 2.238007E+06, 2.299004E+06,
2.359887E+06, 2.420867E+06, 2.481477E+06, 2.542041E+06, 2.602768E+06,
2.663046E+06, 2.723258E+06, 2.783720E+06, 2.844346E+06, 2.904724E+06,
2.965035E+06, 3.025430E+06, 3.085661E+06, 3.145949E+06, 3.206166E+06,
3.266374E+06, 3.326406E+06, 3.380687E+06, 3.412046E+06, 3.442253E+06,
3.472469E+06, 3.502621E+06, 3.532827E+06, 3.562934E+06, 3.593040E+06,
3.623146E+06, 3.653245E+06, 3.683366E+06, 3.713523E+06, 3.743638E+06,
3.773718E+06, 3.803830E+06, 3.833914E+06, 3.864014E+06, 3.894090E+06,
3.924155E+06, 3.954217E+06, 3.984273E+06, 4.014276E+06, 4.044324E+06,
4.074353E+06, 4.104387E+06, 4.134372E+06, 4.164371E+06, 4.194336E+06,

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4.224303E+06,4.254265E+06,4.284215E+06,4.314148E+06,4.344033E+06,
4.373920E+06,4.403811E+06,4.433687E+06,4.463553E+06,4.493412E+06,
4.523267E+06,4.553109E+06,4.582955E+06,4.612797E+06,4.642639E+06,
4.672448E+06,4.702271E+06,4.732250E+06,4.762167E+06,4.792011E+06,
4.821814E+06,4.851607E+06,4.875259E+06,4.875435E+06,4.875480E+06,
4.875531E+06,4.875630E+06,4.875703E+06,4.875824E+06,4.875933E+06,
4.876011E+06,4.876146E+06,4.876262E+06,4.876350E+06,4.876483E+06,
4.876584E+06,4.876708E+06,4.876823E+06,4.876947E+06,4.877063E+06,
4.877194E+06,4.877299E+06,4.877433E+06,4.877549E+06,4.877638E+06,
4.877774E+06,4.877907E+06,4.878008E+06,4.878106E+06,4.878233E+06,
4.878339E+06,4.878472E+06,4.878574E+06,4.878697E+06,4.878813E+06,
4.878926E+06,4.879041E+06,4.879136E+06,4.879225E+06,4.879338E+06,
4.879412E+06,4.879506E+06,4.879576E+06,4.879658E+06,4.879735E+06,
4.879809E+06,4.879879E+06,4.879943E+06,4.880011E+06,4.880070E+06,
4.880129E+06,4.880188E+06,4.880242E+06,4.880302E+06,4.880359E+06,
4.880417E+06,4.880474E+06,4.880529E+06,4.880584E+06,4.880641E+06,
4.880690E+06,4.880741E+06,4.880789E+06,4.880838E+06,4.880887E+06,
4.880933E+06,4.880979E+06,4.881025E+06,4.881070E+06,4.881118E+06,
4.881162E+06,4.881208E+06,4.881251E+06,4.881297E+06,4.881346E+06,
4.881389E+06,4.881433E+06,4.881475E+06,4.881518E+06,4.881558E+06,
4.881599E+06,4.881638E+06,4.881680E+06,4.881720E+06,4.881761E+06,
4.881798E+06,4.881835E+06,4.881872E+06,4.881907E+06,4.881941E+06,
4.881976E+06,4.882011E+06,4.882045E+06,4.882079E+06,4.882111E+06,
4.882143E+06,4.882176E+06,4.885821E+06,4.885821E+06

POROSITY SURFACE #1; GAS GENERATION RATE #3.

SDATA (NSDATA =3,NTDATA=1:214,MKLOS =1)

8.810350E-01,7.887582E-01,7.708505E-01,6.448627E-01,5.588016E-01,
4.881833E-01,4.288228E-01,3.776416E-01,3.330553E-01,2.945655E-01,
2.628787E-01,2.393555E-01,2.198566E-01,2.035457E-01,1.898214E-01,
1.777870E-01,1.669751E-01,1.574966E-01,1.489963E-01,1.414614E-01,
1.348647E-01,1.292179E-01,1.242092E-01,1.160533E-01,1.098931E-01,
1.049382E-01,1.007977E-01,9.733366E-02,9.448464E-02,9.212851E-02,
9.021971E-02,8.849761E-02,8.708955E-02,8.584327E-02,8.474533E-02,
8.380801E-02,8.299521E-02,8.226313E-02,8.164614E-02,8.109227E-02,
8.063482E-02,8.024122E-02,7.991148E-02,7.964648E-02,7.943990E-02,
7.926879E-02,7.913692E-02,7.903197E-02,7.895734E-02,7.889238E-02,
7.883516E-02,7.877749E-02,7.873438E-02,7.869563E-02,7.865377E-02,
7.862730E-02,7.860425E-02,7.857508E-02,7.854233E-02,7.851716E-02,
7.849570E-02,7.847268E-02,7.845516E-02,7.843660E-02,7.842072E-02,
7.840556E-02,7.839498E-02,7.838444E-02,7.837605E-02,7.836696E-02,
7.835781E-02,7.835018E-02,7.834122E-02,7.833511E-02,7.832873E-02,

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7.832275E-02,7.831706E-02,7.831089E-02,7.830404E-02,7.829814E-02,
7.829303E-02,7.828732E-02,7.828248E-02,7.827739E-02,7.827265E-02,
7.826848E-02,7.826404E-02,7.826004E-02,7.825669E-02,7.825307E-02,
7.824975E-02,7.824654E-02,7.824415E-02,7.824144E-02,7.823953E-02,
7.823763E-02,7.823602E-02,7.823442E-02,7.823331E-02,7.823276E-02,
7.823262E-02,7.823234E-02,7.823201E-02,7.823234E-02,7.823234E-02,
7.823275E-02,7.823299E-02,7.823364E-02,7.823397E-02,7.823463E-02,
7.823510E-02,7.823560E-02,7.823637E-02,7.823502E-02,7.823502E-02,
7.823560E-02,7.823631E-02,7.823724E-02,7.823694E-02,7.823613E-02,
7.823540E-02,7.823389E-02,7.823255E-02,7.823061E-02,7.822888E-02,
7.822743E-02,7.822537E-02,7.822355E-02,7.822201E-02,7.821976E-02,
7.821817E-02,7.821605E-02,7.821431E-02,7.821208E-02,7.821018E-02,
7.820812E-02,7.820638E-02,7.820433E-02,7.820237E-02,7.820087E-02,
7.819881E-02,7.819642E-02,7.819482E-02,7.819328E-02,7.819121E-02,
7.818938E-02,7.818718E-02,7.818554E-02,7.818362E-02,7.818170E-02,
7.817984E-02,7.817788E-02,7.817629E-02,7.817496E-02,7.817309E-02,
7.817183E-02,7.817041E-02,7.816929E-02,7.816772E-02,7.816671E-02,
7.816526E-02,7.816414E-02,7.816332E-02,7.816205E-02,7.816111E-02,
7.816016E-02,7.815919E-02,7.815839E-02,7.815727E-02,7.815647E-02,
7.815535E-02,7.815456E-02,7.815361E-02,7.815264E-02,7.815184E-02,
7.815104E-02,7.815026E-02,7.814946E-02,7.814866E-02,7.814787E-02,
7.814707E-02,7.814627E-02,7.814548E-02,7.814469E-02,7.814389E-02,
7.814313E-02,7.814262E-02,7.814182E-02,7.814103E-02,7.814023E-02,
7.813944E-02,7.813897E-02,7.813818E-02,7.813738E-02,7.813692E-02,
7.813612E-02,7.813532E-02,7.813485E-02,7.813406E-02,7.813359E-02,
7.813279E-02,7.813232E-02,7.813153E-02,7.813107E-02,7.813059E-02,
7.812980E-02,7.812933E-02,7.812886E-02,7.812839E-02,7.812779E-02,
7.812713E-02,7.812666E-02,7.806707E-02,7.806707E-02

POROSITY SURFACE #1; GAS GENERATION RATE #4.

PDATA(NSDATA =4,NTDATAB=1:214,MKLOS =1)

1.013250E+05,1.019367E+05,1.025844E+05,1.100541E+05,1.199691E+05,
1.323559E+05,1.474737E+05,1.658334E+05,1.881738E+05,2.154314E+05,
2.465620E+05,2.796533E+05,3.157922E+05,3.549270E+05,3.966103E+05,
4.408549E+05,4.877774E+05,5.376286E+05,5.911094E+05,6.460473E+05,
7.026135E+05,7.603417E+05,8.188491E+05,9.372309E+05,1.057284E+06,
1.176930E+06,1.297715E+06,1.418972E+06,1.539169E+06,1.659222E+06,
1.778579E+06,1.896584E+06,2.014003E+06,2.129844E+06,2.245098E+06,
2.358814E+06,2.471331E+06,2.582536E+06,2.692048E+06,2.800229E+06,
2.906426E+06,3.011053E+06,3.114472E+06,3.216943E+06,3.319211E+06,
3.420912E+06,3.522289E+06,3.623834E+06,3.725236E+06,3.826369E+06,
3.927415E+06,4.028407E+06,4.129262E+06,4.230136E+06,4.330991E+06,

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4.431765E+06,4.532456E+06,4.633080E+06,4.733710E+06,4.834251E+06,
4.934765E+06,5.035245E+06,5.135664E+06,5.236045E+06,5.336371E+06,
5.436633E+06,5.536848E+06,5.627395E+06,5.679444E+06,5.729521E+06,
5.779600E+06,5.829685E+06,5.879741E+06,5.929795E+06,5.979851E+06,
6.029893E+06,6.079903E+06,6.129888E+06,6.179867E+06,6.229815E+06,
6.279757E+06,6.329679E+06,6.379601E+06,6.429495E+06,6.479369E+06,
6.529234E+06,6.579058E+06,6.628887E+06,6.678665E+06,6.728481E+06,
6.778280E+06,6.828094E+06,6.877864E+06,6.927647E+06,6.977392E+06,
7.027104E+06,7.076834E+06,7.126520E+06,7.176196E+06,7.225835E+06,
7.275453E+06,7.325076E+06,7.374656E+06,7.424226E+06,7.473799E+06,
7.523363E+06,7.572886E+06,7.622423E+06,7.671946E+06,7.721447E+06,
7.770879E+06,7.820321E+06,7.870018E+06,7.919389E+06,7.968738E+06,
8.018026E+06,8.067326E+06,8.106327E+06,8.106085E+06,8.105670E+06,
8.105311E+06,8.105033E+06,8.104803E+06,8.104611E+06,8.104452E+06,
8.104315E+06,8.104200E+06,8.104108E+06,8.104028E+06,8.103958E+06,
8.103906E+06,8.103852E+06,8.103808E+06,8.103767E+06,8.103731E+06,
8.103700E+06,8.103671E+06,8.103647E+06,8.103623E+06,8.103604E+06,
8.103582E+06,8.103562E+06,8.103547E+06,8.103529E+06,8.103518E+06,
8.103504E+06,8.103497E+06,8.103488E+06,8.103481E+06,8.103476E+06,
8.103474E+06,8.103474E+06,8.103474E+06,8.103478E+06,8.103481E+06,
8.103487E+06,8.103492E+06,8.103500E+06,8.103507E+06,8.103516E+06,
8.103523E+06,8.103531E+06,8.103543E+06,8.103551E+06,8.103560E+06,
8.103569E+06,8.103581E+06,8.103589E+06,8.103600E+06,8.103611E+06,
8.103619E+06,8.103629E+06,8.103641E+06,8.103652E+06,8.103662E+06,
8.103674E+06,8.103683E+06,8.103694E+06,8.103703E+06,8.103712E+06,
8.103721E+06,8.103732E+06,8.103744E+06,8.103752E+06,8.103766E+06,
8.103773E+06,8.103784E+06,8.103795E+06,8.103804E+06,8.103815E+06,
8.103822E+06,8.103833E+06,8.103846E+06,8.103853E+06,8.103861E+06,
8.103873E+06,8.103883E+06,8.103891E+06,8.103901E+06,8.103913E+06,
8.103920E+06,8.103927E+06,8.103937E+06,8.103948E+06,8.103956E+06,
8.103964E+06,8.103973E+06,8.103979E+06,8.103989E+06,8.103997E+06,
8.104007E+06,8.104015E+06,8.105364E+06,8.105364E+06

POROSITY SURFACE #1; GAS GENERATION RATE #4.

SDATA(NSDATA =4,NTDATA=1:214,MKLOS =1)

8.810350E-01,7.878199E-01,7.701936E-01,6.429939E-01,5.568310E-01,
4.869273E-01,4.283253E-01,3.778764E-01,3.341083E-01,2.962066E-01,
2.648303E-01,2.416281E-01,2.223626E-01,2.066053E-01,1.933625E-01,
1.819241E-01,1.718378E-01,1.628374E-01,1.546817E-01,1.476748E-01,
1.415362E-01,1.361786E-01,1.315973E-01,1.241585E-01,1.183105E-01,
1.138504E-01,1.101584E-01,1.071175E-01,1.046620E-01,1.025945E-01,
1.008677E-01,9.944060E-02,9.822504E-02,9.722167E-02,9.635598E-02,

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9.564221E-02,9.504542E-02,9.455261E-02,9.416329E-02,9.385254E-02,
9.363118E-02,9.347698E-02,9.337058E-02,9.329983E-02,9.323959E-02,
9.319877E-02,9.316605E-02,9.313412E-02,9.310732E-02,9.308890E-02,
9.307358E-02,9.306041E-02,9.305001E-02,9.304067E-02,9.303236E-02,
9.302581E-02,9.302142E-02,9.301860E-02,9.301584E-02,9.301440E-02,
9.301412E-02,9.301421E-02,9.301567E-02,9.301788E-02,9.302081E-02,
9.302482E-02,9.302892E-02,9.303233E-02,9.303546E-02,9.303823E-02,
9.304061E-02,9.304299E-02,9.304575E-02,9.304852E-02,9.305127E-02,
9.305412E-02,9.305743E-02,9.306110E-02,9.306479E-02,9.306884E-02,
9.307305E-02,9.307728E-02,9.308188E-02,9.308649E-02,9.309147E-02,
9.309629E-02,9.310143E-02,9.310696E-02,9.311210E-02,9.311725E-02,
9.312278E-02,9.312793E-02,9.313346E-02,9.313900E-02,9.314507E-02,
9.315114E-02,9.315721E-02,9.316366E-02,9.317011E-02,9.317655E-02,
9.318377E-02,9.319081E-02,9.319817E-02,9.320533E-02,9.321260E-02,
9.321992E-02,9.322728E-02,9.323466E-02,9.324204E-02,9.324982E-02,
9.325755E-02,9.326564E-02,9.327360E-02,9.328190E-02,9.329027E-02,
9.329911E-02,9.330793E-02,9.331602E-02,9.332265E-02,9.332730E-02,
9.333160E-02,9.333482E-02,9.333732E-02,9.333956E-02,9.334141E-02,
9.334324E-02,9.334455E-02,9.334546E-02,9.334639E-02,9.334731E-02,
9.334785E-02,9.334856E-02,9.334894E-02,9.334949E-02,9.335003E-02,
9.335020E-02,9.335074E-02,9.335081E-02,9.335119E-02,9.335158E-02,
9.335158E-02,9.335196E-02,9.335196E-02,9.335233E-02,9.335233E-02,
9.335271E-02,9.335271E-02,9.335271E-02,9.335271E-02,9.335288E-02,
9.335309E-02,9.335309E-02,9.335309E-02,9.335271E-02,9.335271E-02,
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9.335196E-02,9.335158E-02,9.335158E-02,9.335158E-02,9.335119E-02,
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9.335052E-02,9.335045E-02,9.335045E-02,9.335041E-02,9.335006E-02,
9.335006E-02,9.335006E-02,9.334968E-02,9.334968E-02,9.334968E-02,
9.334930E-02,9.334930E-02,9.334930E-02,9.334892E-02,9.334892E-02,
9.334892E-02,9.334865E-02,9.334856E-02,9.334856E-02,9.334854E-02,
9.334816E-02,9.334816E-02,9.334816E-02,9.334786E-02,9.334779E-02,
9.334779E-02,9.334775E-02,9.334741E-02,9.334741E-02,9.334741E-02,
9.334710E-02,9.334704E-02,9.334704E-02,9.334704E-02,9.334666E-02,
9.334666E-02,9.334666E-02,9.333074E-02,9.333074E-02

POROSITY SURFACE #1; GAS GENERATION RATE #5.

PDATA(NSDATA =5,NTDATA=1:214,MKLOS =1)

1.013250E+05,1.028230E+05,1.043268E+05,1.193632E+05,1.433537E+05,
1.701278E+05,1.969022E+05,2.346395E+05,2.843196E+05,3.339881E+05,
3.873079E+05,4.557298E+05,5.241518E+05,5.925607E+05,6.727943E+05,

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7.541983E+05, 8.356024E+05, 9.246392E+05, 1.018289E+06, 1.111932E+06,
1.206610E+06, 1.303274E+06, 1.400036E+06, 1.593405E+06, 1.786766E+06,
1.979315E+06, 2.171063E+06, 2.359950E+06, 2.546125E+06, 2.730495E+06,
2.910511E+06, 3.089306E+06, 3.265849E+06, 3.439798E+06, 3.612334E+06,
3.780358E+06, 3.947017E+06, 4.111553E+06, 4.274565E+06, 4.436999E+06,
4.598934E+06, 4.760584E+06, 4.921913E+06, 5.082896E+06, 5.243779E+06,
5.404466E+06, 5.564854E+06, 5.725364E+06, 5.885693E+06, 6.045949E+06,
6.206051E+06, 6.366065E+06, 6.525971E+06, 6.685665E+06, 6.845326E+06,
7.004935E+06, 7.164395E+06, 7.323776E+06, 7.482948E+06, 7.642017E+06,
7.801056E+06, 7.959724E+06, 8.118271E+06, 8.276814E+06, 8.435227E+06,
8.593497E+06, 8.751544E+06, 8.894922E+06, 8.974895E+06, 9.054036E+06,
9.132480E+06, 9.210949E+06, 9.289403E+06, 9.367899E+06, 9.446414E+06,
9.524942E+06, 9.603409E+06, 9.681870E+06, 9.760321E+06, 9.838720E+06,
9.917128E+06, 9.995479E+06, 1.007383E+07, 1.015218E+07, 1.023045E+07,
1.030870E+07, 1.038686E+07, 1.046511E+07, 1.054336E+07, 1.062184E+07,
1.070029E+07, 1.077852E+07, 1.085662E+07, 1.093466E+07, 1.101268E+07,
1.109068E+07, 1.116866E+07, 1.124655E+07, 1.132438E+07, 1.140173E+07,
1.147919E+07, 1.155683E+07, 1.163420E+07, 1.171145E+07, 1.178853E+07,
1.186561E+07, 1.194268E+07, 1.201971E+07, 1.209671E+07, 1.217372E+07,
1.225091E+07, 1.232844E+07, 1.240577E+07, 1.248250E+07, 1.255913E+07,
1.263556E+07, 1.271189E+07, 1.274761E+07, 1.277038E+07, 1.276847E+07,
1.276692E+07, 1.276559E+07, 1.276443E+07, 1.276326E+07, 1.276207E+07,
1.276109E+07, 1.276019E+07, 1.275939E+07, 1.275862E+07, 1.275790E+07,
1.275719E+07, 1.275649E+07, 1.275582E+07, 1.275519E+07, 1.275461E+07,
1.275410E+07, 1.275357E+07, 1.275298E+07, 1.275245E+07, 1.275197E+07,
1.275150E+07, 1.275106E+07, 1.275065E+07, 1.275026E+07, 1.274989E+07,
1.274955E+07, 1.274923E+07, 1.274891E+07, 1.274861E+07, 1.274832E+07,
1.274805E+07, 1.274778E+07, 1.274751E+07, 1.274726E+07, 1.274703E+07,
1.274680E+07, 1.274658E+07, 1.274635E+07, 1.274614E+07, 1.274594E+07,
1.274575E+07, 1.274557E+07, 1.274539E+07, 1.274523E+07, 1.274506E+07,
1.274490E+07, 1.274475E+07, 1.274461E+07, 1.274447E+07, 1.274435E+07,
1.274422E+07, 1.274411E+07, 1.274399E+07, 1.274389E+07, 1.274379E+07,
1.274369E+07, 1.274360E+07, 1.274352E+07, 1.274342E+07, 1.274334E+07,
1.274326E+07, 1.274319E+07, 1.274312E+07, 1.274306E+07, 1.274299E+07,
1.274293E+07, 1.274287E+07, 1.274281E+07, 1.274276E+07, 1.274271E+07,
1.274266E+07, 1.274262E+07, 1.274258E+07, 1.274254E+07, 1.274250E+07,
1.274247E+07, 1.274243E+07, 1.274240E+07, 1.274237E+07, 1.274234E+07,
1.274231E+07, 1.274228E+07, 1.274226E+07, 1.274224E+07, 1.274221E+07,
1.274219E+07, 1.274217E+07, 1.274215E+07, 1.274213E+07, 1.274212E+07,
1.274210E+07, 1.274209E+07, 1.274260E+07, 1.274260E+07
POROSITY SURFACE #1; GAS GENERATION RATE #5.

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SDATA (NSDATA =5,NTDATA=1:214,MKLOS =1)
  8.810350E-01,8.221918E-01,8.071246E-01,6.564677E-01,5.701580E-01,
  5.038119E-01,4.374655E-01,3.841511E-01,3.450336E-01,3.059252E-01,
  2.707192E-01,2.517662E-01,2.328131E-01,2.138637E-01,2.027257E-01,
  1.923666E-01,1.820076E-01,1.738506E-01,1.670118E-01,1.601735E-01,
  1.542665E-01,1.501642E-01,1.460577E-01,1.394642E-01,1.343107E-01,
  1.306321E-01,1.274171E-01,1.250688E-01,1.231763E-01,1.215867E-01,
  1.204882E-01,1.195114E-01,1.187518E-01,1.181638E-01,1.176658E-01,
  1.173808E-01,1.171502E-01,1.170044E-01,1.169135E-01,1.168436E-01,
  1.167941E-01,1.167538E-01,1.167242E-01,1.167049E-01,1.166891E-01,
  1.166788E-01,1.166711E-01,1.166654E-01,1.166638E-01,1.166636E-01,
  1.166665E-01,1.166707E-01,1.166758E-01,1.166851E-01,1.166947E-01,
  1.167050E-01,1.167169E-01,1.167298E-01,1.167452E-01,1.167610E-01,
  1.167775E-01,1.167985E-01,1.168209E-01,1.168419E-01,1.168641E-01,
  1.168878E-01,1.169124E-01,1.169365E-01,1.169579E-01,1.169780E-01,
  1.169971E-01,1.170154E-01,1.170334E-01,1.170508E-01,1.170677E-01,
  1.170843E-01,1.171011E-01,1.171177E-01,1.171340E-01,1.171506E-01,
  1.171674E-01,1.171843E-01,1.172009E-01,1.172172E-01,1.172341E-01,
  1.172514E-01,1.172690E-01,1.172855E-01,1.173006E-01,1.173144E-01,
  1.173283E-01,1.173440E-01,1.173606E-01,1.173780E-01,1.173952E-01,
  1.174125E-01,1.174300E-01,1.174481E-01,1.174667E-01,1.174895E-01,
  1.175113E-01,1.175307E-01,1.175526E-01,1.175756E-01,1.175999E-01,
  1.176240E-01,1.176475E-01,1.176714E-01,1.176954E-01,1.177189E-01,
  1.177396E-01,1.177573E-01,1.177808E-01,1.178053E-01,1.178302E-01,
  1.178564E-01,1.178837E-01,1.179073E-01,1.179290E-01,1.179468E-01,
  1.179612E-01,1.179735E-01,1.179845E-01,1.179955E-01,1.180063E-01,
  1.180154E-01,1.180237E-01,1.180312E-01,1.180384E-01,1.180453E-01,
  1.180520E-01,1.180585E-01,1.180645E-01,1.180703E-01,1.180758E-01,
  1.180808E-01,1.180858E-01,1.180912E-01,1.180962E-01,1.181009E-01,
  1.181051E-01,1.181093E-01,1.181130E-01,1.181166E-01,1.181201E-01,
  1.181232E-01,1.181263E-01,1.181292E-01,1.181318E-01,1.181344E-01,
  1.181370E-01,1.181396E-01,1.181422E-01,1.181445E-01,1.181468E-01,
  1.181488E-01,1.181508E-01,1.181528E-01,1.181548E-01,1.181568E-01,
  1.181586E-01,1.181603E-01,1.181620E-01,1.181635E-01,1.181650E-01,
  1.181667E-01,1.181681E-01,1.181692E-01,1.181707E-01,1.181720E-01,
  1.181732E-01,1.181741E-01,1.181750E-01,1.181761E-01,1.181772E-01,
  1.181780E-01,1.181789E-01,1.181797E-01,1.181806E-01,1.181813E-01,
  1.181819E-01,1.181825E-01,1.181831E-01,1.181839E-01,1.181847E-01,
  1.181853E-01,1.181858E-01,1.181863E-01,1.181866E-01,1.181871E-01,
  1.181876E-01,1.181879E-01,1.181882E-01,1.181885E-01,1.181890E-01,
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1.181920E-01,1.181923E-01,1.181924E-01,1.181924E-01,1.181926E-01,
1.181928E-01,1.181928E-01,1.181881E-01,1.181881E-01

POROSITY SURFACE #1; GAS GENERATION RATE #6.

PDATA(NSDATA =6,NTDATA=1:214,MKLOS =1)

1.013250E+05,1.044625E+05,1.076827E+05,1.398820E+05,1.794587E+05,
2.373400E+05,2.952216E+05,3.532305E+05,4.536252E+05,5.539963E+05,
6.543954E+05,7.735449E+05,9.000448E+05,1.026521E+06,1.159067E+06,
1.299483E+06,1.439899E+06,1.581173E+06,1.727523E+06,1.873864E+06,
2.020205E+06,2.165059E+06,2.309830E+06,2.597337E+06,2.880419E+06,
3.157021E+06,3.430495E+06,3.696883E+06,3.960480E+06,4.219164E+06,
4.473529E+06,4.725867E+06,4.973911E+06,5.220712E+06,5.465891E+06,
5.710379E+06,5.954540E+06,6.197938E+06,6.441180E+06,6.684264E+06,
6.926950E+06,7.169520E+06,7.411938E+06,7.654174E+06,7.896307E+06,
8.138193E+06,8.379660E+06,8.621203E+06,8.862472E+06,9.103591E+06,
9.344282E+06,9.584796E+06,9.824935E+06,1.006486E+07,1.030464E+07,
1.054408E+07,1.078338E+07,1.102249E+07,1.126128E+07,1.149984E+07,
1.173802E+07,1.197591E+07,1.221353E+07,1.245089E+07,1.268804E+07,
1.292461E+07,1.315145E+07,1.337148E+07,1.349249E+07,1.360831E+07,
1.372464E+07,1.384081E+07,1.395684E+07,1.407235E+07,1.418804E+07,
1.430404E+07,1.441985E+07,1.453548E+07,1.464989E+07,1.476439E+07,
1.487906E+07,1.499289E+07,1.510658E+07,1.522063E+07,1.533432E+07,
1.544771E+07,1.556063E+07,1.567337E+07,1.578549E+07,1.589726E+07,
1.600872E+07,1.612005E+07,1.623117E+07,1.634195E+07,1.645236E+07,
1.656256E+07,1.667193E+07,1.678104E+07,1.688975E+07,1.699730E+07,
1.710450E+07,1.721166E+07,1.731814E+07,1.742383E+07,1.752869E+07,
1.763300E+07,1.773558E+07,1.783730E+07,1.793825E+07,1.803919E+07,
1.813954E+07,1.823851E+07,1.833659E+07,1.843319E+07,1.852693E+07,
1.861932E+07,1.870917E+07,1.874216E+07,1.874759E+07,1.872865E+07,
1.871105E+07,1.869554E+07,1.868232E+07,1.867011E+07,1.866083E+07,
1.865226E+07,1.864450E+07,1.863753E+07,1.863089E+07,1.862492E+07,
1.861933E+07,1.861404E+07,1.860907E+07,1.860417E+07,1.859958E+07,
1.859497E+07,1.859035E+07,1.858591E+07,1.858149E+07,1.857710E+07,
1.857263E+07,1.856812E+07,1.856384E+07,1.855958E+07,1.855533E+07,
1.855108E+07,1.854683E+07,1.854264E+07,1.853855E+07,1.853455E+07,
1.853046E+07,1.852637E+07,1.852236E+07,1.851831E+07,1.851418E+07,
1.851025E+07,1.850635E+07,1.850249E+07,1.849859E+07,1.849466E+07,
1.849081E+07,1.848695E+07,1.848307E+07,1.847931E+07,1.847561E+07,
1.847191E+07,1.846826E+07,1.846462E+07,1.846096E+07,1.845731E+07,
1.845377E+07,1.845023E+07,1.844668E+07,1.844314E+07,1.843961E+07,
1.843605E+07,1.843257E+07,1.842912E+07,1.842568E+07,1.842232E+07,

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1.841915E+07,1.841592E+07,1.841265E+07,1.840906E+07,1.840558E+07,
1.840231E+07,1.839912E+07,1.839600E+07,1.839263E+07,1.838927E+07,
1.838591E+07,1.838280E+07,1.837976E+07,1.837675E+07,1.837366E+07,
1.837048E+07,1.836742E+07,1.836443E+07,1.836148E+07,1.835849E+07,
1.835546E+07,1.835254E+07,1.834963E+07,1.834678E+07,1.834392E+07,
1.834106E+07,1.833825E+07,1.833540E+07,1.833253E+07,1.832976E+07,
1.832701E+07,1.832421E+07,1.784436E+07,1.784436E+07

POROSITY SURFACE #1; GAS GENERATION RATE #6.

SDATA (NSDATA =6,NTD DATA=1:214,MKLOS =1)

8.810350E-01,8.093810E-01,7.967799E-01,6.707830E-01,5.639549E-01,
5.046195E-01,4.452838E-01,3.860223E-01,3.514972E-01,3.169802E-01,
2.824536E-01,2.613405E-01,2.454832E-01,2.296289E-01,2.169938E-01,
2.085653E-01,2.001368E-01,1.922331E-01,1.873091E-01,1.823854E-01,
1.774618E-01,1.743318E-01,1.714792E-01,1.664243E-01,1.629469E-01,
1.603927E-01,1.583400E-01,1.570668E-01,1.559932E-01,1.552698E-01,
1.547867E-01,1.544129E-01,1.542299E-01,1.540944E-01,1.540203E-01,
1.539730E-01,1.539369E-01,1.539243E-01,1.539160E-01,1.539118E-01,
1.539168E-01,1.539241E-01,1.539345E-01,1.539477E-01,1.539629E-01,
1.539810E-01,1.540005E-01,1.540230E-01,1.540490E-01,1.540769E-01,
1.541094E-01,1.541437E-01,1.541811E-01,1.542208E-01,1.542615E-01,
1.543047E-01,1.543484E-01,1.543927E-01,1.544393E-01,1.544869E-01,
1.545374E-01,1.545902E-01,1.546450E-01,1.546998E-01,1.547560E-01,
1.548166E-01,1.548844E-01,1.549573E-01,1.550161E-01,1.550711E-01,
1.551192E-01,1.551683E-01,1.552180E-01,1.552727E-01,1.553247E-01,
1.553725E-01,1.554211E-01,1.554712E-01,1.555337E-01,1.555940E-01,
1.556515E-01,1.557172E-01,1.557837E-01,1.558448E-01,1.559087E-01,
1.559752E-01,1.560445E-01,1.561155E-01,1.561902E-01,1.562685E-01,
1.563491E-01,1.564295E-01,1.565107E-01,1.565938E-01,1.566797E-01,
1.567670E-01,1.568600E-01,1.569548E-01,1.570523E-01,1.571585E-01,
1.572676E-01,1.573751E-01,1.574877E-01,1.576063E-01,1.577305E-01,
1.578587E-01,1.580000E-01,1.581477E-01,1.583010E-01,1.584522E-01,
1.586063E-01,1.587708E-01,1.589471E-01,1.591292E-01,1.593325E-01,
1.595460E-01,1.597794E-01,1.600163E-01,1.602519E-01,1.604151E-01,
1.605668E-01,1.607007E-01,1.608149E-01,1.609205E-01,1.610011E-01,
1.610754E-01,1.611428E-01,1.612033E-01,1.612610E-01,1.613128E-01,
1.613616E-01,1.614077E-01,1.614511E-01,1.614938E-01,1.615341E-01,
1.615743E-01,1.616145E-01,1.616532E-01,1.616919E-01,1.617305E-01,
1.617698E-01,1.618092E-01,1.618467E-01,1.618840E-01,1.619215E-01,
1.619586E-01,1.619957E-01,1.620324E-01,1.620684E-01,1.621036E-01,
1.621398E-01,1.621759E-01,1.622111E-01,1.622467E-01,1.622830E-01,
1.623179E-01,1.623525E-01,1.623865E-01,1.624207E-01,1.624552E-01,

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1.624892E-01,1.625234E-01,1.625578E-01,1.625912E-01,1.626239E-01,
1.626567E-01,1.626890E-01,1.627210E-01,1.627534E-01,1.627858E-01,
1.628175E-01,1.628490E-01,1.628802E-01,1.629115E-01,1.629428E-01,
1.629744E-01,1.630055E-01,1.630363E-01,1.630669E-01,1.630967E-01,
1.631249E-01,1.631537E-01,1.631829E-01,1.632151E-01,1.632461E-01,
1.632750E-01,1.633034E-01,1.633313E-01,1.633615E-01,1.633916E-01,
1.634217E-01,1.634494E-01,1.634763E-01,1.635033E-01,1.635310E-01,
1.635595E-01,1.635870E-01,1.636139E-01,1.636404E-01,1.636672E-01,
1.636942E-01,1.637204E-01,1.637465E-01,1.637722E-01,1.637979E-01,
1.638237E-01,1.638486E-01,1.638741E-01,1.638999E-01,1.639248E-01,
1.639495E-01,1.639748E-01,1.684095E-01,1.684095E-01

POROSITY SURFACE #1; GAS GENERATION RATE #7.

PDATA(NSDATA =7,NTDATA=1:214,MKLOS =1)

1.013250E+05,1.055196E+05,1.098189E+05,1.528066E+05,1.957910E+05,
2.668437E+05,3.453648E+05,4.238860E+05,5.281031E+05,6.574334E+05,
7.867997E+05,9.214743E+05,1.074906E+06,1.228308E+06,1.381749E+06,
1.546069E+06,1.711129E+06,1.876158E+06,2.040590E+06,2.204672E+06,
2.368753E+06,2.531402E+06,2.691798E+06,3.011992E+06,3.324302E+06,
3.632379E+06,3.934849E+06,4.230771E+06,4.523804E+06,4.810694E+06,
5.094979E+06,5.376370E+06,5.654931E+06,5.932741E+06,6.209750E+06,
6.486522E+06,6.763080E+06,7.039269E+06,7.315322E+06,7.591097E+06,
7.866675E+06,8.142118E+06,8.417200E+06,8.692286E+06,8.967441E+06,
9.242122E+06,9.516225E+06,9.790190E+06,1.006400E+07,1.033759E+07,
1.061057E+07,1.088331E+07,1.115567E+07,1.142788E+07,1.169984E+07,
1.197145E+07,1.224287E+07,1.251382E+07,1.278420E+07,1.305403E+07,
1.332235E+07,1.359021E+07,1.385728E+07,1.412324E+07,1.438853E+07,
1.465211E+07,1.490242E+07,1.512735E+07,1.528460E+07,1.541277E+07,
1.554234E+07,1.567167E+07,1.580063E+07,1.592901E+07,1.605713E+07,
1.618474E+07,1.631208E+07,1.643913E+07,1.656570E+07,1.669197E+07,
1.681755E+07,1.694250E+07,1.706696E+07,1.719027E+07,1.731311E+07,
1.743497E+07,1.755582E+07,1.767614E+07,1.779332E+07,1.791078E+07,
1.802861E+07,1.814545E+07,1.826169E+07,1.837600E+07,1.848886E+07,
1.859977E+07,1.870648E+07,1.881244E+07,1.892100E+07,1.902293E+07,
1.911822E+07,1.919616E+07,1.926996E+07,1.933932E+07,1.940584E+07,
1.947021E+07,1.952877E+07,1.958591E+07,1.964057E+07,1.969298E+07,
1.974410E+07,1.979159E+07,1.983798E+07,1.988172E+07,1.992384E+07,
1.996497E+07,2.000206E+07,1.999858E+07,1.994188E+07,1.988652E+07,
1.983349E+07,1.979203E+07,1.975437E+07,1.972018E+07,1.969142E+07,
1.966459E+07,1.964171E+07,1.962086E+07,1.960150E+07,1.958512E+07,
1.956936E+07,1.955462E+07,1.954060E+07,1.952682E+07,1.951172E+07,
1.949750E+07,1.948478E+07,1.947242E+07,1.946036E+07,1.945016E+07,

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1.943907E+07,1.942682E+07,1.941470E+07,1.940271E+07,1.939112E+07,
1.938016E+07,1.936969E+07,1.935932E+07,1.934946E+07,1.934126E+07,
1.933237E+07,1.932298E+07,1.931433E+07,1.930557E+07,1.929638E+07,
1.928770E+07,1.927923E+07,1.927025E+07,1.926142E+07,1.925285E+07,
1.924510E+07,1.923751E+07,1.922854E+07,1.921959E+07,1.921065E+07,
1.920156E+07,1.919261E+07,1.918402E+07,1.917623E+07,1.916915E+07,
1.916236E+07,1.915561E+07,1.914883E+07,1.914182E+07,1.913465E+07,
1.912758E+07,1.912085E+07,1.911469E+07,1.910809E+07,1.910130E+07,
1.909528E+07,1.908958E+07,1.908442E+07,1.907865E+07,1.907274E+07,
1.906756E+07,1.906221E+07,1.905677E+07,1.905164E+07,1.904649E+07,
1.904088E+07,1.903549E+07,1.903030E+07,1.902528E+07,1.902035E+07,
1.901560E+07,1.901069E+07,1.900574E+07,1.900151E+07,1.899740E+07,
1.899346E+07,1.898928E+07,1.898500E+07,1.898106E+07,1.897712E+07,
1.897320E+07,1.896861E+07,1.896384E+07,1.895977E+07,1.895595E+07,
1.895243E+07,1.894900E+07,1.842811E+07,1.842811E+07

POROSITY SURFACE #1; GAS GENERATION RATE #7.

SDATA (NSDATA =7,NTDATA=1:214,MKLOS =1)

8.810350E-01,8.121463E-01,8.005424E-01,6.845162E-01,5.684990E-01,
5.018084E-01,4.482483E-01,3.946883E-01,3.526027E-01,3.217522E-01,
2.908930E-01,2.638419E-01,2.502192E-01,2.365990E-01,2.229754E-01,
2.153148E-01,2.080600E-01,2.008065E-01,1.957599E-01,1.918941E-01,
1.880283E-01,1.847747E-01,1.825730E-01,1.782471E-01,1.756175E-01,
1.734363E-01,1.719252E-01,1.709245E-01,1.701347E-01,1.697052E-01,
1.693939E-01,1.692148E-01,1.691420E-01,1.690972E-01,1.690798E-01,
1.690701E-01,1.690667E-01,1.690725E-01,1.690812E-01,1.690952E-01,
1.691129E-01,1.691328E-01,1.691574E-01,1.691809E-01,1.692022E-01,
1.692305E-01,1.692622E-01,1.692992E-01,1.693376E-01,1.693780E-01,
1.694253E-01,1.694748E-01,1.695255E-01,1.695776E-01,1.696313E-01,
1.696869E-01,1.697435E-01,1.698032E-01,1.698682E-01,1.699374E-01,
1.700226E-01,1.701116E-01,1.702066E-01,1.703111E-01,1.704212E-01,
1.705445E-01,1.706685E-01,1.707934E-01,1.708990E-01,1.709951E-01,
1.710735E-01,1.711535E-01,1.712357E-01,1.713228E-01,1.714118E-01,
1.715046E-01,1.715992E-01,1.716956E-01,1.717947E-01,1.718956E-01,
1.720017E-01,1.721130E-01,1.722284E-01,1.723527E-01,1.724807E-01,
1.726159E-01,1.727591E-01,1.729068E-01,1.730806E-01,1.732515E-01,
1.734164E-01,1.735883E-01,1.737641E-01,1.739552E-01,1.741583E-01,
1.743779E-01,1.746331E-01,1.748938E-01,1.751261E-01,1.754172E-01,
1.757679E-01,1.762730E-01,1.768140E-01,1.773909E-01,1.779900E-01,
1.786058E-01,1.792691E-01,1.799434E-01,1.806357E-01,1.813449E-01,
1.820627E-01,1.828091E-01,1.835699E-01,1.843445E-01,1.851300E-01,
1.859223E-01,1.867485E-01,1.875208E-01,1.882222E-01,1.887846E-01,

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1.892914E-01,1.896900E-01,1.900532E-01,1.903844E-01,1.906639E-01,
1.909251E-01,1.911488E-01,1.913530E-01,1.915432E-01,1.917041E-01,
1.918590E-01,1.920043E-01,1.921430E-01,1.922797E-01,1.924289E-01,
1.925698E-01,1.926964E-01,1.928195E-01,1.929396E-01,1.930411E-01,
1.931519E-01,1.932745E-01,1.933956E-01,1.935155E-01,1.936321E-01,
1.937421E-01,1.938472E-01,1.939518E-01,1.940513E-01,1.941335E-01,
1.942234E-01,1.943188E-01,1.944061E-01,1.944947E-01,1.945881E-01,
1.946759E-01,1.947616E-01,1.948527E-01,1.949425E-01,1.950302E-01,
1.951091E-01,1.951862E-01,1.952781E-01,1.953696E-01,1.954605E-01,
1.955537E-01,1.956455E-01,1.957336E-01,1.958135E-01,1.958860E-01,
1.959558E-01,1.960253E-01,1.960948E-01,1.961671E-01,1.962413E-01,
1.963142E-01,1.963837E-01,1.964473E-01,1.965154E-01,1.965854E-01,
1.966480E-01,1.967072E-01,1.967606E-01,1.968202E-01,1.968813E-01,
1.969353E-01,1.969909E-01,1.970471E-01,1.971007E-01,1.971547E-01,
1.972130E-01,1.972689E-01,1.973226E-01,1.973750E-01,1.974265E-01,
1.974762E-01,1.975277E-01,1.975794E-01,1.976237E-01,1.976668E-01,
1.977078E-01,1.977516E-01,1.977967E-01,1.978377E-01,1.978788E-01,
1.979199E-01,1.979682E-01,1.980187E-01,1.980613E-01,1.981013E-01,
1.981383E-01,1.981741E-01,2.038069E-01,2.038069E-01

POROSITY SURFACE #1; GAS GENERATION RATE #8.

PDATA(NSDATA =8,NTDATA=1:214,MKLOS =1)

1.013250E+05,1.060899E+05,1.109714E+05,1.597815E+05,2.163145E+05,
3.029852E+05,3.896565E+05,4.763278E+05,6.155277E+05,7.592791E+05,
9.030706E+05,1.066291E+06,1.240678E+06,1.415032E+06,1.592615E+06,
1.776087E+06,1.959559E+06,2.142916E+06,2.325173E+06,2.507420E+06,
2.689666E+06,2.865567E+06,3.039882E+06,3.385855E+06,3.724639E+06,
4.056405E+06,4.384162E+06,4.703791E+06,5.020997E+06,5.333714E+06,
5.643902E+06,5.952860E+06,6.260512E+06,6.567859E+06,6.874713E+06,
7.181142E+06,7.487368E+06,7.793197E+06,8.098833E+06,8.404239E+06,
8.709459E+06,9.014545E+06,9.319274E+06,9.623696E+06,9.927895E+06,
1.023161E+07,1.053473E+07,1.083783E+07,1.114056E+07,1.144306E+07,
1.174509E+07,1.204698E+07,1.234850E+07,1.264630E+07,1.294261E+07,
1.324427E+07,1.354535E+07,1.384556E+07,1.414355E+07,1.444037E+07,
1.473448E+07,1.502694E+07,1.531758E+07,1.560757E+07,1.589672E+07,
1.618287E+07,1.645582E+07,1.671788E+07,1.686658E+07,1.700390E+07,
1.714201E+07,1.727953E+07,1.741664E+07,1.755248E+07,1.768760E+07,
1.782135E+07,1.795405E+07,1.808616E+07,1.821574E+07,1.834516E+07,
1.847444E+07,1.860025E+07,1.872431E+07,1.884356E+07,1.895870E+07,
1.906948E+07,1.916968E+07,1.926607E+07,1.935492E+07,1.943908E+07,
1.951947E+07,1.959278E+07,1.966404E+07,1.973166E+07,1.979514E+07,
1.985619E+07,1.991243E+07,1.996685E+07,2.001798E+07,2.006561E+07,

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2.011172E+07, 2.015639E+07, 2.019924E+07, 2.023956E+07, 2.027864E+07,
2.031691E+07, 2.035225E+07, 2.038673E+07, 2.042032E+07, 2.045148E+07,
2.048159E+07, 2.050942E+07, 2.053787E+07, 2.056649E+07, 2.059106E+07,
2.061547E+07, 2.064034E+07, 2.061009E+07, 2.054883E+07, 2.047610E+07,
2.040909E+07, 2.035272E+07, 2.030315E+07, 2.025660E+07, 2.021877E+07,
2.018344E+07, 2.015143E+07, 2.012286E+07, 2.009574E+07, 2.007172E+07,
2.004987E+07, 2.003020E+07, 2.001189E+07, 1.999403E+07, 1.997772E+07,
1.996258E+07, 1.994828E+07, 1.993587E+07, 1.992313E+07, 1.990924E+07,
1.989670E+07, 1.988491E+07, 1.987378E+07, 1.986257E+07, 1.985113E+07,
1.984010E+07, 1.982919E+07, 1.981846E+07, 1.980737E+07, 1.979583E+07,
1.978469E+07, 1.977365E+07, 1.976264E+07, 1.975191E+07, 1.974133E+07,
1.973158E+07, 1.972190E+07, 1.971208E+07, 1.970243E+07, 1.969290E+07,
1.968432E+07, 1.967569E+07, 1.966681E+07, 1.965746E+07, 1.964788E+07,
1.963862E+07, 1.962963E+07, 1.962096E+07, 1.961287E+07, 1.960505E+07,
1.959778E+07, 1.959014E+07, 1.958203E+07, 1.957496E+07, 1.956815E+07,
1.956125E+07, 1.955443E+07, 1.954760E+07, 1.954044E+07, 1.953353E+07,
1.952758E+07, 1.952114E+07, 1.951437E+07, 1.950793E+07, 1.950122E+07,
1.949384E+07, 1.948783E+07, 1.948257E+07, 1.947617E+07, 1.946993E+07,
1.946393E+07, 1.945789E+07, 1.945183E+07, 1.944589E+07, 1.944011E+07,
1.943452E+07, 1.942928E+07, 1.942414E+07, 1.941871E+07, 1.941291E+07,
1.940677E+07, 1.940059E+07, 1.939455E+07, 1.938894E+07, 1.938390E+07,
1.937925E+07, 1.937388E+07, 1.936831E+07, 1.936254E+07, 1.935756E+07,
1.935292E+07, 1.934765E+07, 1.869588E+07, 1.869588E+07

POROSITY SURFACE #1; GAS GENERATION RATE #8.

SDATA(NSDATA =8,NTDATA=1:214,MKLOS =1)

8.810350E-01, 8.106902E-01, 7.982643E-01, 6.740181E-01, 5.634896E-01,
5.063996E-01, 4.493093E-01, 3.922190E-01, 3.578168E-01, 3.254026E-01,
2.929795E-01, 2.718085E-01, 2.571004E-01, 2.423950E-01, 2.303067E-01,
2.230742E-01, 2.158418E-01, 2.088351E-01, 2.050054E-01, 2.011759E-01,
1.973465E-01, 1.949998E-01, 1.930654E-01, 1.896092E-01, 1.873886E-01,
1.858034E-01, 1.846282E-01, 1.840132E-01, 1.835299E-01, 1.832800E-01,
1.831386E-01, 1.830504E-01, 1.830131E-01, 1.829866E-01, 1.829768E-01,
1.829786E-01, 1.829853E-01, 1.830007E-01, 1.830196E-01, 1.830424E-01,
1.830669E-01, 1.830929E-01, 1.831242E-01, 1.831592E-01, 1.831976E-01,
1.832409E-01, 1.832863E-01, 1.833359E-01, 1.833886E-01, 1.834434E-01,
1.835004E-01, 1.835582E-01, 1.836172E-01, 1.837278E-01, 1.838580E-01,
1.839050E-01, 1.839582E-01, 1.840207E-01, 1.841086E-01, 1.842085E-01,
1.843380E-01, 1.844834E-01, 1.846466E-01, 1.848092E-01, 1.849780E-01,
1.851730E-01, 1.853699E-01, 1.855685E-01, 1.857275E-01, 1.858782E-01,
1.860171E-01, 1.861601E-01, 1.863054E-01, 1.864613E-01, 1.866235E-01,
1.867976E-01, 1.869796E-01, 1.871663E-01, 1.873748E-01, 1.875823E-01,

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1.877888E-01,1.880269E-01,1.882807E-01,1.885783E-01,1.889138E-01,
1.892897E-01,1.897639E-01,1.902735E-01,1.908500E-01,1.914693E-01,
1.921222E-01,1.928367E-01,1.935680E-01,1.943296E-01,1.951269E-01,
1.959453E-01,1.968031E-01,1.976760E-01,1.985767E-01,1.995064E-01,
2.004494E-01,2.014000E-01,2.023661E-01,2.033537E-01,2.043491E-01,
2.053505E-01,2.063760E-01,2.074077E-01,2.084453E-01,2.095035E-01,
2.105695E-01,2.116559E-01,2.127402E-01,2.138122E-01,2.149224E-01,
2.160321E-01,2.171345E-01,2.181832E-01,2.192013E-01,2.199872E-01,
2.207119E-01,2.213259E-01,2.218691E-01,2.223811E-01,2.227996E-01,
2.231914E-01,2.235478E-01,2.238669E-01,2.241702E-01,2.244397E-01,
2.246852E-01,2.249070E-01,2.251141E-01,2.253162E-01,2.255006E-01,
2.256725E-01,2.258354E-01,2.259769E-01,2.261221E-01,2.262805E-01,
2.264237E-01,2.265585E-01,2.266862E-01,2.268148E-01,2.269463E-01,
2.270732E-01,2.271986E-01,2.273224E-01,2.274504E-01,2.275836E-01,
2.277125E-01,2.278402E-01,2.279676E-01,2.280923E-01,2.282155E-01,
2.283284E-01,2.284408E-01,2.285556E-01,2.286684E-01,2.287796E-01,
2.288799E-01,2.289806E-01,2.290840E-01,2.291936E-01,2.293064E-01,
2.294149E-01,2.295202E-01,2.296220E-01,2.297176E-01,2.298101E-01,
2.298954E-01,2.299853E-01,2.300813E-01,2.301648E-01,2.302453E-01,
2.303272E-01,2.304080E-01,2.304886E-01,2.305736E-01,2.306556E-01,
2.307263E-01,2.308029E-01,2.308836E-01,2.309602E-01,2.310400E-01,
2.311278E-01,2.311992E-01,2.312616E-01,2.313381E-01,2.314128E-01,
2.314844E-01,2.315569E-01,2.316295E-01,2.317007E-01,2.317698E-01,
2.318365E-01,2.318992E-01,2.319611E-01,2.320266E-01,2.320965E-01,
2.321702E-01,2.322445E-01,2.323173E-01,2.323848E-01,2.324456E-01,
2.325018E-01,2.325664E-01,2.326336E-01,2.327031E-01,2.327633E-01,
2.328193E-01,2.328832E-01,2.410464E-01,2.410464E-01

POROSITY SURFACE #1; GAS GENERATION RATE #9.

PDATA (NSDATA =9,NTDATA=1:214,MKLOS =1)

1.013250E+05,1.075138E+05,1.137576E+05,1.761884E+05,2.606492E+05,
3.687214E+05,4.767943E+05,5.980646E+05,7.726453E+05,9.471851E+05,
1.121774E+06,1.333713E+06,1.549174E+06,1.764595E+06,1.981759E+06,
2.199905E+06,2.418051E+06,2.632903E+06,2.841627E+06,3.050338E+06,
3.258529E+06,3.458595E+06,3.658864E+06,4.053904E+06,4.440770E+06,
4.819289E+06,5.194672E+06,5.563048E+06,5.929423E+06,6.293441E+06,
6.656425E+06,7.019062E+06,7.381083E+06,7.742886E+06,8.104480E+06,
8.465748E+06,8.826886E+06,9.187801E+06,9.548428E+06,9.908858E+06,
1.026890E+07,1.062863E+07,1.098779E+07,1.134597E+07,1.170370E+07,
1.206049E+07,1.241645E+07,1.277227E+07,1.312724E+07,1.348174E+07,
1.383481E+07,1.418694E+07,1.453789E+07,1.488707E+07,1.523534E+07,
1.558131E+07,1.592564E+07,1.626858E+07,1.660818E+07,1.694624E+07,

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1.728134E+07,1.761259E+07,1.794142E+07,1.826142E+07,1.857749E+07,
1.888612E+07,1.917535E+07,1.944767E+07,1.955385E+07,1.965610E+07,
1.975255E+07,1.984134E+07,1.992675E+07,2.000505E+07,2.007971E+07,
2.015038E+07,2.021588E+07,2.027919E+07,2.033755E+07,2.039318E+07,
2.044661E+07,2.049613E+07,2.054418E+07,2.058930E+07,2.063254E+07,
2.067464E+07,2.071130E+07,2.074769E+07,2.078368E+07,2.081758E+07,
2.085034E+07,2.087926E+07,2.090765E+07,2.093530E+07,2.096164E+07,
2.098736E+07,2.101155E+07,2.103465E+07,2.105660E+07,2.107689E+07,
2.109673E+07,2.111595E+07,2.113411E+07,2.115142E+07,2.116730E+07,
2.118287E+07,2.119795E+07,2.121192E+07,2.122523E+07,2.123722E+07,
2.124850E+07,2.125853E+07,2.127026E+07,2.128265E+07,2.129580E+07,
2.130747E+07,2.131711E+07,2.126464E+07,2.119160E+07,2.109941E+07,
2.101647E+07,2.094313E+07,2.088023E+07,2.082088E+07,2.077048E+07,
2.072382E+07,2.067999E+07,2.064133E+07,2.060470E+07,2.057215E+07,
2.054212E+07,2.051351E+07,2.048691E+07,2.046133E+07,2.043829E+07,
2.041766E+07,2.039817E+07,2.038091E+07,2.036377E+07,2.034677E+07,
2.033339E+07,2.032075E+07,2.030650E+07,2.029488E+07,2.028582E+07,
2.027433E+07,2.026294E+07,2.025332E+07,2.024359E+07,2.023378E+07,
2.022415E+07,2.021484E+07,2.020629E+07,2.019739E+07,2.018821E+07,
2.017961E+07,2.017074E+07,2.016141E+07,2.015203E+07,2.014279E+07,
2.013531E+07,2.012756E+07,2.011947E+07,2.011083E+07,2.010220E+07,
2.009433E+07,2.008617E+07,2.007765E+07,2.006937E+07,2.006110E+07,
2.005275E+07,2.004535E+07,2.003863E+07,2.003148E+07,2.002444E+07,
2.001764E+07,2.001016E+07,2.000231E+07,1.999504E+07,1.998834E+07,
1.998261E+07,1.997633E+07,1.996987E+07,1.996359E+07,1.995713E+07,
1.995042E+07,1.994374E+07,1.993720E+07,1.993096E+07,1.992443E+07,
1.991763E+07,1.991243E+07,1.990714E+07,1.990081E+07,1.989489E+07,
1.988926E+07,1.988371E+07,1.987790E+07,1.987135E+07,1.986567E+07,
1.986043E+07,1.985513E+07,1.984988E+07,1.984473E+07,1.983905E+07,
1.983323E+07,1.982785E+07,1.982260E+07,1.981762E+07,1.981253E+07,
1.980727E+07,1.980139E+07,1.900425E+07,1.900425E+07

POROSITY SURFACE #1; GAS GENERATION RATE #9.

SDATA(NSDATA =9,NTDATA=1:214,MKLOS =1)

8.810350E-01,8.178201E-01,8.042962E-01,6.690713E-01,5.705597E-01,
5.113449E-01,4.521297E-01,3.982915E-01,3.661736E-01,3.340631E-01,
3.019437E-01,2.849836E-01,2.694525E-01,2.539244E-01,2.438808E-01,
2.370716E-01,2.302623E-01,2.247339E-01,2.216370E-01,2.185403E-01,
2.155390E-01,2.140244E-01,2.125082E-01,2.100669E-01,2.085529E-01,
2.076479E-01,2.069941E-01,2.067317E-01,2.065589E-01,2.064911E-01,
2.064637E-01,2.064495E-01,2.064543E-01,2.064647E-01,2.064799E-01,
2.065013E-01,2.065246E-01,2.065512E-01,2.065817E-01,2.066149E-01,

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2.066522E-01, 2.066936E-01, 2.067436E-01, 2.068072E-01, 2.068777E-01,
2.069571E-01, 2.070399E-01, 2.071280E-01, 2.072236E-01, 2.073234E-01,
2.074374E-01, 2.075606E-01, 2.076943E-01, 2.078454E-01, 2.080049E-01,
2.081856E-01, 2.083808E-01, 2.085882E-01, 2.088243E-01, 2.090725E-01,
2.093464E-01, 2.096554E-01, 2.099861E-01, 2.103996E-01, 2.108489E-01,
2.113659E-01, 2.119899E-01, 2.126659E-01, 2.134247E-01, 2.142211E-01,
2.150730E-01, 2.159986E-01, 2.169558E-01, 2.179791E-01, 2.190362E-01,
2.201305E-01, 2.212709E-01, 2.224311E-01, 2.236362E-01, 2.248651E-01,
2.261142E-01, 2.273971E-01, 2.286926E-01, 2.300135E-01, 2.313499E-01,
2.326956E-01, 2.340936E-01, 2.354924E-01, 2.368887E-01, 2.383055E-01,
2.397329E-01, 2.411975E-01, 2.426651E-01, 2.441381E-01, 2.456216E-01,
2.471102E-01, 2.486120E-01, 2.501242E-01, 2.516472E-01, 2.531848E-01,
2.547268E-01, 2.562730E-01, 2.578294E-01, 2.593938E-01, 2.609726E-01,
2.625539E-01, 2.641378E-01, 2.657342E-01, 2.673374E-01, 2.689542E-01,
2.705772E-01, 2.722160E-01, 2.738402E-01, 2.754441E-01, 2.770353E-01,
2.786439E-01, 2.802775E-01, 2.818505E-01, 2.833638E-01, 2.846099E-01,
2.857372E-01, 2.867411E-01, 2.876099E-01, 2.884327E-01, 2.891369E-01,
2.897912E-01, 2.904075E-01, 2.909543E-01, 2.914738E-01, 2.919378E-01,
2.923668E-01, 2.927763E-01, 2.931585E-01, 2.935265E-01, 2.938591E-01,
2.941572E-01, 2.944393E-01, 2.946903E-01, 2.949396E-01, 2.951868E-01,
2.953819E-01, 2.955668E-01, 2.957751E-01, 2.959455E-01, 2.960789E-01,
2.962476E-01, 2.964148E-01, 2.965561E-01, 2.966994E-01, 2.968443E-01,
2.969861E-01, 2.971234E-01, 2.972500E-01, 2.973813E-01, 2.975164E-01,
2.976442E-01, 2.977760E-01, 2.979146E-01, 2.980539E-01, 2.981913E-01,
2.983025E-01, 2.984182E-01, 2.985394E-01, 2.986684E-01, 2.987973E-01,
2.989145E-01, 2.990365E-01, 2.991643E-01, 2.992884E-01, 2.994123E-01,
2.995376E-01, 2.996484E-01, 2.997488E-01, 2.998568E-01, 2.999632E-01,
3.000657E-01, 3.001784E-01, 3.002969E-01, 3.004067E-01, 3.005076E-01,
3.005940E-01, 3.006890E-01, 3.007868E-01, 3.008815E-01, 3.009794E-01,
3.010814E-01, 3.011828E-01, 3.012821E-01, 3.013769E-01, 3.014761E-01,
3.015792E-01, 3.016585E-01, 3.017394E-01, 3.018362E-01, 3.019262E-01,
3.020113E-01, 3.020965E-01, 3.021857E-01, 3.022854E-01, 3.023720E-01,
3.024519E-01, 3.025337E-01, 3.026144E-01, 3.026934E-01, 3.027806E-01,
3.028700E-01, 3.029518E-01, 3.030321E-01, 3.031086E-01, 3.031874E-01,
3.032685E-01, 3.033588E-01, 3.161523E-01, 3.161523E-01

POROSITY SURFACE #1; GAS GENERATION RATE #10.

PDATA(NSDATA =10,NTDATA=1:214,MKLOS =1)

1.013250E+05, 1.086925E+05, 1.161023E+05, 1.901929E+05, 3.072118E+05,
4.320126E+05, 5.568141E+05, 7.235048E+05, 9.227972E+05, 1.122043E+06,
1.336062E+06, 1.588336E+06, 1.840610E+06, 2.092837E+06, 2.336651E+06,
2.580391E+06, 2.824131E+06, 3.061090E+06, 3.295341E+06, 3.529578E+06,

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3.759670E+06,3.984094E+06,4.208745E+06,4.648559E+06,5.081475E+06,
5.503549E+06,5.923576E+06,6.339410E+06,6.754157E+06,7.168293E+06,
7.581461E+06,7.994421E+06,8.406974E+06,8.819289E+06,9.231451E+06,
9.643133E+06,1.005456E+07,1.046570E+07,1.087617E+07,1.128624E+07,
1.169505E+07,1.210323E+07,1.251083E+07,1.291733E+07,1.332339E+07,
1.372833E+07,1.413129E+07,1.453369E+07,1.493358E+07,1.533241E+07,
1.572905E+07,1.612313E+07,1.651567E+07,1.690391E+07,1.729020E+07,
1.767311E+07,1.804912E+07,1.842162E+07,1.878447E+07,1.913899E+07,
1.948317E+07,1.979765E+07,2.009695E+07,2.035470E+07,2.058875E+07,
2.080032E+07,2.097749E+07,2.110928E+07,2.110510E+07,2.110748E+07,
2.111450E+07,2.112918E+07,2.114590E+07,2.116630E+07,2.118757E+07,
2.120928E+07,2.122981E+07,2.125087E+07,2.127281E+07,2.129374E+07,
2.131417E+07,2.133310E+07,2.135198E+07,2.137079E+07,2.138817E+07,
2.140511E+07,2.142161E+07,2.143722E+07,2.145201E+07,2.146616E+07,
2.147974E+07,2.149176E+07,2.150268E+07,2.151287E+07,2.152426E+07,
2.153523E+07,2.154512E+07,2.155460E+07,2.156384E+07,2.157105E+07,
2.157860E+07,2.158671E+07,2.159387E+07,2.160065E+07,2.160692E+07,
2.161302E+07,2.161891E+07,2.162403E+07,2.162909E+07,2.163465E+07,
2.164002E+07,2.164522E+07,2.165070E+07,2.165582E+07,2.165982E+07,
2.166361E+07,2.166727E+07,2.160653E+07,2.153142E+07,2.143088E+07,
2.134323E+07,2.126225E+07,2.119426E+07,2.112978E+07,2.107233E+07,
2.102076E+07,2.097175E+07,2.092781E+07,2.088615E+07,2.084711E+07,
2.081186E+07,2.077790E+07,2.074620E+07,2.071690E+07,2.069020E+07,
2.066544E+07,2.064206E+07,2.062208E+07,2.060181E+07,2.058135E+07,
2.056205E+07,2.054317E+07,2.052513E+07,2.050945E+07,2.049483E+07,
2.048190E+07,2.046848E+07,2.045435E+07,2.044277E+07,2.043203E+07,
2.042153E+07,2.041142E+07,2.040177E+07,2.039345E+07,2.038534E+07,
2.037730E+07,2.036962E+07,2.036224E+07,2.035485E+07,2.034748E+07,
2.034014E+07,2.033294E+07,2.032585E+07,2.031918E+07,2.031253E+07,
2.030579E+07,2.029894E+07,2.029197E+07,2.028461E+07,2.027763E+07,
2.027123E+07,2.026538E+07,2.025957E+07,2.025283E+07,2.024592E+07,
2.023876E+07,2.023310E+07,2.022755E+07,2.022136E+07,2.021541E+07,
2.020966E+07,2.020436E+07,2.019888E+07,2.019280E+07,2.018706E+07,
2.018152E+07,2.017598E+07,2.017029E+07,2.016422E+07,2.015835E+07,
2.015257E+07,2.014682E+07,2.014133E+07,2.013621E+07,2.013100E+07,
2.012575E+07,2.012041E+07,2.011496E+07,2.010933E+07,2.010322E+07,
2.009741E+07,2.009309E+07,2.008862E+07,2.008403E+07,2.007928E+07,
2.007459E+07,2.007008E+07,2.006470E+07,2.005891E+07,2.005422E+07,
2.004950E+07,2.004473E+07,1.918239E+07,1.918239E+07

POROSITY SURFACE #1; GAS GENERATION RATE #10.
SDATA (NSDATA =10,NTDATA=1:214,MKLOS =1)

Information Only

8.810350E-01, 8.186546E-01, 8.036798E-01, 6.539479E-01, 5.778739E-01,
5.151116E-01, 4.523489E-01, 4.065616E-01, 3.739860E-01, 3.414181E-01,
3.132264E-01, 2.964396E-01, 2.796528E-01, 2.628692E-01, 2.566008E-01,
2.504054E-01, 2.442100E-01, 2.404081E-01, 2.375888E-01, 2.347696E-01,
2.325940E-01, 2.312921E-01, 2.299890E-01, 2.282314E-01, 2.271121E-01,
2.266635E-01, 2.263499E-01, 2.262456E-01, 2.261891E-01, 2.261593E-01,
2.261630E-01, 2.261723E-01, 2.261918E-01, 2.262157E-01, 2.262419E-01,
2.262761E-01, 2.263134E-01, 2.263549E-01, 2.264061E-01, 2.264631E-01,
2.265395E-01, 2.266227E-01, 2.267125E-01, 2.268130E-01, 2.269182E-01,
2.270340E-01, 2.271667E-01, 2.273121E-01, 2.274830E-01, 2.276644E-01,
2.278669E-01, 2.280949E-01, 2.283369E-01, 2.286201E-01, 2.289211E-01,
2.292528E-01, 2.296548E-01, 2.300919E-01, 2.306219E-01, 2.312351E-01,
2.319544E-01, 2.329887E-01, 2.341829E-01, 2.358112E-01, 2.376791E-01,
2.397740E-01, 2.422055E-01, 2.446613E-01, 2.470384E-01, 2.492772E-01,
2.514182E-01, 2.534645E-01, 2.554836E-01, 2.574551E-01, 2.594113E-01,
2.613598E-01, 2.633172E-01, 2.652653E-01, 2.671980E-01, 2.691384E-01,
2.710837E-01, 2.730426E-01, 2.749994E-01, 2.769539E-01, 2.789231E-01,
2.808960E-01, 2.828692E-01, 2.848527E-01, 2.868433E-01, 2.888403E-01,
2.908437E-01, 2.928652E-01, 2.948984E-01, 2.969405E-01, 2.989640E-01,
3.009921E-01, 3.030325E-01, 3.050769E-01, 3.071241E-01, 3.091969E-01,
3.112644E-01, 3.133224E-01, 3.153923E-01, 3.174670E-01, 3.195472E-01,
3.216296E-01, 3.237140E-01, 3.258082E-01, 3.279026E-01, 3.299881E-01,
3.320737E-01, 3.341625E-01, 3.362568E-01, 3.383433E-01, 3.404463E-01,
3.425514E-01, 3.446589E-01, 3.466867E-01, 3.485897E-01, 3.502333E-01,
3.516786E-01, 3.530211E-01, 3.541613E-01, 3.552463E-01, 3.562186E-01,
3.570970E-01, 3.579343E-01, 3.586909E-01, 3.594100E-01, 3.600860E-01,
3.606985E-01, 3.612897E-01, 3.618449E-01, 3.623590E-01, 3.628284E-01,
3.632658E-01, 3.636794E-01, 3.640335E-01, 3.643932E-01, 3.647565E-01,
3.651011E-01, 3.654382E-01, 3.657611E-01, 3.660420E-01, 3.663042E-01,
3.665369E-01, 3.667784E-01, 3.670330E-01, 3.672421E-01, 3.674362E-01,
3.676263E-01, 3.678091E-01, 3.679836E-01, 3.681342E-01, 3.682815E-01,
3.684284E-01, 3.685681E-01, 3.687019E-01, 3.688367E-01, 3.689715E-01,
3.691055E-01, 3.692365E-01, 3.693657E-01, 3.694879E-01, 3.696095E-01,
3.697316E-01, 3.698568E-01, 3.699844E-01, 3.701201E-01, 3.702484E-01,
3.703660E-01, 3.704732E-01, 3.705797E-01, 3.707035E-01, 3.708308E-01,
3.709634E-01, 3.710679E-01, 3.711703E-01, 3.712847E-01, 3.713942E-01,
3.714999E-01, 3.715979E-01, 3.716991E-01, 3.718112E-01, 3.719171E-01,
3.720194E-01, 3.721228E-01, 3.722286E-01, 3.723408E-01, 3.724497E-01,
3.725571E-01, 3.726647E-01, 3.727671E-01, 3.728623E-01, 3.729595E-01,
3.730573E-01, 3.731560E-01, 3.732576E-01, 3.733629E-01, 3.734768E-01,
3.735850E-01, 3.736656E-01, 3.737491E-01, 3.738348E-01, 3.739239E-01,

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3.740120E-01, 3.740965E-01, 3.741970E-01, 3.743052E-01, 3.743936E-01,
3.744824E-01, 3.745721E-01, 3.915004E-01, 3.915004E-01
POROSITY SURFACE #1; GAS GENERATION RATE #11.
PDATA (NSDATA =11, NTDATA=1:214, MKLOS =1)
1.013250E+05, 1.107756E+05, 1.202943E+05, 2.154709E+05, 3.335003E+05,
4.950159E+05, 6.565325E+05, 8.228237E+05, 1.063589E+06, 1.304297E+06,
1.545073E+06, 1.821084E+06, 2.107289E+06, 2.393440E+06, 2.671510E+06,
2.941113E+06, 3.210716E+06, 3.476908E+06, 3.730259E+06, 3.983594E+06,
4.236929E+06, 4.481544E+06, 4.725673E+06, 5.208759E+06, 5.681620E+06,
6.148741E+06, 6.613720E+06, 7.076054E+06, 7.538127E+06, 7.999771E+06,
8.461013E+06, 8.922083E+06, 9.382660E+06, 9.842990E+06, 1.030301E+07,
1.076225E+07, 1.122107E+07, 1.167876E+07, 1.213562E+07, 1.259176E+07,
1.304666E+07, 1.350095E+07, 1.395389E+07, 1.440477E+07, 1.485438E+07,
1.530099E+07, 1.574563E+07, 1.618814E+07, 1.662755E+07, 1.706522E+07,
1.749603E+07, 1.792311E+07, 1.834446E+07, 1.875560E+07, 1.916105E+07,
1.954825E+07, 1.991438E+07, 2.025710E+07, 2.054926E+07, 2.082030E+07,
2.104520E+07, 2.124423E+07, 2.142182E+07, 2.156791E+07, 2.170243E+07,
2.181378E+07, 2.190347E+07, 2.197988E+07, 2.191353E+07, 2.185488E+07,
2.181821E+07, 2.179576E+07, 2.178009E+07, 2.177305E+07, 2.176860E+07,
2.176792E+07, 2.176823E+07, 2.176924E+07, 2.177313E+07, 2.177730E+07,
2.178179E+07, 2.178563E+07, 2.178950E+07, 2.179398E+07, 2.179920E+07,
2.180500E+07, 2.181310E+07, 2.182009E+07, 2.182347E+07, 2.182763E+07,
2.183225E+07, 2.183578E+07, 2.183913E+07, 2.184218E+07, 2.184635E+07,
2.185096E+07, 2.185479E+07, 2.185813E+07, 2.186078E+07, 2.186335E+07,
2.186607E+07, 2.186992E+07, 2.187336E+07, 2.187638E+07, 2.187792E+07,
2.187943E+07, 2.188181E+07, 2.188344E+07, 2.188450E+07, 2.188602E+07,
2.188732E+07, 2.188792E+07, 2.188933E+07, 2.189119E+07, 2.189143E+07,
2.189243E+07, 2.189479E+07, 2.183620E+07, 2.175163E+07, 2.165108E+07,
2.155800E+07, 2.147518E+07, 2.140299E+07, 2.133455E+07, 2.127503E+07,
2.121949E+07, 2.116793E+07, 2.112041E+07, 2.107469E+07, 2.103310E+07,
2.099440E+07, 2.095786E+07, 2.092450E+07, 2.089180E+07, 2.086118E+07,
2.083235E+07, 2.080447E+07, 2.077880E+07, 2.075405E+07, 2.073091E+07,
2.070886E+07, 2.068741E+07, 2.066804E+07, 2.064952E+07, 2.063196E+07,
2.061624E+07, 2.060109E+07, 2.058677E+07, 2.057320E+07, 2.056038E+07,
2.054714E+07, 2.053422E+07, 2.052267E+07, 2.051127E+07, 2.049987E+07,
2.048980E+07, 2.048028E+07, 2.047188E+07, 2.046337E+07, 2.045482E+07,
2.044795E+07, 2.044117E+07, 2.043454E+07, 2.042810E+07, 2.042176E+07,
2.041565E+07, 2.040986E+07, 2.040441E+07, 2.039924E+07, 2.039408E+07,
2.038855E+07, 2.038309E+07, 2.037768E+07, 2.037252E+07, 2.036745E+07,
2.036254E+07, 2.035733E+07, 2.035186E+07, 2.034660E+07, 2.034131E+07,
2.033591E+07, 2.033064E+07, 2.032544E+07, 2.032022E+07, 2.031519E+07,

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2.031049E+07,2.030607E+07,2.030177E+07,2.029706E+07,2.029232E+07,
2.028757E+07,2.028292E+07,2.027832E+07,2.027394E+07,2.026957E+07,
2.026520E+07,2.026039E+07,2.025565E+07,2.025118E+07,2.024682E+07,
2.024255E+07,2.023806E+07,2.023374E+07,2.022985E+07,2.022651E+07,
2.022343E+07,2.021993E+07,2.021634E+07,2.021272E+07,2.020874E+07,
2.020459E+07,2.019998E+07,1.929467E+07,1.929467E+07

POROSITY SURFACE #1; GAS GENERATION RATE #11.

SDATA(NSDATA =11,NTDATA=1:214,MKLOS =1)

8.810350E-01,8.206745E-01,8.074997E-01,6.757653E-01,5.703730E-01,
5.150381E-01,4.597029E-01,4.060090E-01,3.779154E-01,3.498283E-01,
3.217335E-01,3.045506E-01,2.905232E-01,2.764985E-01,2.669150E-01,
2.619383E-01,2.569616E-01,2.526152E-01,2.506863E-01,2.487575E-01,
2.468288E-01,2.459176E-01,2.450916E-01,2.437899E-01,2.432324E-01,
2.429616E-01,2.428315E-01,2.428168E-01,2.428118E-01,2.428219E-01,
2.428409E-01,2.428641E-01,2.428963E-01,2.429325E-01,2.429734E-01,
2.430269E-01,2.430870E-01,2.431643E-01,2.432531E-01,2.433519E-01,
2.434627E-01,2.435802E-01,2.437128E-01,2.438706E-01,2.440445E-01,
2.442501E-01,2.444701E-01,2.447184E-01,2.449968E-01,2.452923E-01,
2.456604E-01,2.460675E-01,2.465330E-01,2.471074E-01,2.477420E-01,
2.485707E-01,2.496356E-01,2.509632E-01,2.528500E-01,2.549648E-01,
2.575751E-01,2.604551E-01,2.635588E-01,2.669786E-01,2.705169E-01,
2.742938E-01,2.781395E-01,2.820253E-01,2.855150E-01,2.888579E-01,
2.919281E-01,2.948145E-01,2.976125E-01,3.002976E-01,3.029472E-01,
3.055454E-01,3.081295E-01,3.107034E-01,3.132359E-01,3.157621E-01,
3.182833E-01,3.208135E-01,3.233427E-01,3.258610E-01,3.283672E-01,
3.308637E-01,3.333227E-01,3.357988E-01,3.383260E-01,3.408423E-01,
3.433508E-01,3.458756E-01,3.484019E-01,3.509330E-01,3.534441E-01,
3.559476E-01,3.584638E-01,3.609870E-01,3.635200E-01,3.660535E-01,
3.685851E-01,3.710960E-01,3.736131E-01,3.761367E-01,3.786858E-01,
3.812354E-01,3.837683E-01,3.863140E-01,3.888690E-01,3.914166E-01,
3.939656E-01,3.965280E-01,3.990897E-01,4.016279E-01,4.041945E-01,
4.067463E-01,4.092735E-01,4.116982E-01,4.140508E-01,4.159864E-01,
4.177881E-01,4.194063E-01,4.208288E-01,4.221831E-01,4.233714E-01,
4.244840E-01,4.255210E-01,4.264842E-01,4.274137E-01,4.282641E-01,
4.290571E-01,4.298071E-01,4.304957E-01,4.311726E-01,4.318096E-01,
4.324106E-01,4.329922E-01,4.335305E-01,4.340501E-01,4.345368E-01,
4.350010E-01,4.354530E-01,4.358636E-01,4.362564E-01,4.366291E-01,
4.369637E-01,4.372865E-01,4.375936E-01,4.378842E-01,4.381587E-01,
4.384416E-01,4.387180E-01,4.389662E-01,4.392119E-01,4.394582E-01,
4.396752E-01,4.398803E-01,4.400608E-01,4.402446E-01,4.404297E-01,
4.405785E-01,4.407257E-01,4.408699E-01,4.410096E-01,4.411470E-01,

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4.412800E-01, 4.414059E-01, 4.415247E-01, 4.416372E-01, 4.417493E-01,
4.418683E-01, 4.419873E-01, 4.421065E-01, 4.422187E-01, 4.423287E-01,
4.424361E-01, 4.425501E-01, 4.426693E-01, 4.427843E-01, 4.428998E-01,
4.430176E-01, 4.431335E-01, 4.432482E-01, 4.433630E-01, 4.434730E-01,
4.435749E-01, 4.436719E-01, 4.437668E-01, 4.438704E-01, 4.439748E-01,
4.440802E-01, 4.441816E-01, 4.442816E-01, 4.443790E-01, 4.444756E-01,
4.445713E-01, 4.446782E-01, 4.447831E-01, 4.448807E-01, 4.449763E-01,
4.450706E-01, 4.451712E-01, 4.452670E-01, 4.453516E-01, 4.454255E-01,
4.454941E-01, 4.455723E-01, 4.456520E-01, 4.457319E-01, 4.458203E-01,
4.459127E-01, 4.460138E-01, 4.670521E-01, 4.670521E-01

POROSITY SURFACE #1; GAS GENERATION RATE #12.

PDATA (NSDATA =12, NTDATA=1:214, MKLOS =1)

1.013250E+05, 1.139705E+05, 1.268619E+05, 2.557623E+05, 4.022974E+05,
6.154264E+05, 8.285568E+05, 1.041687E+06, 1.331579E+06, 1.627615E+06,
1.923733E+06, 2.245559E+06, 2.581824E+06, 2.918025E+06, 3.249504E+06,
3.572263E+06, 3.895022E+06, 4.215587E+06, 4.508465E+06, 4.801325E+06,
5.094184E+06, 5.378677E+06, 5.661206E+06, 6.223365E+06, 6.778216E+06,
7.330958E+06, 7.883256E+06, 8.434602E+06, 8.985734E+06, 9.536451E+06,
1.008654E+07, 1.063632E+07, 1.118499E+07, 1.173291E+07, 1.227966E+07,
1.282482E+07, 1.336919E+07, 1.391159E+07, 1.445228E+07, 1.499101E+07,
1.552600E+07, 1.605935E+07, 1.658904E+07, 1.711380E+07, 1.763452E+07,
1.814581E+07, 1.865154E+07, 1.914671E+07, 1.962477E+07, 2.009219E+07,
2.049482E+07, 2.086785E+07, 2.118478E+07, 2.145133E+07, 2.169242E+07,
2.187818E+07, 2.204561E+07, 2.218623E+07, 2.229916E+07, 2.240059E+07,
2.248103E+07, 2.255252E+07, 2.261430E+07, 2.266183E+07, 2.270492E+07,
2.274113E+07, 2.275744E+07, 2.275767E+07, 2.265094E+07, 2.254658E+07,
2.247785E+07, 2.242339E+07, 2.237748E+07, 2.234903E+07, 2.232406E+07,
2.230522E+07, 2.228899E+07, 2.227411E+07, 2.226285E+07, 2.225219E+07,
2.224238E+07, 2.223551E+07, 2.222953E+07, 2.222376E+07, 2.221813E+07,
2.221265E+07, 2.221082E+07, 2.220916E+07, 2.220556E+07, 2.220214E+07,
2.219886E+07, 2.219630E+07, 2.219403E+07, 2.219235E+07, 2.219020E+07,
2.218777E+07, 2.218539E+07, 2.218274E+07, 2.217958E+07, 2.217825E+07,
2.217751E+07, 2.217445E+07, 2.217159E+07, 2.216901E+07, 2.216582E+07,
2.216260E+07, 2.216023E+07, 2.215807E+07, 2.215612E+07, 2.215301E+07,
2.214980E+07, 2.214695E+07, 2.214445E+07, 2.214223E+07, 2.214194E+07,
2.214095E+07, 2.213789E+07, 2.207738E+07, 2.198498E+07, 2.187999E+07,
2.178178E+07, 2.169593E+07, 2.161930E+07, 2.154650E+07, 2.148395E+07,
2.142437E+07, 2.136869E+07, 2.131803E+07, 2.126942E+07, 2.122495E+07,
2.118244E+07, 2.114184E+07, 2.110444E+07, 2.106785E+07, 2.103389E+07,
2.100144E+07, 2.097005E+07, 2.094126E+07, 2.091325E+07, 2.088666E+07,
2.086143E+07, 2.083695E+07, 2.081434E+07, 2.079233E+07, 2.077116E+07,

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2.075117E+07,2.073166E+07,2.071333E+07,2.069575E+07,2.067911E+07,
2.066324E+07,2.064769E+07,2.063285E+07,2.061880E+07,2.060539E+07,
2.059250E+07,2.057981E+07,2.056764E+07,2.055604E+07,2.054486E+07,
2.053444E+07,2.052434E+07,2.051486E+07,2.050618E+07,2.049791E+07,
2.048958E+07,2.048175E+07,2.047464E+07,2.046774E+07,2.046096E+07,
2.045464E+07,2.044874E+07,2.044336E+07,2.043824E+07,2.043332E+07,
2.042907E+07,2.042476E+07,2.042035E+07,2.041648E+07,2.041262E+07,
2.040858E+07,2.040462E+07,2.040074E+07,2.039697E+07,2.039319E+07,
2.038936E+07,2.038548E+07,2.038162E+07,2.037788E+07,2.037432E+07,
2.037104E+07,2.036786E+07,2.036464E+07,2.036075E+07,2.035704E+07,
2.035353E+07,2.035008E+07,2.034678E+07,2.034390E+07,2.034086E+07,
2.033767E+07,2.033499E+07,2.033232E+07,2.032944E+07,2.032635E+07,
2.032312E+07,2.032029E+07,2.031731E+07,2.031408E+07,2.031066E+07,
2.030716E+07,2.030437E+07,1.942159E+07,1.942159E+07

POROSITY SURFACE #1; GAS GENERATION RATE #12.

SDATA(NSDATA =12,NTDATA=1:214,MKLOS =1)

8.810350E-01,8.128521E-01,8.005670E-01,6.777283E-01,5.699072E-01,
5.186972E-01,4.674869E-01,4.162765E-01,3.897323E-01,3.651903E-01,
3.406414E-01,3.240459E-01,3.119130E-01,2.997825E-01,2.902756E-01,
2.855218E-01,2.807681E-01,2.762674E-01,2.750491E-01,2.738309E-01,
2.726127E-01,2.720759E-01,2.717232E-01,2.711621E-01,2.710289E-01,
2.709689E-01,2.709556E-01,2.709740E-01,2.709979E-01,2.710314E-01,
2.710765E-01,2.711279E-01,2.711972E-01,2.712793E-01,2.713807E-01,
2.715052E-01,2.716400E-01,2.717978E-01,2.719782E-01,2.721840E-01,
2.724350E-01,2.727041E-01,2.730115E-01,2.733785E-01,2.737957E-01,
2.743178E-01,2.748947E-01,2.755981E-01,2.765033E-01,2.775339E-01,
2.793655E-01,2.815535E-01,2.844135E-01,2.878576E-01,2.915949E-01,
2.959553E-01,3.005203E-01,3.053844E-01,3.105622E-01,3.158674E-01,
3.214068E-01,3.270476E-01,3.327986E-01,3.387227E-01,3.446988E-01,
3.507505E-01,3.568332E-01,3.629388E-01,3.682466E-01,3.732771E-01,
3.777672E-01,3.820377E-01,3.861752E-01,3.900337E-01,3.938355E-01,
3.975370E-01,4.011988E-01,4.048399E-01,4.084203E-01,4.119908E-01,
4.155499E-01,4.190581E-01,4.225509E-01,4.260417E-01,4.295317E-01,
4.330206E-01,4.364374E-01,4.398525E-01,4.433041E-01,4.467560E-01,
4.502055E-01,4.536432E-01,4.570739E-01,4.604931E-01,4.639236E-01,
4.673606E-01,4.707973E-01,4.742399E-01,4.776938E-01,4.811095E-01,
4.845143E-01,4.879686E-01,4.914195E-01,4.948658E-01,4.983272E-01,
5.017899E-01,5.052330E-01,5.086723E-01,5.121064E-01,5.155707E-01,
5.190346E-01,5.224922E-01,5.259607E-01,5.294027E-01,5.328000E-01,
5.362135E-01,5.396795E-01,5.429765E-01,5.461785E-01,5.488211E-01,
5.513031E-01,5.534940E-01,5.554662E-01,5.573483E-01,5.589799E-01,

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5.605399E-01,5.620058E-01,5.633484E-01,5.646407E-01,5.658313E-01,
5.669728E-01,5.680662E-01,5.690793E-01,5.700719E-01,5.709960E-01,
5.718824E-01,5.727422E-01,5.735339E-01,5.743057E-01,5.750414E-01,
5.757403E-01,5.764190E-01,5.770478E-01,5.776613E-01,5.782532E-01,
5.788133E-01,5.793607E-01,5.798748E-01,5.803698E-01,5.808402E-01,
5.812874E-01,5.817259E-01,5.821481E-01,5.825477E-01,5.829289E-01,
5.832960E-01,5.836572E-01,5.840034E-01,5.843335E-01,5.846522E-01,
5.849522E-01,5.852429E-01,5.855142E-01,5.857627E-01,5.859990E-01,
5.862378E-01,5.864628E-01,5.866690E-01,5.868678E-01,5.870628E-01,
5.872465E-01,5.874165E-01,5.875695E-01,5.877186E-01,5.878622E-01,
5.879836E-01,5.881078E-01,5.882357E-01,5.883478E-01,5.884596E-01,
5.885774E-01,5.886921E-01,5.888047E-01,5.889150E-01,5.890253E-01,
5.891355E-01,5.892486E-01,5.893613E-01,5.894691E-01,5.895720E-01,
5.896671E-01,5.897602E-01,5.898547E-01,5.899677E-01,5.900760E-01,
5.901789E-01,5.902786E-01,5.903740E-01,5.904590E-01,5.905480E-01,
5.906407E-01,5.907175E-01,5.907948E-01,5.908797E-01,5.909709E-01,
5.910663E-01,5.911493E-01,5.912360E-01,5.913289E-01,5.914288E-01,
5.915313E-01,5.916139E-01,6.186466E-01,6.186466E-01

POROSITY SURFACE #1; GAS GENERATION RATE #13.

PDATA(NSDATA =13,NTDATA=1:214,MKLOS =1)

1.013250E+05,1.134578E+05,1.262180E+05,2.762811E+05,4.663713E+05,
6.930938E+05,9.537801E+05,1.245543E+06,1.565859E+06,1.905497E+06,
2.258470E+06,2.621871E+06,2.990341E+06,3.359211E+06,3.722429E+06,
4.078590E+06,4.426367E+06,4.765534E+06,5.097235E+06,5.423515E+06,
5.745820E+06,6.064451E+06,6.380449E+06,7.007127E+06,7.631034E+06,
8.252956E+06,8.874625E+06,9.495989E+06,1.011680E+07,1.073664E+07,
1.135533E+07,1.197400E+07,1.259034E+07,1.320502E+07,1.381789E+07,
1.442908E+07,1.503726E+07,1.564275E+07,1.624492E+07,1.684318E+07,
1.743616E+07,1.802241E+07,1.860004E+07,1.916678E+07,1.971999E+07,
2.024894E+07,2.073022E+07,2.114975E+07,2.150410E+07,2.180404E+07,
2.205244E+07,2.225696E+07,2.242392E+07,2.256178E+07,2.267104E+07,
2.276384E+07,2.283979E+07,2.290218E+07,2.295476E+07,2.299645E+07,
2.303026E+07,2.305656E+07,2.308194E+07,2.310241E+07,2.311732E+07,
2.312957E+07,2.314026E+07,2.311710E+07,2.296195E+07,2.284994E+07,
2.276414E+07,2.270023E+07,2.265208E+07,2.261045E+07,2.257637E+07,
2.254677E+07,2.251987E+07,2.250015E+07,2.248420E+07,2.246929E+07,
2.245650E+07,2.244493E+07,2.243259E+07,2.242088E+07,2.241191E+07,
2.240283E+07,2.239486E+07,2.238733E+07,2.238204E+07,2.237582E+07,
2.236957E+07,2.236384E+07,2.235552E+07,2.234989E+07,2.234439E+07,
2.233965E+07,2.233383E+07,2.232932E+07,2.232274E+07,2.231798E+07,
2.231412E+07,2.230859E+07,2.230388E+07,2.229790E+07,2.229243E+07,

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2.228716E+07, 2.228358E+07, 2.227823E+07, 2.227411E+07, 2.226863E+07,
2.226355E+07, 2.225794E+07, 2.225376E+07, 2.224959E+07, 2.224453E+07,
2.223920E+07, 2.223432E+07, 2.219944E+07, 2.207663E+07, 2.196667E+07,
2.186890E+07, 2.178274E+07, 2.170412E+07, 2.163138E+07, 2.156502E+07,
2.150343E+07, 2.144689E+07, 2.139336E+07, 2.134358E+07, 2.129663E+07,
2.125225E+07, 2.121085E+07, 2.117110E+07, 2.113307E+07, 2.109684E+07,
2.106243E+07, 2.102951E+07, 2.099774E+07, 2.096743E+07, 2.093813E+07,
2.090996E+07, 2.088291E+07, 2.085723E+07, 2.083239E+07, 2.080855E+07,
2.078586E+07, 2.076397E+07, 2.074323E+07, 2.072327E+07, 2.070406E+07,
2.068564E+07, 2.066781E+07, 2.065073E+07, 2.063419E+07, 2.061836E+07,
2.060320E+07, 2.058879E+07, 2.057490E+07, 2.056140E+07, 2.054858E+07,
2.053613E+07, 2.052421E+07, 2.051274E+07, 2.050179E+07, 2.049116E+07,
2.048094E+07, 2.047096E+07, 2.046177E+07, 2.045244E+07, 2.044381E+07,
2.043559E+07, 2.042750E+07, 2.041982E+07, 2.041231E+07, 2.040530E+07,
2.039848E+07, 2.039224E+07, 2.038645E+07, 2.038039E+07, 2.037489E+07,
2.036945E+07, 2.036428E+07, 2.035940E+07, 2.035493E+07, 2.035071E+07,
2.034645E+07, 2.034241E+07, 2.033885E+07, 2.033529E+07, 2.033202E+07,
2.032885E+07, 2.032577E+07, 2.032314E+07, 2.032058E+07, 2.031790E+07,
2.031520E+07, 2.031306E+07, 2.031054E+07, 2.030786E+07, 2.030599E+07,
2.030366E+07, 2.030183E+07, 2.029979E+07, 2.029786E+07, 2.029605E+07,
2.029380E+07, 2.029190E+07, 2.028993E+07, 2.028801E+07, 2.028575E+07,
2.028364E+07, 2.028181E+07, 1.955846E+07, 1.955846E+07

POROSITY SURFACE #1; GAS GENERATION RATE #13.

SDATA (NSDATA =13, NTDATA=1:214, MKLOS =1)

8.810350E-01, 7.875822E-01, 7.691885E-01, 6.495094E-01, 5.695103E-01,
5.089608E-01, 4.618662E-01, 4.249945E-01, 3.964172E-01, 3.736529E-01,
3.556851E-01, 3.412639E-01, 3.300894E-01, 3.214436E-01, 3.149950E-01,
3.102492E-01, 3.068731E-01, 3.046081E-01, 3.030951E-01, 3.020709E-01,
3.013774E-01, 3.009435E-01, 3.006971E-01, 3.004796E-01, 3.004093E-01,
3.003997E-01, 3.004225E-01, 3.004500E-01, 3.004931E-01, 3.005570E-01,
3.006456E-01, 3.007256E-01, 3.008527E-01, 3.010065E-01, 3.011855E-01,
3.013859E-01, 3.016296E-01, 3.019068E-01, 3.022254E-01, 3.025919E-01,
3.030257E-01, 3.035432E-01, 3.041715E-01, 3.049340E-01, 3.058653E-01,
3.071138E-01, 3.089994E-01, 3.117225E-01, 3.152959E-01, 3.195538E-01,
3.244534E-01, 3.298979E-01, 3.358011E-01, 3.420655E-01, 3.486913E-01,
3.555140E-01, 3.625493E-01, 3.697558E-01, 3.770871E-01, 3.845618E-01,
3.921484E-01, 3.998443E-01, 4.075373E-01, 4.153031E-01, 4.231570E-01,
4.310503E-01, 4.389612E-01, 4.469029E-01, 4.540244E-01, 4.603685E-01,
4.662352E-01, 4.716917E-01, 4.768405E-01, 4.818776E-01, 4.867671E-01,
4.915726E-01, 4.963325E-01, 5.009436E-01, 5.054744E-01, 5.099888E-01,
5.144628E-01, 5.189142E-01, 5.233841E-01, 5.278478E-01, 5.322502E-01,

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5.366584E-01,5.410426E-01,5.454201E-01,5.497396E-01,5.540894E-01,
5.584427E-01,5.627869E-01,5.671946E-01,5.715411E-01,5.758846E-01,
5.802096E-01,5.845662E-01,5.888911E-01,5.932711E-01,5.976058E-01,
6.019160E-01,6.062743E-01,6.106134E-01,6.149907E-01,6.193536E-01,
6.237133E-01,6.280292E-01,6.323930E-01,6.367279E-01,6.411025E-01,
6.454626E-01,6.498447E-01,6.542088E-01,6.585495E-01,6.629157E-01,
6.672919E-01,6.716569E-01,6.759878E-01,6.798750E-01,6.832972E-01,
6.863670E-01,6.890915E-01,6.915981E-01,6.939371E-01,6.960824E-01,
6.980863E-01,6.999334E-01,7.016960E-01,7.033383E-01,7.048945E-01,
7.063753E-01,7.077632E-01,7.090978E-01,7.103780E-01,7.116016E-01,
7.127735E-01,7.138919E-01,7.149804E-01,7.160180E-01,7.170250E-01,
7.179933E-01,7.189300E-01,7.198193E-01,7.206834E-01,7.215116E-01,
7.222995E-01,7.230694E-01,7.237945E-01,7.244927E-01,7.251711E-01,
7.258194E-01,7.264501E-01,7.270530E-01,7.276372E-01,7.281992E-01,
7.287392E-01,7.292498E-01,7.297438E-01,7.302267E-01,7.306868E-01,
7.311311E-01,7.315567E-01,7.319682E-01,7.323578E-01,7.327433E-01,
7.331092E-01,7.334714E-01,7.338012E-01,7.341375E-01,7.344468E-01,
7.347457E-01,7.350377E-01,7.353152E-01,7.355856E-01,7.358396E-01,
7.360901E-01,7.363121E-01,7.365217E-01,7.367436E-01,7.369430E-01,
7.371441E-01,7.373328E-01,7.375091E-01,7.376715E-01,7.378215E-01,
7.379800E-01,7.381282E-01,7.382539E-01,7.383854E-01,7.385065E-01,
7.386229E-01,7.387346E-01,7.388297E-01,7.389218E-01,7.390197E-01,
7.391189E-01,7.391997E-01,7.392901E-01,7.393867E-01,7.394560E-01,
7.395437E-01,7.396087E-01,7.396866E-01,7.397576E-01,7.398231E-01,
7.399021E-01,7.399742E-01,7.400475E-01,7.401146E-01,7.401974E-01,
7.402756E-01,7.403433E-01,7.678674E-01,7.678674E-01

POROSTIY SURFACE #2, FOR NORTH END w/o BACKFILL.

PDATA(1:NSDATA,1:NTDATA,1:MKLOS); NSDATA=13, NTDATA=214, MKLOS=4

FOR POROSITY SURFACE 2 ONLY 7 GAS GENERATION RATES ARE USED. THE OTHERS ARE SET TO 0.

POROSITY SURFACE #2; GAS GENERATION RATE #1.

PDATA(NSDATA =1,NTDATA=1:214,MKLOS =2)

214*1.01325E+05

POROSITY SURFACE #2; GAS GENERATION RATE #1.

SDATA(NSDATA =1,NTDATA=1:214,MKLOS =2)

1.000000E+00,9.534095E-01,9.470812E-01,8.838051E-01,8.276433E-01,
7.861733E-01,7.484064E-01,7.173585E-01,6.885050E-01,6.631673E-01,
6.394564E-01,6.180607E-01,5.981670E-01,5.801631E-01,5.627327E-01,
5.459486E-01,5.297384E-01,5.141009E-01,4.990251E-01,4.844499E-01,
4.704125E-01,4.567995E-01,4.437878E-01,4.192401E-01,3.964874E-01,
3.751767E-01,3.552082E-01,3.364898E-01,3.189151E-01,3.023835E-01,
2.868185E-01,2.720948E-01,2.581651E-01,2.449692E-01,2.324318E-01,

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2.204926E-01,2.091042E-01,1.982134E-01,1.877656E-01,1.777485E-01,
1.681373E-01,1.588992E-01,1.500107E-01,1.414343E-01,1.331526E-01,
1.251745E-01,1.174815E-01,1.100259E-01,1.028175E-01,9.584869E-02,
8.909149E-02,8.254756E-02,7.693901E-02,7.451250E-02,7.300237E-02,
7.189021E-02,7.096414E-02,7.005430E-02,6.912653E-02,6.817738E-02,
6.726335E-02,6.663430E-02,6.604091E-02,6.545031E-02,6.486270E-02,
6.426792E-02,6.365769E-02,6.304918E-02,6.245663E-02,6.186586E-02,
6.127057E-02,6.068765E-02,6.029795E-02,5.993036E-02,5.956467E-02,
5.919965E-02,5.883590E-02,5.846985E-02,5.810694E-02,5.775345E-02,
5.739881E-02,5.704474E-02,5.669228E-02,5.634425E-02,5.600357E-02,
5.566500E-02,5.532663E-02,5.499063E-02,5.466124E-02,5.433156E-02,
5.400286E-02,5.367802E-02,5.335247E-02,5.303295E-02,5.271830E-02,
5.240880E-02,5.210035E-02,5.180037E-02,5.154411E-02,5.133337E-02,
5.112551E-02,5.092030E-02,5.071740E-02,5.051430E-02,5.031270E-02,
5.011605E-02,4.992288E-02,4.973039E-02,4.953898E-02,4.935035E-02,
4.916469E-02,4.897645E-02,4.878863E-02,4.860686E-02,4.842723E-02,
4.824879E-02,4.807188E-02,4.789492E-02,4.772270E-02,4.754869E-02,
4.737678E-02,4.720621E-02,4.703845E-02,4.687104E-02,4.670247E-02,
4.653825E-02,4.637758E-02,4.621634E-02,4.606176E-02,4.590184E-02,
4.574245E-02,4.558406E-02,4.543160E-02,4.527579E-02,4.512643E-02,
4.497860E-02,4.483008E-02,4.467961E-02,4.453317E-02,4.438445E-02,
4.424214E-02,4.410265E-02,4.395699E-02,4.381356E-02,4.367305E-02,
4.353236E-02,4.339238E-02,4.325384E-02,4.311681E-02,4.298572E-02,
4.285369E-02,4.271757E-02,4.258749E-02,4.246131E-02,4.233546E-02,
4.220638E-02,4.208240E-02,4.196041E-02,4.184144E-02,4.172026E-02,
4.159814E-02,4.147748E-02,4.136008E-02,4.124329E-02,4.112522E-02,
4.100843E-02,4.089352E-02,4.078081E-02,4.067128E-02,4.056127E-02,
4.044993E-02,4.033861E-02,4.023044E-02,4.012223E-02,4.001501E-02,
3.991086E-02,3.980735E-02,3.970315E-02,3.960160E-02,3.950125E-02,
3.940188E-02,3.929886E-02,3.919949E-02,3.910088E-02,3.900398E-02,
3.890766E-02,3.880925E-02,3.871312E-02,3.861761E-02,3.852258E-02,
3.842907E-02,3.833798E-02,3.824781E-02,3.815684E-02,3.806357E-02,
3.797260E-02,3.788361E-02,3.779672E-02,3.770721E-02,3.761810E-02,
3.752975E-02,3.744690E-02,3.737379E-02,3.730308E-02,3.723242E-02,
3.716311E-02,3.709546E-02,3.702772E-02,3.695971E-02,3.689402E-02,
3.682877E-02,3.676412E-02,2.272370E-02,2.272370E-02
POROSITY SURFACE #2; GAS GENERATION RATE #2.
PDATA (NSDATA =2,NTDATAB=1:214,MKLOS =2)
1.013250E+05,1.014093E+05,1.015523E+05,1.031616E+05,1.048276E+05,
1.068422E+05,1.089119E+05,1.112513E+05,1.136401E+05,1.162275E+05,
1.188864E+05,1.217844E+05,1.247580E+05,1.279487E+05,1.312437E+05,

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1.347958E+05,1.384441E+05,1.422999E+05,1.463145E+05,1.506277E+05,
1.550551E+05,1.596720E+05,1.644783E+05,1.747817E+05,1.858761E+05,
1.979292E+05,2.108541E+05,2.248434E+05,2.398929E+05,2.560424E+05,
2.733766E+05,2.919586E+05,3.118325E+05,3.331196E+05,3.559474E+05,
3.803980E+05,4.065253E+05,4.344409E+05,4.642741E+05,4.960894E+05,
5.299836E+05,5.660611E+05,6.044208E+05,6.452472E+05,6.886736E+05,
7.347832E+05,7.837028E+05,8.356391E+05,8.905844E+05,9.487232E+05,
1.010075E+06,1.074721E+06,1.142717E+06,1.214201E+06,1.289146E+06,
1.367447E+06,1.449172E+06,1.534210E+06,1.622367E+06,1.713500E+06,
1.790713E+06,1.842637E+06,1.890687E+06,1.940466E+06,1.991106E+06,
2.041159E+06,2.086093E+06,2.130789E+06,2.156297E+06,2.183154E+06,
2.210975E+06,2.239099E+06,2.267275E+06,2.295954E+06,2.324395E+06,
2.353343E+06,2.382465E+06,2.411465E+06,2.440401E+06,2.466799E+06,
2.491822E+06,2.517263E+06,2.542601E+06,2.568024E+06,2.593250E+06,
2.618748E+06,2.644177E+06,2.669713E+06,2.695147E+06,2.720852E+06,
2.746441E+06,2.772027E+06,2.797572E+06,2.823127E+06,2.848799E+06,
2.874385E+06,2.899873E+06,2.925409E+06,2.951050E+06,2.976655E+06,
3.002245E+06,3.027851E+06,3.053427E+06,3.079021E+06,3.104568E+06,
3.130066E+06,3.155509E+06,3.180970E+06,3.206431E+06,3.231807E+06,
3.257115E+06,3.282395E+06,3.307837E+06,3.333101E+06,3.358333E+06,
3.383535E+06,3.414603E+06,3.430426E+06,3.433367E+06,3.436070E+06,
3.438645E+06,3.441352E+06,3.444171E+06,3.446829E+06,3.449510E+06,
3.452169E+06,3.454931E+06,3.457696E+06,3.460426E+06,3.463018E+06,
3.465728E+06,3.468426E+06,3.471103E+06,3.473837E+06,3.476593E+06,
3.479455E+06,3.482072E+06,3.484664E+06,3.487188E+06,3.490022E+06,
3.492730E+06,3.495227E+06,3.497872E+06,3.500402E+06,3.502972E+06,
3.505673E+06,3.508370E+06,3.510792E+06,3.513372E+06,3.515871E+06,
3.518338E+06,3.520822E+06,3.523284E+06,3.525750E+06,3.528186E+06,
3.530631E+06,3.532989E+06,3.535450E+06,3.537854E+06,3.540237E+06,
3.542773E+06,3.545129E+06,3.547447E+06,3.549794E+06,3.552195E+06,
3.554652E+06,3.557018E+06,3.559281E+06,3.561572E+06,3.563860E+06,
3.566201E+06,3.568491E+06,3.570821E+06,3.573039E+06,3.575216E+06,
3.577390E+06,3.579614E+06,3.581895E+06,3.584184E+06,3.586490E+06,
3.588661E+06,3.590758E+06,3.592852E+06,3.595005E+06,3.597172E+06,
3.599267E+06,3.601346E+06,3.603600E+06,3.605719E+06,3.607811E+06,
3.609893E+06,3.611913E+06,3.613967E+06,3.616097E+06,3.618278E+06,
3.620339E+06,3.622438E+06,3.624383E+06,3.626389E+06,3.628372E+06,
3.630401E+06,3.632423E+06,3.634293E+06,3.636176E+06,3.638208E+06,
3.640222E+06,3.642184E+06,3.644082E+06,3.646202E+06,3.647983E+06,
3.649877E+06,3.651749E+06,4.110656E+06,4.110656E+06

POROSITY SURFACE #2; GAS GENERATION RATE #2.

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SDATA (NSDATA =2,NTDATAB=1:214,MKLOS =2)
1.000000E+00,9.565004E-01,9.436509E-01,8.868655E-01,8.322576E-01,
7.909592E-01,7.512482E-01,7.193079E-01,6.888833E-01,6.645635E-01,
6.410119E-01,6.200830E-01,5.997678E-01,5.812253E-01,5.630845E-01,
5.459556E-01,5.292066E-01,5.132826E-01,4.978331E-01,4.832920E-01,
4.692086E-01,4.558917E-01,4.430069E-01,4.189573E-01,3.967271E-01,
3.762620E-01,3.571731E-01,3.392695E-01,3.225206E-01,3.068566E-01,
2.921286E-01,2.782606E-01,2.652192E-01,2.528790E-01,2.411461E-01,
2.299981E-01,2.194328E-01,2.094044E-01,1.998646E-01,1.908099E-01,
1.822177E-01,1.740624E-01,1.663240E-01,1.589588E-01,1.519455E-01,
1.452796E-01,1.389390E-01,1.329021E-01,1.271757E-01,1.217345E-01,
1.165771E-01,1.116931E-01,1.070704E-01,1.026923E-01,9.855422E-02,
9.465543E-02,9.097910E-02,8.751992E-02,8.427484E-02,8.123457E-02,
7.915322E-02,7.838058E-02,7.783170E-02,7.723851E-02,7.664140E-02,
7.609826E-02,7.577639E-02,7.547761E-02,7.517153E-02,7.485395E-02,
7.452646E-02,7.419691E-02,7.387396E-02,7.354265E-02,7.322774E-02,
7.290437E-02,7.258368E-02,7.227496E-02,7.197582E-02,7.176074E-02,
7.159178E-02,7.141390E-02,7.124276E-02,7.107270E-02,7.091170E-02,
7.074624E-02,7.058590E-02,7.042597E-02,7.027141E-02,7.011311E-02,
6.996097E-02,6.981182E-02,6.966638E-02,6.952360E-02,6.938050E-02,
6.924218E-02,6.910882E-02,6.897672E-02,6.884442E-02,6.871519E-02,
6.858877E-02,6.846415E-02,6.834243E-02,6.822237E-02,6.810541E-02,
6.799153E-02,6.788065E-02,6.777135E-02,6.766383E-02,6.755986E-02,
6.745864E-02,6.735986E-02,6.726170E-02,6.716596E-02,6.707231E-02,
6.698100E-02,6.689089E-02,6.681383E-02,6.675485E-02,6.670072E-02,
6.664926E-02,6.659524E-02,6.653909E-02,6.648622E-02,6.643298E-02,
6.638025E-02,6.632559E-02,6.627095E-02,6.621709E-02,6.616603E-02,
6.611274E-02,6.605977E-02,6.600729E-02,6.595378E-02,6.589992E-02,
6.584409E-02,6.579313E-02,6.574273E-02,6.569371E-02,6.563877E-02,
6.558636E-02,6.553811E-02,6.548707E-02,6.543831E-02,6.538887E-02,
6.533700E-02,6.528527E-02,6.523891E-02,6.518958E-02,6.514188E-02,
6.509484E-02,6.504755E-02,6.500074E-02,6.495395E-02,6.490777E-02,
6.486150E-02,6.481691E-02,6.477048E-02,6.472516E-02,6.468031E-02,
6.463265E-02,6.458843E-02,6.454499E-02,6.450106E-02,6.445618E-02,
6.441032E-02,6.436624E-02,6.432411E-02,6.428152E-02,6.423903E-02,
6.419563E-02,6.415323E-02,6.411016E-02,6.406919E-02,6.402904E-02,
6.398900E-02,6.394808E-02,6.390618E-02,6.386417E-02,6.382191E-02,
6.378217E-02,6.374384E-02,6.370561E-02,6.366637E-02,6.362691E-02,
6.358879E-02,6.355102E-02,6.351012E-02,6.347172E-02,6.343384E-02,
6.339621E-02,6.335974E-02,6.332267E-02,6.328430E-02,6.324506E-02,
6.320801E-02,6.317035E-02,6.313546E-02,6.309954E-02,6.306406E-02,
```

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6.302779E-02, 6.299169E-02, 6.295837E-02, 6.292484E-02, 6.288867E-02,
6.285289E-02, 6.281804E-02, 6.278440E-02, 6.274686E-02, 6.271534E-02,
6.268188E-02, 6.264882E-02, 5.547806E-02, 5.547806E-02
POROSITY SURFACE #2; GAS GENERATION RATE #3.
PDATA (NSDATA =3, NTDATA=1:214, MKLOS =2)
1.013250E+05, 1.015771E+05, 1.018292E+05, 1.147067E+05, 1.306487E+05,
1.491446E+05, 1.682754E+05, 1.892675E+05, 2.106405E+05, 2.342118E+05,
2.581500E+05, 2.845363E+05, 3.112294E+05, 3.403808E+05, 3.697596E+05,
4.017414E+05, 4.338682E+05, 4.688076E+05, 5.038403E+05, 5.417496E+05,
5.797587E+05, 6.205020E+05, 6.614677E+05, 7.487837E+05, 8.414315E+05,
9.384733E+05, 1.039827E+06, 1.145171E+06, 1.254268E+06, 1.367179E+06,
1.483761E+06, 1.603423E+06, 1.725992E+06, 1.851095E+06, 1.978518E+06,
2.107852E+06, 2.238724E+06, 2.371138E+06, 2.504740E+06, 2.639191E+06,
2.774245E+06, 2.909738E+06, 3.045664E+06, 3.181756E+06, 3.317693E+06,
3.453398E+06, 3.588739E+06, 3.723851E+06, 3.858402E+06, 3.992369E+06,
4.125670E+06, 4.258275E+06, 4.390145E+06, 4.521291E+06, 4.651631E+06,
4.781165E+06, 4.909911E+06, 5.037843E+06, 5.164938E+06, 5.291161E+06,
5.416672E+06, 5.541417E+06, 5.665388E+06, 5.788610E+06, 5.911139E+06,
6.032976E+06, 6.154115E+06, 6.274577E+06, 6.346582E+06, 6.407251E+06,
6.471258E+06, 6.535135E+06, 6.598847E+06, 6.662413E+06, 6.725774E+06,
6.788943E+06, 6.851917E+06, 6.914722E+06, 6.977287E+06, 7.039640E+06,
7.101820E+06, 7.163803E+06, 7.225581E+06, 7.287183E+06, 7.348608E+06,
7.409845E+06, 7.470912E+06, 7.531804E+06, 7.592472E+06, 7.652989E+06,
7.713422E+06, 7.773676E+06, 7.833734E+06, 7.893666E+06, 7.953460E+06,
8.013141E+06, 8.072675E+06, 8.132100E+06, 8.191401E+06, 8.250536E+06,
8.309604E+06, 8.368560E+06, 8.427428E+06, 8.486178E+06, 8.544846E+06,
8.603414E+06, 8.661856E+06, 8.720267E+06, 8.778582E+06, 8.836821E+06,
8.894960E+06, 8.953074E+06, 9.011429E+06, 9.069399E+06, 9.127280E+06,
9.185108E+06, 9.254526E+06, 9.302475E+06, 9.302899E+06, 9.303409E+06,
9.303921E+06, 9.304431E+06, 9.304969E+06, 9.305512E+06, 9.306051E+06,
9.306619E+06, 9.307180E+06, 9.307750E+06, 9.308342E+06, 9.308901E+06,
9.309474E+06, 9.310067E+06, 9.310694E+06, 9.311310E+06, 9.311903E+06,
9.312534E+06, 9.313181E+06, 9.313788E+06, 9.314421E+06, 9.315068E+06,
9.315715E+06, 9.316362E+06, 9.317010E+06, 9.317657E+06, 9.318311E+06,
9.318959E+06, 9.319653E+06, 9.320306E+06, 9.320954E+06, 9.321603E+06,
9.322300E+06, 9.322953E+06, 9.323652E+06, 9.324302E+06, 9.324957E+06,
9.325659E+06, 9.326308E+06, 9.327009E+06, 9.327661E+06, 9.328361E+06,
9.329009E+06, 9.329663E+06, 9.330361E+06, 9.331016E+06, 9.331713E+06,
9.332377E+06, 9.333071E+06, 9.333720E+06, 9.334382E+06, 9.335073E+06,
9.335736E+06, 9.336427E+06, 9.337078E+06, 9.337727E+06, 9.338394E+06,
9.339089E+06, 9.339739E+06, 9.340389E+06, 9.341059E+06, 9.341744E+06,

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9.342395E+06,9.343046E+06,9.343697E+06,9.344348E+06,9.345023E+06,
9.345705E+06,9.346362E+06,9.347013E+06,9.347665E+06,9.348317E+06,
9.348941E+06,9.349567E+06,9.350218E+06,9.350871E+06,9.351522E+06,
9.352175E+06,9.352834E+06,9.353452E+06,9.354085E+06,9.354738E+06,
9.355391E+06,9.356006E+06,9.356643E+06,9.357295E+06,9.357910E+06,
9.358548E+06,9.359201E+06,9.359818E+06,9.360461E+06,9.361114E+06,
9.361724E+06,9.362368E+06,9.649179E+06,9.649179E+06

POROSITY SURFACE #2; GAS GENERATION RATE #3.

SDATA (NSDATA =3,NTDATA=1:214,MKLOS =2)

1.000000E+00,9.751257E-01,9.560622E-01,8.804212E-01,8.388185E-01,
8.082005E-01,7.803164E-01,7.558443E-01,7.320703E-01,7.097225E-01,
6.876007E-01,6.668157E-01,6.461978E-01,6.274485E-01,6.088610E-01,
5.919256E-01,5.750822E-01,5.596248E-01,5.442045E-01,5.301203E-01,
5.160812E-01,5.032843E-01,4.905514E-01,4.674176E-01,4.465329E-01,
4.279986E-01,4.114445E-01,3.965919E-01,3.832112E-01,3.710218E-01,
3.598670E-01,3.497286E-01,3.404744E-01,3.320368E-01,3.243227E-01,
3.172866E-01,3.108793E-01,3.050032E-01,2.996258E-01,2.947152E-01,
2.902342E-01,2.861395E-01,2.823803E-01,2.789375E-01,2.758001E-01,
2.729359E-01,2.703129E-01,2.679124E-01,2.657244E-01,2.637272E-01,
2.619064E-01,2.602461E-01,2.587307E-01,2.573500E-01,2.560942E-01,
2.549524E-01,2.539137E-01,2.529710E-01,2.521176E-01,2.513464E-01,
2.506473E-01,2.500157E-01,2.494470E-01,2.489360E-01,2.484764E-01,
2.480647E-01,2.476966E-01,2.473673E-01,2.470531E-01,2.467466E-01,
2.464519E-01,2.461680E-01,2.458953E-01,2.456339E-01,2.453853E-01,
2.451483E-01,2.449228E-01,2.447077E-01,2.445049E-01,2.443128E-01,
2.441306E-01,2.439585E-01,2.437963E-01,2.436429E-01,2.434982E-01,
2.433620E-01,2.432332E-01,2.431128E-01,2.429999E-01,2.428954E-01,
2.427952E-01,2.427023E-01,2.426165E-01,2.425364E-01,2.424618E-01,
2.423917E-01,2.423273E-01,2.422670E-01,2.422114E-01,2.421609E-01,
2.421136E-01,2.420705E-01,2.420304E-01,2.419942E-01,2.419610E-01,
2.419310E-01,2.419045E-01,2.418799E-01,2.418581E-01,2.418388E-01,
2.418209E-01,2.418049E-01,2.417912E-01,2.417790E-01,2.417683E-01,
2.417590E-01,2.417505E-01,2.417414E-01,2.417302E-01,2.417168E-01,
2.417034E-01,2.416900E-01,2.416759E-01,2.416616E-01,2.416475E-01,
2.416326E-01,2.416178E-01,2.416029E-01,2.415873E-01,2.415727E-01,
2.415576E-01,2.415421E-01,2.415256E-01,2.415095E-01,2.414939E-01,
2.414774E-01,2.414604E-01,2.414445E-01,2.414280E-01,2.414110E-01,
2.413940E-01,2.413771E-01,2.413601E-01,2.413431E-01,2.413260E-01,
2.413091E-01,2.412909E-01,2.412738E-01,2.412569E-01,2.412399E-01,
2.412216E-01,2.412046E-01,2.411863E-01,2.411693E-01,2.411521E-01,
2.411338E-01,2.411168E-01,2.410985E-01,2.410815E-01,2.410632E-01,

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2.410462E-01,2.410292E-01,2.410110E-01,2.409939E-01,2.409757E-01,
2.409584E-01,2.409402E-01,2.409232E-01,2.409060E-01,2.408880E-01,
2.408706E-01,2.408527E-01,2.408357E-01,2.408188E-01,2.408014E-01,
2.407833E-01,2.407663E-01,2.407494E-01,2.407319E-01,2.407141E-01,
2.406971E-01,2.406801E-01,2.406632E-01,2.406463E-01,2.406287E-01,
2.406109E-01,2.405938E-01,2.405769E-01,2.405599E-01,2.405429E-01,
2.405267E-01,2.405104E-01,2.404935E-01,2.404766E-01,2.404596E-01,
2.404426E-01,2.404255E-01,2.404095E-01,2.403930E-01,2.403760E-01,
2.403591E-01,2.403431E-01,2.403266E-01,2.403096E-01,2.402937E-01,
2.402771E-01,2.402602E-01,2.402441E-01,2.402274E-01,2.402105E-01,
2.401947E-01,2.401781E-01,2.329632E-01,2.329632E-01

POROSITY SURFACE #2; GAS GENERATION RATE #4.

PDATA (NSDATA =4,NTD DATA=1:214,MKLOS =2)

1.013250E+05,1.019288E+05,1.025327E+05,1.300565E+05,1.614025E+05,
1.986491E+05,2.367147E+05,2.781497E+05,3.199284E+05,3.662243E+05,
4.128385E+05,4.642963E+05,5.159247E+05,5.726598E+05,6.295555E+05,
6.913039E+05,7.533107E+05,8.198411E+05,8.867198E+05,9.572510E+05,
1.028228E+06,1.102708E+06,1.177711E+06,1.333387E+06,1.493866E+06,
1.658546E+06,1.827100E+06,1.999581E+06,2.175030E+06,2.352510E+06,
2.531243E+06,2.710956E+06,2.891399E+06,3.072793E+06,3.254575E+06,
3.436070E+06,3.617196E+06,3.797580E+06,3.977201E+06,4.155853E+06,
4.333736E+06,4.510513E+06,4.686196E+06,4.860878E+06,5.034447E+06,
5.206854E+06,5.377927E+06,5.548093E+06,5.717168E+06,5.885200E+06,
6.052211E+06,6.218272E+06,6.383402E+06,6.547739E+06,6.711306E+06,
6.874140E+06,7.036300E+06,7.197844E+06,7.358839E+06,7.519326E+06,
7.679431E+06,7.839164E+06,7.998604E+06,8.157785E+06,8.316751E+06,
8.475526E+06,8.634132E+06,8.792575E+06,8.879369E+06,8.954693E+06,
9.034189E+06,9.113674E+06,9.193112E+06,9.272542E+06,9.351939E+06,
9.431302E+06,9.510629E+06,9.589955E+06,9.669213E+06,9.748441E+06,
9.827658E+06,9.906835E+06,9.986008E+06,1.006511E+07,1.014421E+07,
1.022327E+07,1.030224E+07,1.038121E+07,1.046009E+07,1.053896E+07,
1.061779E+07,1.069660E+07,1.077531E+07,1.085402E+07,1.093266E+07,
1.101128E+07,1.108985E+07,1.116840E+07,1.124691E+07,1.132538E+07,
1.140384E+07,1.148227E+07,1.156068E+07,1.163906E+07,1.171742E+07,
1.179577E+07,1.187407E+07,1.195236E+07,1.203065E+07,1.210889E+07,
1.218700E+07,1.226512E+07,1.234367E+07,1.242170E+07,1.249961E+07,
1.257755E+07,1.267275E+07,1.273261E+07,1.273182E+07,1.273123E+07,
1.273075E+07,1.273032E+07,1.272995E+07,1.272962E+07,1.272931E+07,
1.272904E+07,1.272879E+07,1.272856E+07,1.272836E+07,1.272816E+07,
1.272799E+07,1.272784E+07,1.272768E+07,1.272753E+07,1.272738E+07,
1.272723E+07,1.272711E+07,1.272701E+07,1.272687E+07,1.272676E+07,

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1.272666E+07,1.272656E+07,1.272646E+07,1.272636E+07,1.272630E+07,
1.272621E+07,1.272611E+07,1.272601E+07,1.272595E+07,1.272585E+07,
1.272580E+07,1.272570E+07,1.272565E+07,1.272560E+07,1.272550E+07,
1.272545E+07,1.272540E+07,1.272534E+07,1.272525E+07,1.272524E+07,
1.272515E+07,1.272514E+07,1.272504E+07,1.272500E+07,1.272499E+07,
1.272494E+07,1.272489E+07,1.272484E+07,1.272479E+07,1.272475E+07,
1.272474E+07,1.272469E+07,1.272465E+07,1.272463E+07,1.272458E+07,
1.272455E+07,1.272453E+07,1.272450E+07,1.272448E+07,1.272445E+07,
1.272443E+07,1.272438E+07,1.272435E+07,1.272435E+07,1.272433E+07,
1.272430E+07,1.272427E+07,1.272425E+07,1.272422E+07,1.272420E+07,
1.272420E+07,1.272417E+07,1.272415E+07,1.272412E+07,1.272410E+07,
1.272410E+07,1.272410E+07,1.272407E+07,1.272405E+07,1.272405E+07,
1.272401E+07,1.272400E+07,1.272400E+07,1.272400E+07,1.272396E+07,
1.272395E+07,1.272395E+07,1.272395E+07,1.272391E+07,1.272390E+07,
1.272390E+07,1.272390E+07,1.272415E+07,1.272415E+07

POROSITY SURFACE #2; GAS GENERATION RATE #4.

SDATA (NSDATA =4,NTD DATA=1:214,MKLOS =2)

1.000000E+00,9.724346E-01,9.541304E-01,8.917347E-01,8.508140E-01,
8.181004E-01,7.865272E-01,7.634814E-01,7.413054E-01,7.199909E-01,
6.987284E-01,6.788974E-01,6.591168E-01,6.409217E-01,6.227728E-01,
6.063495E-01,5.900173E-01,5.752889E-01,5.607140E-01,5.478763E-01,
5.352014E-01,5.238148E-01,5.126271E-01,4.930414E-01,4.761990E-01,
4.615490E-01,4.487267E-01,4.372760E-01,4.271189E-01,4.181672E-01,
4.103113E-01,4.033790E-01,3.972383E-01,3.917184E-01,3.867844E-01,
3.824227E-01,3.785509E-01,3.751336E-01,3.721073E-01,3.694377E-01,
3.670603E-01,3.649658E-01,3.631202E-01,3.614865E-01,3.600509E-01,
3.587943E-01,3.576967E-01,3.567406E-01,3.559119E-01,3.551955E-01,
3.545806E-01,3.540541E-01,3.536052E-01,3.532256E-01,3.529060E-01,
3.526401E-01,3.524210E-01,3.522424E-01,3.520983E-01,3.519824E-01,
3.518915E-01,3.518213E-01,3.517669E-01,3.517259E-01,3.516959E-01,
3.516750E-01,3.516597E-01,3.516476E-01,3.516332E-01,3.516176E-01,
3.516042E-01,3.515915E-01,3.515799E-01,3.515698E-01,3.515610E-01,
3.515538E-01,3.515479E-01,3.515422E-01,3.515391E-01,3.515363E-01,
3.515347E-01,3.515346E-01,3.515346E-01,3.515373E-01,3.515402E-01,
3.515444E-01,3.515502E-01,3.515573E-01,3.515644E-01,3.515744E-01,
3.515857E-01,3.515973E-01,3.516114E-01,3.516259E-01,3.516430E-01,
3.516601E-01,3.516785E-01,3.516971E-01,3.517169E-01,3.517370E-01,
3.517582E-01,3.517794E-01,3.518010E-01,3.518236E-01,3.518463E-01,
3.518689E-01,3.518920E-01,3.519160E-01,3.519401E-01,3.519646E-01,
3.519905E-01,3.520174E-01,3.520445E-01,3.520719E-01,3.521008E-01,
3.521304E-01,3.521608E-01,3.521891E-01,3.522111E-01,3.522274E-01,

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3.522408E-01, 3.522527E-01, 3.522632E-01, 3.522724E-01, 3.522809E-01,
3.522885E-01, 3.522956E-01, 3.523017E-01, 3.523074E-01, 3.523130E-01,
3.523178E-01, 3.523220E-01, 3.523262E-01, 3.523305E-01, 3.523348E-01,
3.523390E-01, 3.523421E-01, 3.523450E-01, 3.523489E-01, 3.523521E-01,
3.523549E-01, 3.523577E-01, 3.523605E-01, 3.523633E-01, 3.523649E-01,
3.523676E-01, 3.523705E-01, 3.523733E-01, 3.523748E-01, 3.523776E-01,
3.523791E-01, 3.523819E-01, 3.523832E-01, 3.523846E-01, 3.523875E-01,
3.523889E-01, 3.523903E-01, 3.523918E-01, 3.523944E-01, 3.523947E-01,
3.523972E-01, 3.523976E-01, 3.524002E-01, 3.524014E-01, 3.524016E-01,
3.524030E-01, 3.524044E-01, 3.524058E-01, 3.524072E-01, 3.524083E-01,
3.524087E-01, 3.524101E-01, 3.524111E-01, 3.524115E-01, 3.524130E-01,
3.524139E-01, 3.524144E-01, 3.524153E-01, 3.524158E-01, 3.524167E-01,
3.524173E-01, 3.524187E-01, 3.524195E-01, 3.524195E-01, 3.524202E-01,
3.524209E-01, 3.524216E-01, 3.524223E-01, 3.524230E-01, 3.524236E-01,
3.524236E-01, 3.524244E-01, 3.524250E-01, 3.524259E-01, 3.524264E-01,
3.524264E-01, 3.524264E-01, 3.524273E-01, 3.524278E-01, 3.524278E-01,
3.524288E-01, 3.524292E-01, 3.524292E-01, 3.524292E-01, 3.524303E-01,
3.524306E-01, 3.524306E-01, 3.524306E-01, 3.524318E-01, 3.524320E-01,
3.524320E-01, 3.524320E-01, 3.524250E-01, 3.524250E-01

POROSITY SURFACE #2; GAS GENERATION RATE #5.

PDATA(NSDATA =5,NTDATA=1:214,MKLOS =2)

1.013250E+05, 1.026735E+05, 1.040221E+05, 1.607512E+05, 2.228597E+05,
2.965181E+05, 3.712018E+05, 4.545696E+05, 5.384155E+05, 6.316594E+05,
7.252057E+05, 8.275393E+05, 9.301412E+05, 1.039961E+06, 1.150150E+06,
1.265237E+06, 1.380796E+06, 1.500871E+06, 1.621431E+06, 1.745206E+06,
1.869480E+06, 1.996490E+06, 2.124048E+06, 2.383006E+06, 2.644644E+06,
2.907113E+06, 3.169191E+06, 3.431185E+06, 3.692633E+06, 3.952942E+06,
4.211742E+06, 4.468770E+06, 4.724031E+06, 4.977272E+06, 5.228455E+06,
5.477898E+06, 5.725619E+06, 5.971700E+06, 6.216289E+06, 6.459450E+06,
6.701329E+06, 6.942031E+06, 7.181728E+06, 7.420592E+06, 7.658834E+06,
7.896570E+06, 8.133632E+06, 8.370753E+06, 8.607682E+06, 8.844459E+06,
9.081135E+06, 9.317727E+06, 9.554166E+06, 9.790605E+06, 1.002695E+07,
1.026320E+07, 1.049935E+07, 1.073535E+07, 1.097119E+07, 1.120670E+07,
1.144204E+07, 1.167721E+07, 1.191222E+07, 1.214705E+07, 1.238172E+07,
1.261620E+07, 1.285038E+07, 1.308424E+07, 1.320837E+07, 1.331891E+07,
1.343523E+07, 1.355151E+07, 1.366766E+07, 1.378373E+07, 1.389967E+07,
1.401550E+07, 1.413117E+07, 1.424663E+07, 1.436191E+07, 1.447698E+07,
1.459192E+07, 1.470667E+07, 1.482119E+07, 1.493553E+07, 1.504957E+07,
1.516339E+07, 1.527691E+07, 1.539017E+07, 1.550308E+07, 1.561578E+07,
1.572820E+07, 1.584032E+07, 1.595206E+07, 1.606354E+07, 1.617464E+07,
1.628533E+07, 1.639566E+07, 1.650560E+07, 1.661510E+07, 1.672414E+07,

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1.683277E+07,1.694097E+07,1.704870E+07,1.715589E+07,1.726259E+07,
1.736876E+07,1.747432E+07,1.757935E+07,1.768382E+07,1.778767E+07,
1.789081E+07,1.799343E+07,1.809597E+07,1.819716E+07,1.829759E+07,
1.839735E+07,1.852289E+07,1.859165E+07,1.857597E+07,1.856196E+07,
1.854899E+07,1.853691E+07,1.852557E+07,1.851477E+07,1.850466E+07,
1.849506E+07,1.848597E+07,1.847731E+07,1.846900E+07,1.846102E+07,
1.845338E+07,1.844602E+07,1.843887E+07,1.843190E+07,1.842523E+07,
1.841875E+07,1.841246E+07,1.840633E+07,1.840038E+07,1.839456E+07,
1.838887E+07,1.838332E+07,1.837784E+07,1.837252E+07,1.836722E+07,
1.836212E+07,1.835709E+07,1.835216E+07,1.834735E+07,1.834264E+07,
1.833799E+07,1.833339E+07,1.832891E+07,1.832448E+07,1.832011E+07,
1.831585E+07,1.831165E+07,1.830755E+07,1.830345E+07,1.829946E+07,
1.829552E+07,1.829159E+07,1.828776E+07,1.828395E+07,1.828023E+07,
1.827653E+07,1.827292E+07,1.826936E+07,1.826582E+07,1.826237E+07,
1.825892E+07,1.825553E+07,1.825220E+07,1.824891E+07,1.824565E+07,
1.824245E+07,1.823931E+07,1.823620E+07,1.823312E+07,1.823008E+07,
1.822711E+07,1.822414E+07,1.822122E+07,1.821835E+07,1.821551E+07,
1.821272E+07,1.820993E+07,1.820720E+07,1.820449E+07,1.820181E+07,
1.819919E+07,1.819660E+07,1.819403E+07,1.819151E+07,1.818901E+07,
1.818652E+07,1.818404E+07,1.818164E+07,1.817925E+07,1.817686E+07,
1.817451E+07,1.817222E+07,1.816990E+07,1.816765E+07,1.816541E+07,
1.816319E+07,1.816101E+07,1.815881E+07,1.815663E+07,1.815451E+07,
1.815239E+07,1.815031E+07,1.782467E+07,1.782467E+07

POROSITY SURFACE #2; GAS GENERATION RATE #5.

SDATA (NSDATA =5,NTDATAB=1:214,MKLOS =2)

1.000000E+00,9.748433E-01,9.570604E-01,8.993860E-01,8.566730E-01,
8.261634E-01,7.967376E-01,7.714288E-01,7.463467E-01,7.237408E-01,
7.012057E-01,6.816788E-01,6.622614E-01,6.458001E-01,6.295390E-01,
6.162211E-01,6.031002E-01,5.918746E-01,5.808760E-01,5.715093E-01,
5.623564E-01,5.543895E-01,5.466391E-01,5.333857E-01,5.222797E-01,
5.130504E-01,5.055043E-01,4.991576E-01,4.938125E-01,4.893376E-01,
4.856066E-01,4.825148E-01,4.799491E-01,4.778509E-01,4.761508E-01,
4.747646E-01,4.736467E-01,4.727547E-01,4.720491E-01,4.715028E-01,
4.710900E-01,4.707870E-01,4.705720E-01,4.704243E-01,4.703261E-01,
4.702639E-01,4.702274E-01,4.702071E-01,4.701983E-01,4.701982E-01,
4.702032E-01,4.702125E-01,4.702253E-01,4.702409E-01,4.702603E-01,
4.702831E-01,4.703097E-01,4.703414E-01,4.703788E-01,4.704255E-01,
4.704801E-01,4.705395E-01,4.706032E-01,4.706711E-01,4.707425E-01,
4.708187E-01,4.709006E-01,4.709851E-01,4.710580E-01,4.711240E-01,
4.711890E-01,4.712541E-01,4.713214E-01,4.713917E-01,4.714648E-01,
4.715408E-01,4.716209E-01,4.717066E-01,4.717968E-01,4.718912E-01,

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4.719899E-01,4.720930E-01,4.722017E-01,4.723148E-01,4.724350E-01,
4.725610E-01,4.726928E-01,4.728318E-01,4.729764E-01,4.731283E-01,
4.732873E-01,4.734523E-01,4.736256E-01,4.738050E-01,4.739932E-01,
4.741910E-01,4.743963E-01,4.746104E-01,4.748343E-01,4.750671E-01,
4.753096E-01,4.755611E-01,4.758231E-01,4.760961E-01,4.763796E-01,
4.766745E-01,4.769813E-01,4.773002E-01,4.776301E-01,4.779730E-01,
4.783278E-01,4.786944E-01,4.790763E-01,4.794705E-01,4.798787E-01,
4.803021E-01,4.807400E-01,4.811815E-01,4.815897E-01,4.819551E-01,
4.822939E-01,4.826099E-01,4.829070E-01,4.831902E-01,4.834558E-01,
4.837080E-01,4.839472E-01,4.841753E-01,4.843944E-01,4.846050E-01,
4.848067E-01,4.850010E-01,4.851902E-01,4.853747E-01,4.855513E-01,
4.857233E-01,4.858899E-01,4.860528E-01,4.862108E-01,4.863654E-01,
4.865169E-01,4.866645E-01,4.868102E-01,4.869520E-01,4.870934E-01,
4.872294E-01,4.873637E-01,4.874953E-01,4.876240E-01,4.877500E-01,
4.878742E-01,4.879972E-01,4.881172E-01,4.882358E-01,4.883528E-01,
4.884670E-01,4.885798E-01,4.886900E-01,4.888000E-01,4.889071E-01,
4.890130E-01,4.891186E-01,4.892217E-01,4.893243E-01,4.894244E-01,
4.895240E-01,4.896211E-01,4.897172E-01,4.898126E-01,4.899058E-01,
4.899986E-01,4.900900E-01,4.901800E-01,4.902690E-01,4.903570E-01,
4.904436E-01,4.905283E-01,4.906125E-01,4.906959E-01,4.907780E-01,
4.908585E-01,4.909391E-01,4.910183E-01,4.910961E-01,4.911731E-01,
4.912486E-01,4.913242E-01,4.913984E-01,4.914718E-01,4.915445E-01,
4.916157E-01,4.916864E-01,4.917561E-01,4.918245E-01,4.918923E-01,
4.919601E-01,4.920277E-01,4.920931E-01,4.921581E-01,4.922231E-01,
4.922871E-01,4.923496E-01,4.924128E-01,4.924742E-01,4.925349E-01,
4.925956E-01,4.926553E-01,4.927153E-01,4.927746E-01,4.928326E-01,
4.928905E-01,4.929473E-01,5.020043E-01,5.020043E-01

POROSITY SURFACE #2; GAS GENERATION RATE #6.

PDATA (NSDATA =6,NTDATA=1:214,MKLOS =2)

1.013250E+05,1.041277E+05,1.069304E+05,1.997906E+05,2.942560E+05,
4.081954E+05,5.225804E+05,6.487903E+05,7.756826E+05,9.122583E+05,
1.049883E+06,1.197148E+06,1.345512E+06,1.501593E+06,1.658793E+06,
1.821939E+06,1.985730E+06,2.152366E+06,2.319640E+06,2.489115E+06,
2.658574E+06,2.827946E+06,2.997392E+06,3.335452E+06,3.672853E+06,
4.007227E+06,4.338823E+06,4.667183E+06,4.992937E+06,5.316048E+06,
5.636777E+06,5.955357E+06,6.271942E+06,6.586640E+06,6.899697E+06,
7.211508E+06,7.522387E+06,7.832654E+06,8.142551E+06,8.452198E+06,
8.761705E+06,9.071065E+06,9.380312E+06,9.689462E+06,9.998553E+06,
1.030751E+07,1.061590E+07,1.092451E+07,1.123285E+07,1.154087E+07,
1.184858E+07,1.215600E+07,1.246305E+07,1.276991E+07,1.307642E+07,
1.338250E+07,1.368810E+07,1.399312E+07,1.429746E+07,1.460088E+07,

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1.490347E+07, 1.520498E+07, 1.550532E+07, 1.580435E+07, 1.610200E+07,
1.639809E+07, 1.669237E+07, 1.698476E+07, 1.712639E+07, 1.726045E+07,
1.740043E+07, 1.754008E+07, 1.767926E+07, 1.781787E+07, 1.795587E+07,
1.809314E+07, 1.822956E+07, 1.836499E+07, 1.849940E+07, 1.863258E+07,
1.876472E+07, 1.889571E+07, 1.902557E+07, 1.915430E+07, 1.928182E+07,
1.940802E+07, 1.953279E+07, 1.965614E+07, 1.977783E+07, 1.989810E+07,
2.001682E+07, 2.013405E+07, 2.024971E+07, 2.036380E+07, 2.047613E+07,
2.058665E+07, 2.069520E+07, 2.080176E+07, 2.090634E+07, 2.100891E+07,
2.110961E+07, 2.120832E+07, 2.130499E+07, 2.139945E+07, 2.149161E+07,
2.158135E+07, 2.166862E+07, 2.175347E+07, 2.183593E+07, 2.191606E+07,
2.199366E+07, 2.206875E+07, 2.214145E+07, 2.221080E+07, 2.227712E+07,
2.234055E+07, 2.243618E+07, 2.244959E+07, 2.237180E+07, 2.230020E+07,
2.223338E+07, 2.217045E+07, 2.211095E+07, 2.205400E+07, 2.200055E+07,
2.194969E+07, 2.190118E+07, 2.185489E+07, 2.181059E+07, 2.176806E+07,
2.172722E+07, 2.168795E+07, 2.165015E+07, 2.161330E+07, 2.157811E+07,
2.154413E+07, 2.151119E+07, 2.147927E+07, 2.144828E+07, 2.141815E+07,
2.138889E+07, 2.136047E+07, 2.133278E+07, 2.130584E+07, 2.127931E+07,
2.125367E+07, 2.122866E+07, 2.120423E+07, 2.118034E+07, 2.115700E+07,
2.113418E+07, 2.111185E+07, 2.108998E+07, 2.106861E+07, 2.104745E+07,
2.102694E+07, 2.100683E+07, 2.098715E+07, 2.096781E+07, 2.094884E+07,
2.093020E+07, 2.091194E+07, 2.089396E+07, 2.087632E+07, 2.085899E+07,
2.084175E+07, 2.082496E+07, 2.080844E+07, 2.079221E+07, 2.077620E+07,
2.076045E+07, 2.074494E+07, 2.072964E+07, 2.071458E+07, 2.069976E+07,
2.068500E+07, 2.067061E+07, 2.065639E+07, 2.064236E+07, 2.062856E+07,
2.061494E+07, 2.060148E+07, 2.058820E+07, 2.057513E+07, 2.056221E+07,
2.054943E+07, 2.053672E+07, 2.052429E+07, 2.051201E+07, 2.049989E+07,
2.048791E+07, 2.047610E+07, 2.046442E+07, 2.045289E+07, 2.044147E+07,
2.043021E+07, 2.041897E+07, 2.040794E+07, 2.039707E+07, 2.038630E+07,
2.037565E+07, 2.036513E+07, 2.035473E+07, 2.034447E+07, 2.033427E+07,
2.032416E+07, 2.031420E+07, 2.030426E+07, 2.029450E+07, 2.028483E+07,
2.027529E+07, 2.026586E+07, 1.869941E+07, 1.869941E+07

POROSITY SURFACE #2; GAS GENERATION RATE #6.

SDATA (NSDATA =6, NTDATA=1:214, MKLOS =2)

1.000000E+00, 9.725971E-01, 9.501980E-01, 8.946068E-01, 8.430061E-01,
8.128133E-01, 7.828748E-01, 7.597040E-01, 7.368370E-01, 7.182998E-01,
6.999815E-01, 6.838028E-01, 6.679279E-01, 6.541989E-01, 6.408072E-01,
6.292966E-01, 6.182295E-01, 6.091482E-01, 6.004289E-01, 5.930653E-01,
5.861215E-01, 5.804992E-01, 5.752079E-01, 5.667006E-01, 5.599054E-01,
5.546717E-01, 5.506656E-01, 5.476300E-01, 5.452939E-01, 5.435257E-01,
5.421968E-01, 5.412133E-01, 5.405056E-01, 5.400254E-01, 5.397192E-01,
5.395365E-01, 5.394375E-01, 5.393883E-01, 5.393678E-01, 5.393645E-01,

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5.393707E-01,5.393849E-01,5.394052E-01,5.394290E-01,5.394564E-01,
5.394888E-01,5.395276E-01,5.395735E-01,5.396296E-01,5.396978E-01,
5.397768E-01,5.398642E-01,5.399595E-01,5.400626E-01,5.401755E-01,
5.403008E-01,5.404390E-01,5.405938E-01,5.407681E-01,5.409653E-01,
5.411890E-01,5.414419E-01,5.417260E-01,5.420447E-01,5.423983E-01,
5.427906E-01,5.432252E-01,5.436992E-01,5.441471E-01,5.445719E-01,
5.449921E-01,5.454158E-01,5.458461E-01,5.462886E-01,5.467428E-01,
5.472124E-01,5.477004E-01,5.482110E-01,5.487446E-01,5.493050E-01,
5.498902E-01,5.505000E-01,5.511342E-01,5.517930E-01,5.524777E-01,
5.531912E-01,5.539347E-01,5.547103E-01,5.555194E-01,5.563623E-01,
5.572380E-01,5.581453E-01,5.590841E-01,5.600570E-01,5.610672E-01,
5.621160E-01,5.632078E-01,5.643422E-01,5.655187E-01,5.667367E-01,
5.679946E-01,5.692942E-01,5.706367E-01,5.720261E-01,5.734653E-01,
5.749566E-01,5.765006E-01,5.780981E-01,5.797465E-01,5.814445E-01,
5.831940E-01,5.850002E-01,5.868787E-01,5.888118E-01,5.908107E-01,
5.928754E-01,5.950049E-01,5.971756E-01,5.992612E-01,6.011939E-01,
6.030087E-01,6.047281E-01,6.063628E-01,6.079356E-01,6.094196E-01,
6.108380E-01,6.121972E-01,6.134996E-01,6.147516E-01,6.159584E-01,
6.171214E-01,6.182442E-01,6.193287E-01,6.203894E-01,6.214058E-01,
6.223908E-01,6.233482E-01,6.242788E-01,6.251850E-01,6.260687E-01,
6.269293E-01,6.277677E-01,6.285861E-01,6.293850E-01,6.301731E-01,
6.309370E-01,6.316839E-01,6.324153E-01,6.331317E-01,6.338338E-01,
6.345214E-01,6.351957E-01,6.358577E-01,6.365056E-01,6.371488E-01,
6.377734E-01,6.383867E-01,6.389882E-01,6.395802E-01,6.401624E-01,
6.407354E-01,6.412975E-01,6.418521E-01,6.423970E-01,6.429334E-01,
6.434678E-01,6.439890E-01,6.445029E-01,6.450086E-01,6.455081E-01,
6.460002E-01,6.464854E-01,6.469648E-01,6.474374E-01,6.479035E-01,
6.483680E-01,6.488218E-01,6.492706E-01,6.497140E-01,6.501508E-01,
6.505825E-01,6.510098E-01,6.514315E-01,6.518474E-01,6.522591E-01,
6.526667E-01,6.530729E-01,6.534702E-01,6.538632E-01,6.542519E-01,
6.546363E-01,6.550156E-01,6.553912E-01,6.557626E-01,6.561307E-01,
6.564943E-01,6.568574E-01,6.572142E-01,6.575662E-01,6.579154E-01,
6.582610E-01,6.586025E-01,6.589408E-01,6.592748E-01,6.596071E-01,
6.599369E-01,6.602622E-01,6.605868E-01,6.609063E-01,6.612228E-01,
6.615354E-01,6.618451E-01,7.175897E-01,7.175897E-01

POROSITY SURFACE #2; GAS GENERATION RATE #7.

PDATA (NSDATA =7,NTDATA=1:214,MKLOS =2)

1.013250E+05,1.164545E+05,1.328637E+05,2.969381E+05,4.678443E+05,
6.583228E+05,8.551700E+05,1.067707E+06,1.285569E+06,1.514794E+06,
1.745731E+06,1.979752E+06,2.213127E+06,2.445386E+06,2.680436E+06,
2.919471E+06,3.159042E+06,3.399262E+06,3.639050E+06,3.878254E+06,

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4.116121E+06,4.352572E+06,4.587498E+06,5.052158E+06,5.511509E+06,
5.966950E+06,6.420379E+06,6.871780E+06,7.321569E+06,7.770397E+06,
8.218751E+06,8.666901E+06,9.114884E+06,9.562751E+06,1.001048E+07,
1.045806E+07,1.090532E+07,1.135213E+07,1.179844E+07,1.224419E+07,
1.268943E+07,1.313412E+07,1.357821E+07,1.402143E+07,1.446351E+07,
1.490410E+07,1.534227E+07,1.577890E+07,1.621318E+07,1.664491E+07,
1.707389E+07,1.749968E+07,1.792144E+07,1.833862E+07,1.875031E+07,
1.915568E+07,1.955410E+07,1.994550E+07,2.032966E+07,2.070565E+07,
2.107273E+07,2.142949E+07,2.177396E+07,2.210547E+07,2.242261E+07,
2.272422E+07,2.301239E+07,2.328566E+07,2.331447E+07,2.337622E+07,
2.344192E+07,2.350443E+07,2.356230E+07,2.361563E+07,2.366498E+07,
2.371138E+07,2.375509E+07,2.379618E+07,2.383428E+07,2.386932E+07,
2.390150E+07,2.393079E+07,2.395739E+07,2.398164E+07,2.400399E+07,
2.402475E+07,2.404394E+07,2.406149E+07,2.407749E+07,2.409189E+07,
2.410476E+07,2.411630E+07,2.412657E+07,2.413573E+07,2.414391E+07,
2.415116E+07,2.415752E+07,2.416301E+07,2.416766E+07,2.417148E+07,
2.417450E+07,2.417684E+07,2.417852E+07,2.417961E+07,2.418016E+07,
2.418020E+07,2.417978E+07,2.417884E+07,2.417747E+07,2.417571E+07,
2.417353E+07,2.417099E+07,2.416813E+07,2.416492E+07,2.416137E+07,
2.415764E+07,2.420024E+07,2.411991E+07,2.397319E+07,2.383869E+07,
2.371576E+07,2.360247E+07,2.349773E+07,2.339976E+07,2.330951E+07,
2.322528E+07,2.314614E+07,2.307148E+07,2.300081E+07,2.293383E+07,
2.287018E+07,2.280948E+07,2.275151E+07,2.269556E+07,2.264240E+07,
2.259142E+07,2.254229E+07,2.249494E+07,2.244925E+07,2.240516E+07,
2.236250E+07,2.232121E+07,2.228128E+07,2.224253E+07,2.220451E+07,
2.216793E+07,2.213235E+07,2.209773E+07,2.206403E+07,2.203118E+07,
2.199917E+07,2.196793E+07,2.193746E+07,2.190766E+07,2.187827E+07,
2.184984E+07,2.182200E+07,2.179479E+07,2.176815E+07,2.174206E+07,
2.171650E+07,2.169145E+07,2.166690E+07,2.164279E+07,2.161919E+07,
2.159581E+07,2.157304E+07,2.155071E+07,2.152880E+07,2.150726E+07,
2.148607E+07,2.146526E+07,2.144481E+07,2.142470E+07,2.140493E+07,
2.138528E+07,2.136615E+07,2.134732E+07,2.132880E+07,2.131056E+07,
2.129261E+07,2.127494E+07,2.125754E+07,2.124037E+07,2.122348E+07,
2.120683E+07,2.119025E+07,2.117408E+07,2.115811E+07,2.114237E+07,
2.112684E+07,2.111154E+07,2.109643E+07,2.108152E+07,2.106681E+07,
2.105227E+07,2.103780E+07,2.102365E+07,2.100965E+07,2.099584E+07,
2.098221E+07,2.096876E+07,2.095545E+07,2.094230E+07,2.092932E+07,
2.091650E+07,2.090379E+07,2.089115E+07,2.087875E+07,2.086650E+07,
2.085438E+07,2.084242E+07,1.886452E+07,1.886452E+07

POROSITY SURFACE #2; GAS GENERATION RATE #7.
SDATA(NSDATA =7,NTDATA=1:214,MKLOS =2)

Information Only

1.000000E+00, 9.478489E-01, 9.426141E-01, 8.902719E-01, 8.428811E-01,
8.096146E-01, 7.787077E-01, 7.536157E-01, 7.304598E-01, 7.114597E-01,
6.948615E-01, 6.827894E-01, 6.725766E-01, 6.654428E-01, 6.586062E-01,
6.522078E-01, 6.464755E-01, 6.416089E-01, 6.373698E-01, 6.338563E-01,
6.309090E-01, 6.285429E-01, 6.266416E-01, 6.240241E-01, 6.224727E-01,
6.215351E-01, 6.209769E-01, 6.206787E-01, 6.205589E-01, 6.205316E-01,
6.205428E-01, 6.205688E-01, 6.206028E-01, 6.206422E-01, 6.206857E-01,
6.207355E-01, 6.207985E-01, 6.208815E-01, 6.209854E-01, 6.211094E-01,
6.212505E-01, 6.214073E-01, 6.215824E-01, 6.217840E-01, 6.220245E-01,
6.223129E-01, 6.226598E-01, 6.230717E-01, 6.235517E-01, 6.241030E-01,
6.247270E-01, 6.254348E-01, 6.262463E-01, 6.271816E-01, 6.282605E-01,
6.295013E-01, 6.309161E-01, 6.324976E-01, 6.342448E-01, 6.361750E-01,
6.383111E-01, 6.406838E-01, 6.433433E-01, 6.462997E-01, 6.495867E-01,
6.532295E-01, 6.571582E-01, 6.614067E-01, 6.657402E-01, 6.698859E-01,
6.739626E-01, 6.781091E-01, 6.823660E-01, 6.867368E-01, 6.912041E-01,
6.957399E-01, 7.003375E-01, 7.049962E-01, 7.097284E-01, 7.145349E-01,
7.194162E-01, 7.243718E-01, 7.293978E-01, 7.344847E-01, 7.396201E-01,
7.447953E-01, 7.500090E-01, 7.552677E-01, 7.605626E-01, 7.659070E-01,
7.712939E-01, 7.767182E-01, 7.821768E-01, 7.876688E-01, 7.931890E-01,
7.987365E-01, 8.043107E-01, 8.099108E-01, 8.155367E-01, 8.211873E-01,
8.268650E-01, 8.325652E-01, 8.382869E-01, 8.440288E-01, 8.497893E-01,
8.555671E-01, 8.613601E-01, 8.671734E-01, 8.730027E-01, 8.788473E-01,
8.847027E-01, 8.905759E-01, 8.964936E-01, 9.023908E-01, 9.083023E-01,
9.142210E-01, 9.201552E-01, 9.260823E-01, 9.317727E-01, 9.370510E-01,
9.419281E-01, 9.464683E-01, 9.507046E-01, 9.547019E-01, 9.584139E-01,
9.619044E-01, 9.652077E-01, 9.683444E-01, 9.713327E-01, 9.741821E-01,
9.769054E-01, 9.795162E-01, 9.820228E-01, 9.844548E-01, 9.867765E-01,
9.890134E-01, 9.911781E-01, 9.932740E-01, 9.953045E-01, 9.972718E-01,
9.991832E-01, 1.001040E+00, 1.002842E+00, 1.004597E+00, 1.006326E+00,
1.007993E+00, 1.009622E+00, 1.011211E+00, 1.012762E+00, 1.014279E+00,
1.015762E+00, 1.017214E+00, 1.018633E+00, 1.020025E+00, 1.021401E+00,
1.022737E+00, 1.024047E+00, 1.025332E+00, 1.026593E+00, 1.027830E+00,
1.029045E+00, 1.030239E+00, 1.031412E+00, 1.032567E+00, 1.033699E+00,
1.034824E+00, 1.035921E+00, 1.036999E+00, 1.038060E+00, 1.039105E+00,
1.040134E+00, 1.041147E+00, 1.042145E+00, 1.043128E+00, 1.044096E+00,
1.045060E+00, 1.046000E+00, 1.046926E+00, 1.047840E+00, 1.048741E+00,
1.049630E+00, 1.050505E+00, 1.051370E+00, 1.052223E+00, 1.053065E+00,
1.053896E+00, 1.054724E+00, 1.055533E+00, 1.056334E+00, 1.057124E+00,
1.057905E+00, 1.058676E+00, 1.059437E+00, 1.060190E+00, 1.060934E+00,
1.061670E+00, 1.062404E+00, 1.063122E+00, 1.063834E+00, 1.064538E+00,
1.065232E+00, 1.065919E+00, 1.066599E+00, 1.067273E+00, 1.067938E+00,

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1.068595E+00,1.069248E+00,1.069898E+00,1.070537E+00,1.071168E+00,  
1.071794E+00,1.072411E+00,1.185459E+00,1.185459E+00  
POROSITY SURFACE #2; GAS GENERATION RATE #8.  
PDATA(NSDATA =8,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #8.  
SDATA(NSDATA =8,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #9.  
PDATA(NSDATA =9,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #9.  
SDATA(NSDATA =9,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #10.  
PDATA(NSDATA =10,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #10.  
SDATA(NSDATA =10,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #11.  
PDATA(NSDATA =11,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #11.  
SDATA(NSDATA =11,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #12.  
PDATA(NSDATA =12,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #12.  
SDATA(NSDATA =12,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #13.  
PDATA(NSDATA =13,NTDATA=1:214,MKLOS =2)  
214*0.0D0  
POROSITY SURFACE #2; GAS GENERATION RATE #13.  
SDATA(NSDATA =13,NTDATA=1:214,MKLOS =2)  
214*0.0D0
```

Porosity Surface #3, the Original porosity surface, used before SPM2 in January 1995.
PDATA(1:NSDATA,1:NTDATA,1:MKLOS); NSDATA=13, NTDATA=214, MKLOS=4
FOR POROSITY SURFACE 3 ONLY 5 GAS GENERATION RATES ARE USED. THE REST ARE SET TO 0.

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POROSITY SURFACE #3; GAS GENERATION RATE #1.

PDATA (NSDATA =1,NTDATA=1:214,MKLOS =3)

214*1.01325E+05

POROSITY SURFACE #3; GAS GENERATION RATE #1.

SDATA (NSDATA =1,NTDATA=1:214,MKLOS =3)

6.601800E-01, 6.286592E-01, 6.147037E-01, 5.443911E-01, 4.840260E-01,
4.129768E-01, 3.591968E-01, 3.229848E-01, 2.956664E-01, 2.714550E-01,
2.515415E-01, 2.351813E-01, 2.209761E-01, 2.082591E-01, 1.967323E-01,
1.862986E-01, 1.771738E-01, 1.692050E-01, 1.621965E-01, 1.560070E-01,
1.505974E-01, 1.458731E-01, 1.417570E-01, 1.350343E-01, 1.299794E-01,
1.260634E-01, 1.229168E-01, 1.203476E-01, 1.182078E-01, 1.163877E-01,
1.148130E-01, 1.134184E-01, 1.121825E-01, 1.110670E-01, 1.100880E-01,
1.092200E-01, 1.084440E-01, 1.077474E-01, 1.071116E-01, 1.065305E-01,
1.060035E-01, 1.055185E-01, 1.050696E-01, 1.046564E-01, 1.042789E-01,
1.039193E-01, 1.035893E-01, 1.032771E-01, 1.029884E-01, 1.027173E-01,
1.024582E-01, 1.022223E-01, 1.019924E-01, 1.017800E-01, 1.015735E-01,
1.013786E-01, 1.011954E-01, 1.010238E-01, 1.008580E-01, 1.006980E-01,
1.005496E-01, 1.004013E-01, 1.002644E-01, 1.001334E-01, 1.000081E-01,
9.988862E-02, 9.976917E-02, 9.966115E-02, 9.955318E-02, 9.945095E-02,
9.935443E-02, 9.925798E-02, 9.916154E-02, 9.907083E-02, 9.898582E-02,
9.890085E-02, 9.882157E-02, 9.874231E-02, 9.866308E-02, 9.858954E-02,
9.851603E-02, 9.844253E-02, 9.837472E-02, 9.830692E-02, 9.823915E-02,
9.817705E-02, 9.811495E-02, 9.805288E-02, 9.799083E-02, 9.793443E-02,
9.787804E-02, 9.782167E-02, 9.776530E-02, 9.770899E-02, 9.765828E-02,
9.760761E-02, 9.755693E-02, 9.750627E-02, 9.745562E-02, 9.741062E-02,
9.736562E-02, 9.731499E-02, 9.727002E-02, 9.723067E-02, 9.718570E-02,
9.714075E-02, 9.710142E-02, 9.705649E-02, 9.701718E-02, 9.697787E-02,
9.693857E-02, 9.689929E-02, 9.686000E-02, 9.682633E-02, 9.678705E-02,
9.674779E-02, 9.671415E-02, 9.668049E-02, 9.664687E-02, 9.660762E-02,
9.657400E-02, 9.654037E-02, 9.650677E-02, 9.647875E-02, 9.644514E-02,
9.641153E-02, 9.638355E-02, 9.634995E-02, 9.632196E-02, 9.628838E-02,
9.626039E-02, 9.623241E-02, 9.619884E-02, 9.617086E-02, 9.614290E-02,
9.611493E-02, 9.608699E-02, 9.605902E-02, 9.603667E-02, 9.600872E-02,
9.598076E-02, 9.595282E-02, 9.593047E-02, 9.590254E-02, 9.588020E-02,
9.585226E-02, 9.582992E-02, 9.580199E-02, 9.577966E-02, 9.575732E-02,
9.572941E-02, 9.570707E-02, 9.568475E-02, 9.566242E-02, 9.564011E-02,
9.561779E-02, 9.559547E-02, 9.557316E-02, 9.555084E-02, 9.552853E-02,
9.550623E-02, 9.548391E-02, 9.546161E-02, 9.544490E-02, 9.542259E-02,
9.540030E-02, 9.538358E-02, 9.536128E-02, 9.533899E-02, 9.532227E-02,
9.529998E-02, 9.528327E-02, 9.526099E-02, 9.524428E-02, 9.522200E-02,
9.520530E-02, 9.518858E-02, 9.516631E-02, 9.514961E-02, 9.513290E-02,

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9.511063E-02,9.509393E-02,9.507724E-02,9.506055E-02,9.504384E-02,
9.502715E-02,9.500490E-02,9.498820E-02,9.497152E-02,9.495483E-02,
9.493814E-02,9.492145E-02,9.490477E-02,9.488809E-02,9.487141E-02,
9.486029E-02,9.484360E-02,9.482693E-02,9.481025E-02,9.479357E-02,
9.477690E-02,9.476579E-02,9.474911E-02,9.473243E-02,9.471577E-02,
9.470466E-02,9.468799E-02,9.467132E-02,9.466021E-02,9.464355E-02,
9.462687E-02,9.461577E-02,9.461577E-02,9.461577E-02

POROSITY SURFACE #3; GAS GENERATION RATE #2.

PDATA(NSDATA =2,NTDATA=1:214,MKLOS =3)

1.013250E+05,1.028473E+05,1.044385E+05,1.225220E+05,1.451320E+05,
1.758640E+05,2.136050E+05,2.567050E+05,3.045450E+05,3.566050E+05,
4.128750E+05,4.726850E+05,5.363650E+05,6.041950E+05,6.759650E+05,
7.518550E+05,8.314250E+05,9.136650E+05,9.977150E+05,1.083315E+06,
1.170325E+06,1.258325E+06,1.347325E+06,1.526725E+06,1.706225E+06,
1.883125E+06,2.057525E+06,2.230325E+06,2.401725E+06,2.571625E+06,
2.740225E+06,2.907425E+06,3.073225E+06,3.237625E+06,3.400625E+06,
3.562325E+06,3.722725E+06,3.882025E+06,4.040225E+06,4.197325E+06,
4.353425E+06,4.508525E+06,4.662825E+06,4.816125E+06,4.968925E+06,
5.121125E+06,5.273025E+06,5.424625E+06,5.575925E+06,5.726925E+06,
5.877825E+06,6.028525E+06,6.178925E+06,6.329325E+06,6.479425E+06,
6.629425E+06,6.779325E+06,6.929025E+06,7.078625E+06,7.228125E+06,
7.377425E+06,7.526625E+06,7.675725E+06,7.824625E+06,7.973425E+06,
8.122125E+06,8.270625E+06,8.406625E+06,8.480825E+06,8.555125E+06,
8.629325E+06,8.703525E+06,8.777625E+06,8.851725E+06,8.925825E+06,
8.999925E+06,9.074025E+06,9.148025E+06,9.221925E+06,9.295825E+06,
9.369725E+06,9.443625E+06,9.517525E+06,9.591425E+06,9.665225E+06,
9.738925E+06,9.812625E+06,9.886225E+06,9.959925E+06,1.003363E+07,
1.010733E+07,1.018133E+07,1.025433E+07,1.032733E+07,1.040133E+07,
1.047433E+07,1.054833E+07,1.062133E+07,1.069533E+07,1.076833E+07,
1.084133E+07,1.091433E+07,1.098833E+07,1.106133E+07,1.113433E+07,
1.120733E+07,1.128033E+07,1.135333E+07,1.142633E+07,1.149933E+07,
1.157233E+07,1.164533E+07,1.171833E+07,1.179133E+07,1.186433E+07,
1.193733E+07,1.200933E+07,1.206733E+07,1.206733E+07,1.206633E+07,
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Information Only

1.206533E+07,1.206533E+07,1.206533E+07,1.206533E+07,1.206533E+07,
1.206533E+07,1.206633E+07,1.206633E+07,1.206633E+07,1.206633E+07,
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1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07,
1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07,
1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07,
1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07,1.206733E+07

POROSITY SURFACE #3; GAS GENERATION RATE #2.

SDATA (NSDATA =2,NTDATAB=1:214,MKLOS =3)

6.601800E-01,6.286869E-01,6.148647E-01,5.423710E-01,4.815965E-01,
4.122770E-01,3.597437E-01,3.222874E-01,2.941726E-01,2.722588E-01,
2.543437E-01,2.396425E-01,2.270191E-01,2.158591E-01,2.059528E-01,
1.970205E-01,1.890169E-01,1.820006E-01,1.759262E-01,1.706272E-01,
1.659774E-01,1.618630E-01,1.582307E-01,1.521737E-01,1.474610E-01,
1.439027E-01,1.411504E-01,1.389616E-01,1.371806E-01,1.357188E-01,
1.345173E-01,1.335196E-01,1.326969E-01,1.320212E-01,1.314649E-01,
1.310079E-01,1.306363E-01,1.303369E-01,1.300898E-01,1.299015E-01,
1.297587E-01,1.296484E-01,1.295706E-01,1.295187E-01,1.294928E-01,
1.294798E-01,1.294733E-01,1.294733E-01,1.294798E-01,1.294928E-01,
1.295123E-01,1.295317E-01,1.295576E-01,1.295836E-01,1.296095E-01,
1.296354E-01,1.296679E-01,1.297003E-01,1.297327E-01,1.297652E-01,
1.297976E-01,1.298301E-01,1.298690E-01,1.299080E-01,1.299404E-01,
1.299794E-01,1.300184E-01,1.300573E-01,1.300703E-01,1.300898E-01,
1.301094E-01,1.301288E-01,1.301483E-01,1.301678E-01,1.301873E-01,
1.302003E-01,1.302198E-01,1.302394E-01,1.302588E-01,1.302784E-01,
1.302979E-01,1.303174E-01,1.303369E-01,1.303564E-01,1.303759E-01,
1.304020E-01,1.304215E-01,1.304410E-01,1.304605E-01,1.304801E-01,
1.304996E-01,1.305191E-01,1.305386E-01,1.305647E-01,1.305842E-01,
1.306037E-01,1.306233E-01,1.306494E-01,1.306689E-01,1.306884E-01,
1.307145E-01,1.307340E-01,1.307536E-01,1.307731E-01,1.307992E-01,
1.308188E-01,1.308383E-01,1.308644E-01,1.308839E-01,1.309100E-01,
1.309296E-01,1.309492E-01,1.309752E-01,1.309948E-01,1.310209E-01,
1.310405E-01,1.310600E-01,1.310796E-01,1.310796E-01,1.310861E-01,
1.310861E-01,1.310927E-01,1.310927E-01,1.310927E-01,1.310927E-01,
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1.310992E-01,1.310927E-01,1.310927E-01,1.310927E-01,1.310992E-01,
1.310992E-01,1.310992E-01,1.310992E-01,1.310992E-01,1.310992E-01,

Information Only

1.310992E-01,1.310992E-01,1.310992E-01,1.310992E-01,1.310992E-01,
1.310992E-01,1.310992E-01,1.310992E-01,1.310992E-01,1.310992E-01,
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1.310861E-01,1.310861E-01,1.310861E-01,1.310861E-01,1.310861E-01,
1.310861E-01,1.310861E-01,1.310861E-01,1.310861E-01,1.310861E-01,
1.310861E-01,1.310861E-01,1.310861E-01,1.310861E-01,1.310796E-01,
1.310796E-01,1.310796E-01,1.310796E-01,1.310796E-01,1.310796E-01,
1.310796E-01,1.310796E-01,1.310796E-01,1.310796E-01,1.310796E-01,
1.310796E-01,1.310796E-01,1.310796E-01,1.310796E-01,1.310731E-01,
1.310731E-01,1.310731E-01,1.310731E-01,1.310731E-01

POROSITY SURFACE #3; GAS GENERATION RATE #3.

PDATA (NSDATA =3,NTDATA=1:214,MKLOS =3)

1.013250E+05,1.043696E+05,1.075514E+05,1.438140E+05,1.892090E+05,
2.502750E+05,3.250150E+05,4.105250E+05,5.042350E+05,6.050750E+05,
7.129550E+05,8.268350E+05,9.455950E+05,1.070025E+06,1.199525E+06,
1.333925E+06,1.472825E+06,1.615525E+06,1.761325E+06,1.909225E+06,
2.057825E+06,2.206925E+06,2.356125E+06,2.654225E+06,2.950525E+06,
3.243725E+06,3.533125E+06,3.817625E+06,4.097125E+06,4.372425E+06,
4.643825E+06,4.911525E+06,5.175925E+06,5.437225E+06,5.695825E+06,
5.951925E+06,6.206225E+06,6.459625E+06,6.712225E+06,6.964225E+06,
7.215825E+06,7.466925E+06,7.717625E+06,7.968025E+06,8.218025E+06,
8.467625E+06,8.716925E+06,8.965925E+06,9.214625E+06,9.462925E+06,
9.710925E+06,9.958725E+06,1.020633E+07,1.045333E+07,1.070033E+07,
1.094633E+07,1.119233E+07,1.143833E+07,1.168433E+07,1.192733E+07,
1.216533E+07,1.240233E+07,1.263833E+07,1.286933E+07,1.309933E+07,
1.332733E+07,1.355633E+07,1.375833E+07,1.387733E+07,1.398633E+07,
1.409733E+07,1.420733E+07,1.431733E+07,1.442733E+07,1.453733E+07,
1.464533E+07,1.475233E+07,1.485833E+07,1.496633E+07,1.507133E+07,
1.517733E+07,1.528333E+07,1.538733E+07,1.549133E+07,1.559333E+07,
1.569533E+07,1.579833E+07,1.589733E+07,1.599833E+07,1.609633E+07,
1.619333E+07,1.629133E+07,1.631433E+07,1.636033E+07,1.640533E+07,
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1.666233E+07,1.670233E+07,1.674333E+07,1.678233E+07,1.682133E+07,
1.686033E+07,1.689833E+07,1.693533E+07,1.697233E+07,1.700833E+07,
1.704333E+07,1.707933E+07,1.711333E+07,1.714733E+07,1.718133E+07,
1.721433E+07,1.724633E+07,1.725733E+07,1.725333E+07,1.725033E+07,

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1.724633E+07,1.724333E+07,1.723933E+07,1.723633E+07,1.723233E+07,
1.722933E+07,1.722633E+07,1.722233E+07,1.721933E+07,1.721533E+07,
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1.701233E+07,1.701233E+07,1.701233E+07,1.701233E+07

POROSITY SURFACE #3; GAS GENERATION RATE #3.

SDATA(NSDATA =3,NTDData=1:214,MKLOS =3)

6.601800E-01,6.286869E-01,6.149184E-01,5.411589E-01,4.801299E-01,
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2.590345E-01,2.452293E-01,2.338321E-01,2.239533E-01,2.153417E-01,
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1.552341E-01,1.553063E-01,1.553784E-01,1.554578E-01,1.555589E-01,
1.557250E-01,1.558913E-01,1.560794E-01,1.563038E-01,1.565357E-01,
1.567823E-01,1.570074E-01,1.572909E-01,1.573563E-01,1.575236E-01,
1.576620E-01,1.578077E-01,1.579535E-01,1.581067E-01,1.582526E-01,
1.584133E-01,1.585813E-01,1.587568E-01,1.589105E-01,1.591082E-01,
1.592694E-01,1.594454E-01,1.596362E-01,1.598124E-01,1.600109E-01,
1.602094E-01,1.604082E-01,1.606292E-01,1.608356E-01,1.610570E-01,
1.612934E-01,1.615151E-01,1.622559E-01,1.629988E-01,1.637439E-01,
1.644837E-01,1.652332E-01,1.659850E-01,1.667390E-01,1.674952E-01,

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1.682537E-01,1.690145E-01,1.697775E-01,1.705429E-01,1.713105E-01,
1.720805E-01,1.728528E-01,1.736274E-01,1.744043E-01,1.751837E-01,
1.759653E-01,1.767415E-01,1.775279E-01,1.783168E-01,1.791080E-01,
1.799017E-01,1.806977E-01,1.814963E-01,1.815362E-01,1.815682E-01,
1.816082E-01,1.816402E-01,1.816803E-01,1.817123E-01,1.817523E-01,
1.817843E-01,1.818244E-01,1.818644E-01,1.818964E-01,1.819365E-01,
1.819685E-01,1.820086E-01,1.820407E-01,1.820807E-01,1.821128E-01,
1.821368E-01,1.822010E-01,1.822732E-01,1.823213E-01,1.823775E-01,
1.824336E-01,1.824898E-01,1.825782E-01,1.826264E-01,1.826103E-01,
1.826505E-01,1.826746E-01,1.827147E-01,1.827388E-01,1.826665E-01,
1.827308E-01,1.827388E-01,1.827228E-01,1.827710E-01,1.827147E-01,
1.827549E-01,1.828112E-01,1.828031E-01,1.828674E-01,1.828433E-01,
1.828755E-01,1.829800E-01,1.829559E-01,1.830202E-01,1.830524E-01,
1.830605E-01,1.831570E-01,1.831409E-01,1.831490E-01,1.831812E-01,
1.831490E-01,1.832134E-01,1.832134E-01,1.831731E-01,1.832134E-01,
1.831973E-01,1.832134E-01,1.832536E-01,1.832214E-01,1.832456E-01,
1.832939E-01,1.833100E-01,1.833503E-01,1.833422E-01,1.833503E-01,
1.834308E-01,1.834389E-01,1.834389E-01,1.834872E-01,1.834791E-01,
1.835275E-01,1.835517E-01,1.835275E-01,1.835517E-01,1.835436E-01,
1.835517E-01,1.835920E-01,1.835597E-01,1.835678E-01,1.836001E-01,
1.835920E-01,1.836243E-01,1.836243E-01,1.836323E-01,1.836807E-01,
1.836888E-01,1.837210E-01,1.837452E-01,1.837291E-01,1.837775E-01,
1.837936E-01,1.838017E-01,1.838017E-01,1.838017E-01

POROSITY SURFACE #3; GAS GENERATION RATE #4.

PDATA(NSDATA =4,NTDATA=1:214,MKLOS =3)

1.013250E+05,1.058916E+05,1.106643E+05,1.650910E+05,2.324750E+05,
3.230150E+05,4.328650E+05,5.544850E+05,6.894650E+05,8.351650E+05,
9.895350E+05,1.151625E+06,1.319325E+06,1.491625E+06,1.669425E+06,
1.851325E+06,2.036525E+06,2.224825E+06,2.415325E+06,2.607125E+06,
2.799625E+06,2.992325E+06,3.184825E+06,3.567925E+06,3.946625E+06,
4.319625E+06,4.686425E+06,5.046825E+06,5.401225E+06,5.750225E+06,
6.094425E+06,6.434825E+06,6.771325E+06,7.104225E+06,7.435425E+06,
7.765825E+06,8.095325E+06,8.424125E+06,8.752425E+06,9.080125E+06,
9.407325E+06,9.733925E+06,1.005143E+07,1.037833E+07,1.070433E+07,
1.103033E+07,1.135533E+07,1.168133E+07,1.200633E+07,1.233133E+07,
1.265533E+07,1.298033E+07,1.330433E+07,1.360333E+07,1.390133E+07,
1.419733E+07,1.449233E+07,1.478633E+07,1.507833E+07,1.536933E+07,
1.565933E+07,1.594733E+07,1.623433E+07,1.649433E+07,1.675133E+07,
1.700633E+07,1.725933E+07,1.748633E+07,1.757833E+07,1.766933E+07,
1.775833E+07,1.784733E+07,1.793633E+07,1.802333E+07,1.809433E+07,
1.819733E+07,1.828133E+07,1.836533E+07,1.844333E+07,1.852033E+07,

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1.860433E+07,1.867533E+07,1.874433E+07,1.882033E+07,1.889033E+07,
1.895333E+07,1.902033E+07,1.908733E+07,1.914733E+07,1.920733E+07,
1.926933E+07,1.932633E+07,1.938233E+07,1.943733E+07,1.949133E+07,
1.954333E+07,1.959333E+07,1.964333E+07,1.969233E+07,1.973833E+07,
1.978433E+07,1.983033E+07,1.987333E+07,1.991533E+07,1.995733E+07,
1.999633E+07,2.003633E+07,2.007333E+07,2.011033E+07,2.014633E+07,
2.018133E+07,2.021433E+07,2.024733E+07,2.027833E+07,2.030933E+07,
2.033933E+07,2.036733E+07,2.037033E+07,2.029533E+07,2.022633E+07,
2.016333E+07,2.010633E+07,2.005233E+07,2.000233E+07,1.995533E+07,
1.991133E+07,1.986933E+07,1.982933E+07,1.979233E+07,1.975533E+07,
1.972133E+07,1.968833E+07,1.965633E+07,1.962533E+07,1.959633E+07,
1.956733E+07,1.954033E+07,1.951333E+07,1.948733E+07,1.946233E+07,
1.943833E+07,1.941533E+07,1.939233E+07,1.937033E+07,1.934833E+07,
1.932733E+07,1.930733E+07,1.928733E+07,1.926733E+07,1.924833E+07,
1.923033E+07,1.921233E+07,1.919433E+07,1.917733E+07,1.916033E+07,
1.914333E+07,1.912733E+07,1.911133E+07,1.909633E+07,1.908033E+07,
1.906533E+07,1.905133E+07,1.903633E+07,1.902233E+07,1.900833E+07,
1.899533E+07,1.898133E+07,1.896833E+07,1.895533E+07,1.894233E+07,
1.893033E+07,1.891833E+07,1.890633E+07,1.889433E+07,1.888233E+07,
1.887033E+07,1.885933E+07,1.884833E+07,1.883733E+07,1.882633E+07,
1.881533E+07,1.880533E+07,1.879433E+07,1.878433E+07,1.877433E+07,
1.876433E+07,1.875433E+07,1.874533E+07,1.873533E+07,1.872633E+07,
1.871633E+07,1.870733E+07,1.869833E+07,1.868933E+07,1.868033E+07,
1.867133E+07,1.866333E+07,1.865433E+07,1.864633E+07,1.863733E+07,
1.862933E+07,1.862133E+07,1.861333E+07,1.860533E+07,1.859733E+07,
1.858933E+07,1.858133E+07,1.857433E+07,1.856633E+07,1.855933E+07,
1.855133E+07,1.854433E+07,1.854433E+07,1.854433E+07

POROSITY SURFACE #3; GAS GENERATION RATE #4.

SDATA (NSDATA =4,NTDATAB=1:214,MKLOS =3)

6.601800E-01,6.287422E-01,6.149451E-01,5.409078E-01,4.825706E-01,
4.158393E-01,3.654495E-01,3.314161E-01,3.047796E-01,2.839547E-01,
2.674243E-01,2.539491E-01,2.429617E-01,2.338805E-01,2.260185E-01,
2.192508E-01,2.133895E-01,2.082680E-01,2.037876E-01,1.998852E-01,
1.964867E-01,1.935238E-01,1.909497E-01,1.867633E-01,1.836081E-01,
1.812564E-01,1.795204E-01,1.782773E-01,1.773941E-01,1.767808E-01,
1.763806E-01,1.761298E-01,1.760045E-01,1.759810E-01,1.759966E-01,
1.760280E-01,1.760750E-01,1.761376E-01,1.762003E-01,1.762708E-01,
1.763492E-01,1.764355E-01,1.765061E-01,1.765767E-01,1.766473E-01,
1.767180E-01,1.767887E-01,1.768593E-01,1.769301E-01,1.770008E-01,
1.770716E-01,1.771423E-01,1.772131E-01,1.776067E-01,1.780010E-01,
1.783958E-01,1.787992E-01,1.791952E-01,1.795918E-01,1.799891E-01,

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1.803870E-01,1.807855E-01,1.811845E-01,1.818804E-01,1.825701E-01,
1.832697E-01,1.839631E-01,1.846664E-01,1.853635E-01,1.860706E-01,
1.867715E-01,1.874824E-01,1.881870E-01,1.889017E-01,1.896184E-01,
1.901385E-01,1.908503E-01,1.915556E-01,1.923128E-01,1.930722E-01,
1.937583E-01,1.945722E-01,1.953886E-01,1.961399E-01,1.969441E-01,
1.978018E-01,1.986281E-01,1.994485E-01,2.003313E-01,2.012085E-01,
2.020626E-01,2.029541E-01,2.038572E-01,2.047634E-01,2.056725E-01,
2.066023E-01,2.075440E-01,2.084802E-01,2.094284E-01,2.103978E-01,
2.113616E-01,2.123378E-01,2.133265E-01,2.143187E-01,2.153144E-01,
2.163229E-01,2.173351E-01,2.183601E-01,2.193980E-01,2.204306E-01,
2.214763E-01,2.225352E-01,2.235981E-01,2.246651E-01,2.257455E-01,
2.268300E-01,2.279282E-01,2.290021E-01,2.298317E-01,2.306062E-01,
2.313157E-01,2.319692E-01,2.325759E-01,2.331550E-01,2.336965E-01,
2.342100E-01,2.346952E-01,2.351618E-01,2.356097E-01,2.360290E-01,
2.364391E-01,2.368401E-01,2.372121E-01,2.375847E-01,2.379382E-01,
2.382822E-01,2.386069E-01,2.389320E-01,2.392377E-01,2.395437E-01,
2.398402E-01,2.401271E-01,2.404044E-01,2.406720E-01,2.409398E-01,
2.411980E-01,2.414564E-01,2.416952E-01,2.419440E-01,2.421732E-01,
2.424025E-01,2.426321E-01,2.428518E-01,2.430717E-01,2.432817E-01,
2.434919E-01,2.436922E-01,2.438927E-01,2.440933E-01,2.442840E-01,
2.444748E-01,2.446557E-01,2.448367E-01,2.450178E-01,2.451990E-01,
2.453703E-01,2.455417E-01,2.457131E-01,2.458746E-01,2.460362E-01,
2.461978E-01,2.463596E-01,2.465113E-01,2.466630E-01,2.468149E-01,
2.469668E-01,2.471189E-01,2.472609E-01,2.474029E-01,2.475450E-01,
2.476871E-01,2.478192E-01,2.479615E-01,2.480937E-01,2.482260E-01,
2.483481E-01,2.484805E-01,2.486129E-01,2.487352E-01,2.488576E-01,
2.489799E-01,2.491024E-01,2.492249E-01,2.493372E-01,2.494599E-01,
2.495723E-01,2.496848E-01,2.497972E-01,2.499098E-01,2.500224E-01,
2.501351E-01,2.502375E-01,2.503502E-01,2.504527E-01,2.505553E-01,
2.506681E-01,2.507707E-01,2.508631E-01,2.509658E-01,2.510686E-01,
2.511713E-01,2.512638E-01,2.512638E-01,2.512638E-01

POROSITY SURFACE #3; GAS GENERATION RATE #5.

PDATA (NSDATA =5,NTDATA=1:214,MKLOS =3)

1.013250E+05,1.089360E+05,1.168900E+05,2.072550E+05,3.181050E+05,
4.659750E+05,6.437450E+05,8.487950E+05,1.064795E+06,1.292425E+06,
1.529625E+06,1.774725E+06,2.025825E+06,2.279525E+06,2.535525E+06,
2.793325E+06,3.052025E+06,3.310425E+06,3.568125E+06,3.825025E+06,
4.080525E+06,4.334125E+06,4.585925E+06,5.082825E+06,5.570825E+06,
6.050625E+06,6.524025E+06,6.993025E+06,7.458425E+06,7.920925E+06,
8.380725E+06,8.838525E+06,9.294125E+06,9.747425E+06,1.019033E+07,
1.063833E+07,1.107833E+07,1.151033E+07,1.194233E+07,1.237133E+07,

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1.279233E+07,1.321733E+07,1.360633E+07,1.399533E+07,1.431433E+07,
1.465233E+07,1.498433E+07,1.531033E+07,1.563233E+07,1.594833E+07,
1.625933E+07,1.656533E+07,1.686633E+07,1.716233E+07,1.745333E+07,
1.773933E+07,1.802133E+07,1.829733E+07,1.856933E+07,1.883733E+07,
1.910033E+07,1.935833E+07,1.961333E+07,1.986233E+07,2.010833E+07,
2.034933E+07,2.058633E+07,2.079033E+07,2.083233E+07,2.083933E+07,
2.087533E+07,2.089633E+07,2.092633E+07,2.096133E+07,2.098433E+07,
2.101733E+07,2.104833E+07,2.107033E+07,2.110133E+07,2.112633E+07,
2.114733E+07,2.117333E+07,2.119333E+07,2.121133E+07,2.123233E+07,
2.124833E+07,2.126433E+07,2.128033E+07,2.129233E+07,2.130533E+07,
2.131733E+07,2.132633E+07,2.133633E+07,2.134533E+07,2.135233E+07,
2.135933E+07,2.136533E+07,2.137033E+07,2.137533E+07,2.137933E+07,
2.138233E+07,2.138533E+07,2.138733E+07,2.138933E+07,2.139133E+07,
2.139233E+07,2.139333E+07,2.139333E+07,2.139333E+07,2.139333E+07,
2.139233E+07,2.139233E+07,2.139133E+07,2.139033E+07,2.138833E+07,
2.138733E+07,2.138533E+07,2.135633E+07,2.124533E+07,2.114433E+07,
2.105133E+07,2.096633E+07,2.088733E+07,2.081433E+07,2.074533E+07,
2.068033E+07,2.061933E+07,2.056133E+07,2.050633E+07,2.045433E+07,
2.040433E+07,2.035733E+07,2.031133E+07,2.026833E+07,2.022633E+07,
2.018633E+07,2.014833E+07,2.011133E+07,2.007533E+07,2.004133E+07,
2.000733E+07,1.997533E+07,1.994433E+07,1.991433E+07,1.988433E+07,
1.985633E+07,1.982833E+07,1.980233E+07,1.977633E+07,1.975033E+07,
1.972633E+07,1.970133E+07,1.967833E+07,1.965533E+07,1.963333E+07,
1.961133E+07,1.959033E+07,1.956933E+07,1.954933E+07,1.952933E+07,
1.951033E+07,1.949133E+07,1.947233E+07,1.945433E+07,1.943633E+07,
1.941933E+07,1.940133E+07,1.938533E+07,1.936833E+07,1.935233E+07,
1.933633E+07,1.932133E+07,1.930533E+07,1.929033E+07,1.927533E+07,
1.926133E+07,1.924733E+07,1.923333E+07,1.921933E+07,1.920533E+07,
1.919233E+07,1.917933E+07,1.916633E+07,1.915333E+07,1.914033E+07,
1.912833E+07,1.911633E+07,1.910433E+07,1.909233E+07,1.908033E+07,
1.906933E+07,1.905833E+07,1.904733E+07,1.903533E+07,1.902533E+07,
1.901433E+07,1.900333E+07,1.899333E+07,1.898333E+07,1.897233E+07,
1.896233E+07,1.895233E+07,1.894333E+07,1.893333E+07,1.892333E+07,
1.891433E+07,1.890533E+07,1.889633E+07,1.888633E+07,1.887733E+07,
1.886933E+07,1.886033E+07,1.886033E+07,1.886033E+07

POROSITY SURFACE #3; GAS GENERATION RATE #5.

SDATA (NSDATA =5,NTDATA=1:214,MKLOS =3)

6.601800E-01,6.287145E-01,6.149720E-01,5.426231E-01,4.865704E-01,
4.212892E-01,3.722028E-01,3.348276E-01,3.100184E-01,2.914754E-01,
2.770364E-01,2.654558E-01,2.560523E-01,2.485416E-01,2.423626E-01,
2.372024E-01,2.328750E-01,2.292688E-01,2.262354E-01,2.236822E-01,

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2.215319E-01,2.197295E-01,2.182317E-01,2.159500E-01,2.144362E-01,
2.134526E-01,2.128227E-01,2.124186E-01,2.121584E-01,2.120150E-01,
2.119523E-01,2.119433E-01,2.119881E-01,2.120688E-01,2.123557E-01,
2.125263E-01,2.128497E-01,2.132725E-01,2.136689E-01,2.140929E-01,
2.146080E-01,2.150425E-01,2.160045E-01,2.169152E-01,2.184884E-01,
2.200706E-01,2.216618E-01,2.232620E-01,2.248714E-01,2.264901E-01,
2.281085E-01,2.297457E-01,2.313925E-01,2.330487E-01,2.347146E-01,
2.363903E-01,2.380757E-01,2.397710E-01,2.414763E-01,2.431917E-01,
2.449172E-01,2.466529E-01,2.483990E-01,2.501555E-01,2.519226E-01,
2.537002E-01,2.554886E-01,2.572878E-01,2.590978E-01,2.609190E-01,
2.627512E-01,2.647881E-01,2.666873E-01,2.685223E-01,2.705108E-01,
2.723690E-01,2.742497E-01,2.762201E-01,2.780907E-01,2.800294E-01,
2.820143E-01,2.839204E-01,2.859073E-01,2.879186E-01,2.898844E-01,
2.919214E-01,2.939479E-01,2.959755E-01,2.980522E-01,3.001183E-01,
3.021857E-01,3.042909E-01,3.063976E-01,3.085059E-01,3.106404E-01,
3.127764E-01,3.149266E-01,3.170909E-01,3.192568E-01,3.214242E-01,
3.236188E-01,3.258020E-01,3.279996E-01,3.302118E-01,3.324120E-01,
3.346268E-01,3.368562E-01,3.390732E-01,3.413185E-01,3.435512E-01,
3.457848E-01,3.480330E-01,3.502820E-01,3.525316E-01,3.547959E-01,
3.570465E-01,3.593118E-01,3.615484E-01,3.634353E-01,3.651569E-01,
3.667547E-01,3.682269E-01,3.696164E-01,3.709072E-01,3.721431E-01,
3.732935E-01,3.744026E-01,3.754400E-01,3.764501E-01,3.774025E-01,
3.783119E-01,3.791932E-01,3.800309E-01,3.808400E-01,3.816203E-01,
3.823716E-01,3.830937E-01,3.838018E-01,3.844804E-01,3.851294E-01,
3.857795E-01,3.863997E-01,3.869900E-01,3.875812E-01,3.881422E-01,
3.887040E-01,3.892354E-01,3.897519E-01,3.902692E-01,3.907715E-01,
3.912587E-01,3.917309E-01,3.921879E-01,3.926454E-01,3.930877E-01,
3.935307E-01,3.939424E-01,3.943704E-01,3.947672E-01,3.951643E-01,
3.955619E-01,3.959441E-01,3.963267E-01,3.966936E-01,3.970449E-01,
3.974127E-01,3.977486E-01,3.981010E-01,3.984376E-01,3.987586E-01,
3.990959E-01,3.994174E-01,3.997230E-01,4.000451E-01,4.003351E-01,
4.006415E-01,4.009320E-01,4.012228E-01,4.015138E-01,4.018050E-01,
4.020803E-01,4.023558E-01,4.026152E-01,4.028911E-01,4.031509E-01,
4.034109E-01,4.036711E-01,4.039151E-01,4.041594E-01,4.044200E-01,
4.046483E-01,4.048931E-01,4.051379E-01,4.053667E-01,4.055955E-01,
4.058245E-01,4.060536E-01,4.062665E-01,4.064794E-01,4.067090E-01,
4.069223E-01,4.071356E-01,4.073328E-01,4.075464E-01,4.077437E-01,
4.079575E-01,4.081550E-01,4.083526E-01,4.085504E-01,4.087482E-01,
4.089296E-01,4.091277E-01,4.091277E-01,4.091277E-01

POROSITY SURFACE #3; GAS GENERATION RATE #6.

PDATA (NSDATA =6,NTDATA=1:214,MKLOS =2)

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```
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #6.
SDATA(NSDATA =6,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #7.
PDATA(NSDATA =7,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #7.
SDATA(NSDATA =7,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #8.
PDATA(NSDATA =8,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #8.
SDATA(NSDATA =8,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #9.
PDATA(NSDATA =9,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #9.
SDATA(NSDATA =9,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #10.
PDATA(NSDATA =10,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #10.
SDATA(NSDATA =10,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #11.
PDATA(NSDATA =11,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #11.
SDATA(NSDATA =11,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #12.
PDATA(NSDATA =12,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #12.
SDATA(NSDATA =12,NTDATA=1:214,MKLOS =2)
214*0.0D0
POROSITY SURFACE #3; GAS GENERATION RATE #13.
```

Information Only

PDATA (NSDATA =13,NTDATA=1:214,MKLOS =2)

214*0.0D0

POROSITY SURFACE #3; GAS GENERATION RATE #13.

SDATA (NSDATA =13,NTDATA=1:214,MKLOS =2)

214*0.0D0

Porosity Surface #4, for Waste w/o Backfill. Used in the 1996 CCA calculations.

PDATA(1:NSDATA,1:NTDATA,1:MKLOS); NSDATA=13, NTDATA=214, MKLOS=4

FOR POROSITY SURFACE 4 ALL 13 GAS GENERATION RATES ARE USED.

POROSITY SURFACE #4; GAS GENERATION RATE #1.

PDATA (NSDATA =1,NTDATA=1:214,MKLOS =4)

214*1.01325E+05

POROSITY SURFACE #3; GAS GENERATION RATE #1.

SDATA (NSDATA =1,NTDATA=1:214,MKLOS =4)

8.483506E-01,7.678428E-01,7.532903E-01,6.618482E-01,5.881638E-01,
5.245745E-01,4.730805E-01,4.273885E-01,3.922284E-01,3.655416E-01,
3.426672E-01,3.248504E-01,3.085461E-01,2.942820E-01,2.817888E-01,
2.700120E-01,2.596050E-01,2.499781E-01,2.411298E-01,2.335753E-01,
2.264177E-01,2.199231E-01,2.138299E-01,2.024353E-01,1.923568E-01,
1.832925E-01,1.751700E-01,1.678976E-01,1.613997E-01,1.555435E-01,
1.502041E-01,1.453292E-01,1.408610E-01,1.367447E-01,1.329298E-01,
1.293905E-01,1.260545E-01,1.230789E-01,1.204224E-01,1.179445E-01,
1.156170E-01,1.134198E-01,1.113432E-01,1.094001E-01,1.075878E-01,
1.058807E-01,1.042702E-01,1.027407E-01,1.012968E-01,9.992570E-02,
9.861327E-02,9.736787E-02,9.617720E-02,9.497057E-02,9.375305E-02,
9.268106E-02,9.175387E-02,9.089061E-02,9.005954E-02,8.926152E-02,
8.850467E-02,8.778819E-02,8.708888E-02,8.641811E-02,8.578083E-02,
8.516889E-02,8.458601E-02,8.402581E-02,8.348105E-02,8.294640E-02,
8.243615E-02,8.193762E-02,8.146098E-02,8.098751E-02,8.053389E-02,
8.008932E-02,7.966609E-02,7.924685E-02,7.883700E-02,7.843533E-02,
7.804960E-02,7.767712E-02,7.731047E-02,7.695395E-02,7.660968E-02,
7.626354E-02,7.593400E-02,7.561212E-02,7.529071E-02,7.498190E-02,
7.468013E-02,7.438977E-02,7.409676E-02,7.379402E-02,7.350577E-02,
7.322142E-02,7.295707E-02,7.271977E-02,7.248293E-02,7.224777E-02,
7.201839E-02,7.179235E-02,7.157243E-02,7.135608E-02,7.114224E-02,
7.092882E-02,7.072266E-02,7.051700E-02,7.031783E-02,7.012454E-02,
6.993421E-02,6.974552E-02,6.955972E-02,6.937691E-02,6.919865E-02,
6.902656E-02,6.885707E-02,6.868939E-02,6.852389E-02,6.836029E-02,
6.819610E-02,6.803678E-02,6.788330E-02,6.772873E-02,6.757799E-02,
6.743103E-02,6.728488E-02,6.714114E-02,6.700168E-02,6.686261E-02,
6.672645E-02,6.659151E-02,6.645524E-02,6.632140E-02,6.618937E-02,
6.605848E-02,6.593300E-02,6.580110E-02,6.567227E-02,6.554881E-02,

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6.542683E-02, 6.530940E-02, 6.518675E-02, 6.507169E-02, 6.495712E-02,
6.484661E-02, 6.472992E-02, 6.461901E-02, 6.450641E-02, 6.439884E-02,
6.429229E-02, 6.418251E-02, 6.407217E-02, 6.397099E-02, 6.387098E-02,
6.376211E-02, 6.366289E-02, 6.356182E-02, 6.346667E-02, 6.337336E-02,
6.327214E-02, 6.317669E-02, 6.308820E-02, 6.298988E-02, 6.289590E-02,
6.280897E-02, 6.271845E-02, 6.263361E-02, 6.254847E-02, 6.246069E-02,
6.237855E-02, 6.229433E-02, 6.220630E-02, 6.211854E-02, 6.203881E-02,
6.195632E-02, 6.187841E-02, 6.180172E-02, 6.172317E-02, 6.164795E-02,
6.156999E-02, 6.149125E-02, 6.141602E-02, 6.133857E-02, 6.126763E-02,
6.119770E-02, 6.112126E-02, 6.104996E-02, 6.098326E-02, 6.091140E-02,
6.084418E-02, 6.077985E-02, 6.071217E-02, 6.064259E-02, 6.057543E-02,
6.050815E-02, 6.043750E-02, 6.037122E-02, 6.030519E-02, 6.024162E-02,
6.018000E-02, 6.011421E-02, 6.005227E-02, 5.999056E-02, 5.993175E-02,
5.987501E-02, 5.981561E-02, 5.975109E-02, 5.969391E-02, 5.963009E-02,
5.956814E-02, 5.951255E-02, 4.659957E-02, 4.659957E-02

POROSITY SURFACE #4; GAS GENERATION RATE #2.

PDATA (NSDATA =2, NTDATA=1:214, MKLOS =4)

1.013250E+05, 1.014774E+05, 1.016482E+05, 1.035547E+05, 1.058744E+05,
1.084761E+05, 1.119514E+05, 1.156997E+05, 1.199578E+05, 1.245299E+05,
1.292733E+05, 1.345260E+05, 1.399756E+05, 1.457405E+05, 1.518962E+05,
1.582375E+05, 1.650336E+05, 1.720454E+05, 1.793172E+05, 1.868410E+05,
1.944997E+05, 2.025290E+05, 2.108415E+05, 2.280676E+05, 2.462822E+05,
2.655015E+05, 2.856591E+05, 3.066924E+05, 3.283855E+05, 3.507896E+05,
3.738772E+05, 3.976224E+05, 4.219973E+05, 4.469476E+05, 4.724094E+05,
4.983721E+05, 5.247723E+05, 5.515557E+05, 5.787832E+05, 6.067250E+05,
6.350402E+05, 6.627483E+05, 6.907624E+05, 7.190219E+05, 7.475124E+05,
7.762291E+05, 8.051112E+05, 8.341893E+05, 8.633541E+05, 8.927027E+05,
9.221322E+05, 9.516090E+05, 9.812083E+05, 1.010829E+06, 1.040553E+06,
1.070343E+06, 1.100078E+06, 1.129864E+06, 1.159766E+06, 1.189691E+06,
1.219681E+06, 1.249675E+06, 1.279650E+06, 1.309664E+06, 1.339713E+06,
1.369712E+06, 1.399780E+06, 1.425164E+06, 1.444461E+06, 1.462465E+06,
1.480453E+06, 1.498485E+06, 1.516391E+06, 1.534305E+06, 1.552136E+06,
1.570024E+06, 1.587774E+06, 1.605531E+06, 1.623341E+06, 1.641049E+06,
1.660007E+06, 1.679366E+06, 1.698233E+06, 1.716882E+06, 1.735347E+06,
1.753596E+06, 1.771489E+06, 1.788975E+06, 1.805803E+06, 1.822736E+06,
1.839642E+06, 1.856546E+06, 1.873406E+06, 1.890143E+06, 1.906900E+06,
1.923633E+06, 1.940329E+06, 1.956938E+06, 1.973557E+06, 1.990150E+06,
2.006709E+06, 2.023283E+06, 2.039808E+06, 2.056299E+06, 2.072774E+06,
2.089171E+06, 2.105613E+06, 2.121979E+06, 2.138298E+06, 2.154604E+06,
2.170864E+06, 2.187151E+06, 2.203540E+06, 2.219790E+06, 2.235953E+06,
2.252067E+06, 2.268238E+06, 2.279117E+06, 2.283251E+06, 2.285873E+06,

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2.288547E+06, 2.291267E+06, 2.293935E+06, 2.296515E+06, 2.299229E+06,
2.301849E+06, 2.304285E+06, 2.306623E+06, 2.308922E+06, 2.311259E+06,
2.313513E+06, 2.315833E+06, 2.318191E+06, 2.320589E+06, 2.322827E+06,
2.324994E+06, 2.327308E+06, 2.329832E+06, 2.332247E+06, 2.334598E+06,
2.336945E+06, 2.339020E+06, 2.341292E+06, 2.343448E+06, 2.345653E+06,
2.347838E+06, 2.349809E+06, 2.351981E+06, 2.354166E+06, 2.356281E+06,
2.358290E+06, 2.360707E+06, 2.362494E+06, 2.364599E+06, 2.366594E+06,
2.368651E+06, 2.370755E+06, 2.372839E+06, 2.374700E+06, 2.376635E+06,
2.378535E+06, 2.380546E+06, 2.382838E+06, 2.384522E+06, 2.386413E+06,
2.388315E+06, 2.390165E+06, 2.392261E+06, 2.394107E+06, 2.396023E+06,
2.397772E+06, 2.399612E+06, 2.401404E+06, 2.403232E+06, 2.404922E+06,
2.406635E+06, 2.408430E+06, 2.410261E+06, 2.412056E+06, 2.413828E+06,
2.415503E+06, 2.417151E+06, 2.418949E+06, 2.420724E+06, 2.422384E+06,
2.424063E+06, 2.425753E+06, 2.427463E+06, 2.429494E+06, 2.431196E+06,
2.432850E+06, 2.434454E+06, 2.435976E+06, 2.437637E+06, 2.439355E+06,
2.441099E+06, 2.442630E+06, 2.444184E+06, 2.445773E+06, 2.447507E+06,
2.449018E+06, 2.450629E+06, 2.452203E+06, 2.453676E+06, 2.455262E+06,
2.456674E+06, 2.458291E+06, 2.459849E+06, 2.461464E+06, 2.462882E+06,
2.464230E+06, 2.465692E+06, 2.926491E+06, 2.926491E+06

POROSITY SURFACE #3; GAS GENERATION RATE #2.

SDATA (NSDATA =2,NTDATA=1:214,MKLOS =4)

8.483506E-01, 7.678672E-01, 7.540231E-01, 6.624943E-01, 5.880190E-01,
5.251452E-01, 4.734424E-01, 4.273939E-01, 3.926720E-01, 3.659500E-01,
3.433283E-01, 3.258734E-01, 3.097062E-01, 2.956110E-01, 2.831703E-01,
2.714817E-01, 2.613617E-01, 2.518894E-01, 2.431829E-01, 2.356968E-01,
2.286223E-01, 2.221921E-01, 2.161644E-01, 2.050489E-01, 1.954283E-01,
1.867871E-01, 1.790546E-01, 1.721046E-01, 1.659641E-01, 1.604360E-01,
1.554278E-01, 1.508666E-01, 1.466930E-01, 1.428706E-01, 1.393705E-01,
1.361482E-01, 1.331828E-01, 1.304554E-01, 1.279148E-01, 1.254744E-01,
1.231942E-01, 1.212804E-01, 1.194847E-01, 1.178047E-01, 1.162309E-01,
1.147511E-01, 1.133615E-01, 1.120551E-01, 1.108362E-01, 1.096818E-01,
1.085988E-01, 1.075852E-01, 1.066238E-01, 1.057231E-01, 1.048680E-01,
1.040580E-01, 1.033022E-01, 1.025850E-01, 1.018971E-01, 1.012441E-01,
1.006209E-01, 1.000298E-01, 9.947055E-02, 9.893592E-02, 9.842431E-02,
9.794079E-02, 9.747398E-02, 9.702995E-02, 9.659858E-02, 9.618022E-02,
9.577386E-02, 9.537509E-02, 9.499455E-02, 9.462323E-02, 9.426658E-02,
9.391493E-02, 9.358036E-02, 9.325328E-02, 9.293063E-02, 9.262137E-02,
9.224524E-02, 9.185488E-02, 9.150221E-02, 9.117015E-02, 9.085581E-02,
9.056042E-02, 9.029039E-02, 9.004802E-02, 8.984471E-02, 8.964051E-02,
8.944166E-02, 8.924683E-02, 8.905756E-02, 8.887830E-02, 8.870136E-02,
8.852880E-02, 8.836125E-02, 8.820074E-02, 8.804265E-02, 8.788839E-02,

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8.773848E-02,8.759053E-02,8.744734E-02,8.730809E-02,8.717181E-02,
8.704126E-02,8.691067E-02,8.678567E-02,8.666470E-02,8.654620E-02,
8.643094E-02,8.631673E-02,8.620306E-02,8.609348E-02,8.598910E-02,
8.588808E-02,8.578647E-02,8.568820E-02,8.559165E-02,8.548891E-02,
8.538436E-02,8.527831E-02,8.517453E-02,8.507445E-02,8.496941E-02,
8.486821E-02,8.477438E-02,8.468453E-02,8.459632E-02,8.450685E-02,
8.442074E-02,8.433230E-02,8.424260E-02,8.415159E-02,8.406681E-02,
8.398488E-02,8.389756E-02,8.380253E-02,8.371182E-02,8.362366E-02,
8.353590E-02,8.345845E-02,8.337379E-02,8.329363E-02,8.321178E-02,
8.313087E-02,8.305801E-02,8.297780E-02,8.289733E-02,8.281956E-02,
8.274586E-02,8.265735E-02,8.259200E-02,8.251520E-02,8.244255E-02,
8.236776E-02,8.229138E-02,8.221587E-02,8.214858E-02,8.207870E-02,
8.201022E-02,8.193791E-02,8.185556E-02,8.179524E-02,8.172753E-02,
8.165954E-02,8.159355E-02,8.151891E-02,8.145329E-02,8.138524E-02,
8.132324E-02,8.125815E-02,8.119484E-02,8.113034E-02,8.107085E-02,
8.101059E-02,8.094757E-02,8.088339E-02,8.082056E-02,8.075862E-02,
8.070015E-02,8.064274E-02,8.058016E-02,8.051849E-02,8.046092E-02,
8.040277E-02,8.034431E-02,8.028524E-02,8.021522E-02,8.015659E-02,
8.009972E-02,8.004466E-02,7.999250E-02,7.993561E-02,7.987688E-02,
7.981736E-02,7.976515E-02,7.971226E-02,7.965822E-02,7.959931E-02,
7.954806E-02,7.949353E-02,7.944034E-02,7.939062E-02,7.933711E-02,
7.928955E-02,7.923514E-02,7.918280E-02,7.912860E-02,7.908109E-02,
7.903598E-02,7.898713E-02,6.610390E-02,6.610390E-02

POROSITY SURFACE #4; GAS GENERATION RATE #3.

PDATA(NSDATA =3,NTDATA=1:214,MKLOS =4)

1.013250E+05,1.016297E+05,1.019530E+05,1.057204E+05,1.104215E+05,
1.156266E+05,1.225004E+05,1.300103E+05,1.383559E+05,1.474077E+05,
1.568218E+05,1.672256E+05,1.781407E+05,1.895539E+05,2.017789E+05,
2.143576E+05,2.277335E+05,2.416482E+05,2.559608E+05,2.708600E+05,
2.860190E+05,3.017025E+05,3.179827E+05,3.513858E+05,3.867434E+05,
4.238366E+05,4.625950E+05,5.029679E+05,5.445773E+05,5.873217E+05,
6.310529E+05,6.757711E+05,7.213970E+05,7.675252E+05,8.140367E+05,
8.611600E+05,9.087363E+05,9.566957E+05,1.005103E+06,1.053974E+06,
1.103093E+06,1.152451E+06,1.202102E+06,1.251977E+06,1.302002E+06,
1.352176E+06,1.402368E+06,1.452714E+06,1.503073E+06,1.553470E+06,
1.604003E+06,1.654482E+06,1.704947E+06,1.755511E+06,1.806067E+06,
1.856534E+06,1.906925E+06,1.957265E+06,2.007518E+06,2.057677E+06,
2.107686E+06,2.157613E+06,2.207423E+06,2.257109E+06,2.306689E+06,
2.356140E+06,2.405439E+06,2.446388E+06,2.476542E+06,2.504385E+06,
2.532211E+06,2.559943E+06,2.587608E+06,2.615196E+06,2.642712E+06,
2.670167E+06,2.697568E+06,2.724901E+06,2.752184E+06,2.779612E+06,

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2.806787E+06,2.833929E+06,2.860954E+06,2.887855E+06,2.914713E+06,
2.941478E+06,2.968183E+06,2.994800E+06,3.021321E+06,3.047822E+06,
3.074236E+06,3.100583E+06,3.126842E+06,3.153064E+06,3.179238E+06,
3.205310E+06,3.231325E+06,3.257282E+06,3.283182E+06,3.309020E+06,
3.334808E+06,3.360524E+06,3.386194E+06,3.411805E+06,3.437354E+06,
3.462854E+06,3.488288E+06,3.513675E+06,3.539018E+06,3.564310E+06,
3.589527E+06,3.614701E+06,3.639964E+06,3.665029E+06,3.690048E+06,
3.715009E+06,3.739931E+06,3.756065E+06,3.760908E+06,3.763006E+06,
3.765121E+06,3.767250E+06,3.769395E+06,3.771566E+06,3.773722E+06,
3.775880E+06,3.778037E+06,3.780204E+06,3.782369E+06,3.784532E+06,
3.786692E+06,3.788853E+06,3.791012E+06,3.793187E+06,3.795345E+06,
3.797489E+06,3.799632E+06,3.801769E+06,3.803908E+06,3.806033E+06,
3.808152E+06,3.810266E+06,3.812380E+06,3.814480E+06,3.816597E+06,
3.818694E+06,3.820769E+06,3.822843E+06,3.824913E+06,3.826962E+06,
3.829008E+06,3.831042E+06,3.833073E+06,3.835098E+06,3.837125E+06,
3.839130E+06,3.841121E+06,3.843099E+06,3.845075E+06,3.847042E+06,
3.848998E+06,3.850940E+06,3.852877E+06,3.854804E+06,3.856728E+06,
3.858651E+06,3.860546E+06,3.862436E+06,3.864314E+06,3.866186E+06,
3.868050E+06,3.869900E+06,3.871744E+06,3.873578E+06,3.875404E+06,
3.877239E+06,3.879044E+06,3.880841E+06,3.882629E+06,3.884406E+06,
3.886175E+06,3.887936E+06,3.889688E+06,3.891432E+06,3.893166E+06,
3.894891E+06,3.896627E+06,3.898334E+06,3.900033E+06,3.901727E+06,
3.903409E+06,3.905084E+06,3.906747E+06,3.908407E+06,3.910054E+06,
3.911692E+06,3.913339E+06,3.914963E+06,3.916580E+06,3.918187E+06,
3.919785E+06,3.921378E+06,3.922959E+06,3.924533E+06,3.926101E+06,
3.927661E+06,3.929210E+06,3.930770E+06,3.932305E+06,3.933835E+06,
3.935351E+06,3.936863E+06,4.472104E+06,4.472104E+06
POROSITY SURFACE #3; GAS GENERATION RATE #3.
SDATA (NSDATA =3,NTDATA=1:214,MKLOS =4)
8.483495E-01,7.679417E-01,7.525876E-01,6.611366E-01,5.894121E-01,
5.263598E-01,4.743176E-01,4.294747E-01,3.940904E-01,3.685982E-01,
3.464183E-01,3.282261E-01,3.118852E-01,2.973586E-01,2.851044E-01,
2.735806E-01,2.633561E-01,2.539609E-01,2.451660E-01,2.377703E-01,
2.307459E-01,2.243857E-01,2.186007E-01,2.078450E-01,1.984944E-01,
1.901591E-01,1.827118E-01,1.759932E-01,1.700264E-01,1.646974E-01,
1.599316E-01,1.556257E-01,1.517173E-01,1.482324E-01,1.451221E-01,
1.422782E-01,1.396877E-01,1.373244E-01,1.351456E-01,1.331229E-01,
1.312651E-01,1.295517E-01,1.279582E-01,1.264773E-01,1.251042E-01,
1.238262E-01,1.226404E-01,1.215335E-01,1.205048E-01,1.195446E-01,
1.186379E-01,1.177943E-01,1.170041E-01,1.162560E-01,1.155528E-01,
1.148959E-01,1.142806E-01,1.137019E-01,1.131589E-01,1.126485E-01,

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1.121726E-01,1.117245E-01,1.113038E-01,1.109089E-01,1.105371E-01,
1.101880E-01,1.098605E-01,1.095499E-01,1.092493E-01,1.089571E-01,
1.086723E-01,1.083981E-01,1.081327E-01,1.078766E-01,1.076292E-01,
1.073897E-01,1.071574E-01,1.069327E-01,1.067147E-01,1.064951E-01,
1.062902E-01,1.060907E-01,1.058995E-01,1.057168E-01,1.055392E-01,
1.053684E-01,1.052028E-01,1.050436E-01,1.048901E-01,1.047407E-01,
1.045971E-01,1.044584E-01,1.043248E-01,1.041951E-01,1.040692E-01,
1.039488E-01,1.038323E-01,1.037197E-01,1.036107E-01,1.035053E-01,
1.034034E-01,1.033054E-01,1.032103E-01,1.031186E-01,1.030302E-01,
1.029446E-01,1.028621E-01,1.027825E-01,1.027053E-01,1.026308E-01,
1.025590E-01,1.024899E-01,1.024227E-01,1.023582E-01,1.022959E-01,
1.022360E-01,1.021781E-01,1.021214E-01,1.020640E-01,1.020055E-01,
1.019467E-01,1.018875E-01,1.018279E-01,1.017676E-01,1.017079E-01,
1.016482E-01,1.015885E-01,1.015287E-01,1.014690E-01,1.014094E-01,
1.013499E-01,1.012906E-01,1.012313E-01,1.011716E-01,1.011125E-01,
1.010539E-01,1.009954E-01,1.009370E-01,1.008787E-01,1.008208E-01,
1.007632E-01,1.007058E-01,1.006484E-01,1.005915E-01,1.005342E-01,
1.004775E-01,1.004214E-01,1.003654E-01,1.003096E-01,1.002545E-01,
1.001994E-01,1.001448E-01,1.000903E-01,1.000360E-01,9.998173E-02,
9.992811E-02,9.987489E-02,9.982211E-02,9.976943E-02,9.971702E-02,
9.966499E-02,9.961334E-02,9.956190E-02,9.951081E-02,9.945985E-02,
9.940892E-02,9.935882E-02,9.930888E-02,9.925933E-02,9.920996E-02,
9.916086E-02,9.911221E-02,9.906373E-02,9.901557E-02,9.896768E-02,
9.891956E-02,9.887229E-02,9.882529E-02,9.877858E-02,9.873216E-02,
9.868603E-02,9.864013E-02,9.859449E-02,9.854913E-02,9.850408E-02,
9.845930E-02,9.841424E-02,9.836996E-02,9.832598E-02,9.828216E-02,
9.823868E-02,9.819543E-02,9.815251E-02,9.810972E-02,9.806728E-02,
9.802514E-02,9.798281E-02,9.794107E-02,9.789956E-02,9.785835E-02,
9.781737E-02,9.777656E-02,9.773612E-02,9.769590E-02,9.765584E-02,
9.761603E-02,9.757653E-02,9.753679E-02,9.749771E-02,9.745877E-02,
9.742026E-02,9.738183E-02,8.545658E-02,8.545658E-02

POROSITY SURFACE #4; GAS GENERATION RATE #4.

PDATA (NSDATA =4,NTDATA=1:214,MKLOS =4)

1.013250E+05,1.019346E+05,1.026029E+05,1.102884E+05,1.194610E+05,
1.299878E+05,1.437178E+05,1.585484E+05,1.755090E+05,1.935436E+05,
2.123112E+05,2.330655E+05,2.544944E+05,2.771959E+05,3.011558E+05,
3.257760E+05,3.519634E+05,3.788256E+05,4.067782E+05,4.356074E+05,
4.648607E+05,4.951823E+05,5.261585E+05,5.899170E+05,6.566563E+05,
7.259973E+05,7.978227E+05,8.719307E+05,9.479426E+05,1.025643E+06,
1.104451E+06,1.183959E+06,1.264407E+06,1.345584E+06,1.427392E+06,
1.509860E+06,1.592707E+06,1.676876E+06,1.762162E+06,1.845140E+06,

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1.927777E+06,2.010366E+06,2.092845E+06,2.175338E+06,2.257610E+06,
2.339575E+06,2.422031E+06,2.504527E+06,2.585946E+06,2.666732E+06,
2.747252E+06,2.827563E+06,2.907573E+06,2.987382E+06,3.066968E+06,
3.146196E+06,3.225410E+06,3.304572E+06,3.383317E+06,3.461662E+06,
3.539546E+06,3.616978E+06,3.694025E+06,3.770848E+06,3.847463E+06,
3.923727E+06,3.999783E+06,4.061870E+06,4.105616E+06,4.145447E+06,
4.185212E+06,4.224929E+06,4.264567E+06,4.304174E+06,4.343738E+06,
4.383177E+06,4.422688E+06,4.461980E+06,4.501293E+06,4.540476E+06,
4.579929E+06,4.618818E+06,4.657807E+06,4.696839E+06,4.735600E+06,
4.774566E+06,4.813136E+06,4.851801E+06,4.890425E+06,4.929003E+06,
4.967600E+06,5.006106E+06,5.044713E+06,5.082871E+06,5.121065E+06,
5.159235E+06,5.197465E+06,5.235711E+06,5.273835E+06,5.311948E+06,
5.350033E+06,5.388028E+06,5.425872E+06,5.463740E+06,5.501607E+06,
5.539359E+06,5.577072E+06,5.614746E+06,5.652417E+06,5.690077E+06,
5.727645E+06,5.765193E+06,5.802954E+06,5.840494E+06,5.877976E+06,
5.915430E+06,5.952887E+06,5.976142E+06,5.981307E+06,5.982055E+06,
5.982825E+06,5.983595E+06,5.984354E+06,5.985148E+06,5.985950E+06,
5.986747E+06,5.987554E+06,5.988348E+06,5.989181E+06,5.990044E+06,
5.990881E+06,5.991764E+06,5.992648E+06,5.993528E+06,5.994365E+06,
5.995213E+06,5.996055E+06,5.996957E+06,5.997846E+06,5.998739E+06,
5.999662E+06,6.000560E+06,6.001484E+06,6.002384E+06,6.003286E+06,
6.004245E+06,6.005148E+06,6.006065E+06,6.007048E+06,6.007983E+06,
6.008864E+06,6.009765E+06,6.010673E+06,6.011594E+06,6.012522E+06,
6.013452E+06,6.014421E+06,6.015324E+06,6.016267E+06,6.017190E+06,
6.018164E+06,6.019042E+06,6.019985E+06,6.020883E+06,6.021782E+06,
6.022678E+06,6.023661E+06,6.024690E+06,6.025596E+06,6.026534E+06,
6.027446E+06,6.028335E+06,6.029227E+06,6.030177E+06,6.031128E+06,
6.032075E+06,6.033012E+06,6.033943E+06,6.034831E+06,6.035754E+06,
6.036684E+06,6.037595E+06,6.038457E+06,6.039358E+06,6.040285E+06,
6.041164E+06,6.042070E+06,6.043001E+06,6.043921E+06,6.044832E+06,
6.045728E+06,6.046644E+06,6.047574E+06,6.048490E+06,6.049386E+06,
6.050259E+06,6.051185E+06,6.052100E+06,6.052997E+06,6.053872E+06,
6.054723E+06,6.055629E+06,6.056517E+06,6.057427E+06,6.058260E+06,
6.059140E+06,6.060005E+06,6.060887E+06,6.061792E+06,6.062669E+06,
6.063541E+06,6.064350E+06,6.483598E+06,6.483598E+06

POROSITY SURFACE #3; GAS GENERATION RATE #4.

SDATA (NSDATA =4,NTDATAB=1:214,MKLOS =4)

8.483506E-01,7.678874E-01,7.534420E-01,6.639170E-01,5.886994E-01,
5.264776E-01,4.748047E-01,4.285256E-01,3.948846E-01,3.681094E-01,
3.459574E-01,3.285309E-01,3.124231E-01,2.987258E-01,2.865639E-01,
2.752134E-01,2.657089E-01,2.566832E-01,2.484152E-01,2.411459E-01,

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2.343186E-01, 2.283589E-01, 2.227827E-01, 2.127323E-01, 2.040181E-01,
1.963358E-01, 1.895245E-01, 1.834396E-01, 1.780215E-01, 1.731778E-01,
1.688968E-01, 1.651346E-01, 1.617559E-01, 1.587215E-01, 1.559849E-01,
1.534942E-01, 1.512405E-01, 1.491032E-01, 1.470752E-01, 1.454412E-01,
1.439835E-01, 1.426552E-01, 1.414453E-01, 1.403308E-01, 1.393157E-01,
1.383947E-01, 1.375051E-01, 1.366778E-01, 1.359648E-01, 1.353307E-01,
1.347490E-01, 1.342119E-01, 1.337188E-01, 1.332635E-01, 1.328427E-01,
1.324593E-01, 1.320963E-01, 1.317532E-01, 1.314433E-01, 1.311626E-01,
1.309132E-01, 1.306917E-01, 1.304937E-01, 1.303120E-01, 1.301450E-01,
1.299966E-01, 1.298602E-01, 1.297294E-01, 1.296050E-01, 1.294856E-01,
1.293706E-01, 1.292592E-01, 1.291522E-01, 1.290484E-01, 1.289478E-01,
1.288530E-01, 1.287576E-01, 1.286705E-01, 1.285843E-01, 1.285031E-01,
1.284158E-01, 1.283462E-01, 1.282750E-01, 1.282036E-01, 1.281411E-01,
1.280739E-01, 1.280183E-01, 1.279613E-01, 1.279055E-01, 1.278527E-01,
1.278002E-01, 1.277509E-01, 1.276994E-01, 1.276606E-01, 1.276214E-01,
1.275835E-01, 1.275446E-01, 1.275058E-01, 1.274707E-01, 1.274360E-01,
1.274029E-01, 1.273723E-01, 1.273458E-01, 1.273192E-01, 1.272929E-01,
1.272697E-01, 1.272474E-01, 1.272266E-01, 1.272062E-01, 1.271863E-01,
1.271679E-01, 1.271508E-01, 1.271335E-01, 1.271165E-01, 1.271009E-01,
1.270859E-01, 1.270713E-01, 1.270587E-01, 1.270443E-01, 1.270281E-01,
1.270115E-01, 1.269949E-01, 1.269875E-01, 1.269613E-01, 1.269440E-01,
1.269268E-01, 1.269095E-01, 1.268923E-01, 1.268744E-01, 1.268558E-01,
1.268378E-01, 1.268188E-01, 1.267997E-01, 1.267808E-01, 1.267628E-01,
1.267445E-01, 1.267264E-01, 1.267070E-01, 1.266879E-01, 1.266688E-01,
1.266489E-01, 1.266297E-01, 1.266098E-01, 1.265905E-01, 1.265711E-01,
1.265506E-01, 1.265312E-01, 1.265116E-01, 1.264906E-01, 1.264705E-01,
1.264517E-01, 1.264324E-01, 1.264129E-01, 1.263932E-01, 1.263734E-01,
1.263535E-01, 1.263328E-01, 1.263136E-01, 1.262934E-01, 1.262737E-01,
1.262529E-01, 1.262342E-01, 1.262140E-01, 1.261949E-01, 1.261758E-01,
1.261566E-01, 1.261357E-01, 1.261138E-01, 1.260945E-01, 1.260746E-01,
1.260551E-01, 1.260362E-01, 1.260173E-01, 1.259971E-01, 1.259769E-01,
1.259568E-01, 1.259369E-01, 1.259171E-01, 1.258983E-01, 1.258787E-01,
1.258589E-01, 1.258397E-01, 1.258214E-01, 1.258023E-01, 1.257826E-01,
1.257640E-01, 1.257449E-01, 1.257252E-01, 1.257057E-01, 1.256864E-01,
1.256675E-01, 1.256481E-01, 1.256284E-01, 1.256091E-01, 1.255902E-01,
1.255717E-01, 1.255522E-01, 1.255329E-01, 1.255140E-01, 1.254956E-01,
1.254776E-01, 1.254585E-01, 1.254398E-01, 1.254206E-01, 1.254031E-01,
1.253846E-01, 1.253664E-01, 1.253478E-01, 1.253288E-01, 1.253104E-01,
1.252920E-01, 1.252750E-01, 1.170458E-01, 1.170458E-01

POROSITY SURFACE #4; GAS GENERATION RATE #5.

PDATA (NSDATA =5,NTDATA=1:214,MKLOS =4)

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1.013250E+05, 1.025443E+05, 1.038581E+05, 1.194076E+05, 1.374476E+05,
1.588241E+05, 1.858315E+05, 2.151227E+05, 2.488736E+05, 2.843397E+05,
3.215324E+05, 3.616734E+05, 4.029782E+05, 4.467296E+05, 4.922924E+05,
5.391876E+05, 5.888543E+05, 6.394512E+05, 6.918700E+05, 7.461174E+05,
8.013669E+05, 8.574603E+05, 9.141704E+05, 1.029911E+06, 1.149088E+06,
1.271227E+06, 1.395888E+06, 1.522482E+06, 1.650725E+06, 1.780078E+06,
1.910493E+06, 2.041574E+06, 2.173055E+06, 2.304471E+06, 2.435737E+06,
2.566570E+06, 2.696663E+06, 2.826148E+06, 2.954607E+06, 3.082147E+06,
3.208892E+06, 3.335029E+06, 3.460424E+06, 3.585146E+06, 3.709178E+06,
3.832480E+06, 3.954827E+06, 4.076654E+06, 4.197885E+06, 4.318463E+06,
4.438463E+06, 4.557855E+06, 4.676648E+06, 4.794961E+06, 4.912849E+06,
5.030296E+06, 5.147402E+06, 5.264145E+06, 5.380528E+06, 5.496592E+06,
5.612488E+06, 5.728196E+06, 5.843720E+06, 5.959088E+06, 6.074421E+06,
6.189690E+06, 6.304859E+06, 6.397909E+06, 6.461939E+06, 6.519852E+06,
6.577690E+06, 6.635527E+06, 6.693362E+06, 6.751171E+06, 6.808979E+06,
6.866761E+06, 6.924516E+06, 6.982235E+06, 7.039906E+06, 7.097536E+06,
7.155137E+06, 7.212737E+06, 7.270284E+06, 7.327832E+06, 7.385342E+06,
7.442836E+06, 7.500285E+06, 7.557729E+06, 7.615095E+06, 7.672494E+06,
7.729873E+06, 7.787233E+06, 7.844557E+06, 7.901874E+06, 7.959174E+06,
8.016474E+06, 8.073752E+06, 8.131010E+06, 8.188248E+06, 8.245449E+06,
8.302662E+06, 8.359841E+06, 8.417004E+06, 8.474166E+06, 8.531298E+06,
8.588423E+06, 8.645510E+06, 8.702594E+06, 8.759666E+06, 8.816718E+06,
8.873687E+06, 8.930676E+06, 8.987961E+06, 9.044871E+06, 9.101771E+06,
9.158637E+06, 9.215486E+06, 9.250348E+06, 9.257054E+06, 9.256828E+06,
9.256636E+06, 9.256467E+06, 9.256310E+06, 9.256166E+06, 9.256035E+06,
9.255912E+06, 9.255803E+06, 9.255701E+06, 9.255597E+06, 9.255497E+06,
9.255406E+06, 9.255326E+06, 9.255239E+06, 9.255157E+06, 9.255082E+06,
9.255010E+06, 9.254942E+06, 9.254876E+06, 9.254811E+06, 9.254748E+06,
9.254690E+06, 9.254626E+06, 9.254571E+06, 9.254519E+06, 9.254471E+06,
9.254415E+06, 9.254368E+06, 9.254321E+06, 9.254275E+06, 9.254233E+06,
9.254188E+06, 9.254147E+06, 9.254107E+06, 9.254061E+06, 9.254026E+06,
9.253989E+06, 9.253948E+06, 9.253913E+06, 9.253877E+06, 9.253849E+06,
9.253814E+06, 9.253785E+06, 9.253752E+06, 9.253721E+06, 9.253694E+06,
9.253666E+06, 9.253638E+06, 9.253612E+06, 9.253586E+06, 9.253557E+06,
9.253535E+06, 9.253513E+06, 9.253491E+06, 9.253472E+06, 9.253451E+06,
9.253428E+06, 9.253408E+06, 9.253391E+06, 9.253372E+06, 9.253352E+06,
9.253336E+06, 9.253321E+06, 9.253305E+06, 9.253290E+06, 9.253276E+06,
9.253261E+06, 9.253246E+06, 9.253235E+06, 9.253223E+06, 9.253213E+06,
9.253202E+06, 9.253190E+06, 9.253180E+06, 9.253172E+06, 9.253164E+06,
9.253154E+06, 9.253148E+06, 9.253142E+06, 9.253135E+06, 9.253127E+06,
9.253123E+06, 9.253119E+06, 9.253112E+06, 9.253111E+06, 9.253107E+06,

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9.253104E+06,9.253101E+06,9.253096E+06,9.253098E+06,9.253097E+06,
9.253096E+06,9.253095E+06,9.259519E+06,9.259519E+06
POROSITY SURFACE #3; GAS GENERATION RATE #5.
SDATA (NSDATA =5,NTDATAB=1:214,MKLOS =4)
8.483506E-01,7.678452E-01,7.529217E-01,6.649817E-01,5.886133E-01,
5.277090E-01,4.762030E-01,4.296574E-01,3.974216E-01,3.706221E-01,
3.492238E-01,3.323670E-01,3.169890E-01,3.042621E-01,2.927791E-01,
2.822220E-01,2.731627E-01,2.646062E-01,2.570087E-01,2.499884E-01,
2.432891E-01,2.378687E-01,2.327596E-01,2.238362E-01,2.162365E-01,
2.096394E-01,2.039061E-01,1.989088E-01,1.945214E-01,1.906792E-01,
1.872761E-01,1.842678E-01,1.816046E-01,1.792650E-01,1.772000E-01,
1.753856E-01,1.738041E-01,1.724120E-01,1.712079E-01,1.701600E-01,
1.692419E-01,1.684271E-01,1.677109E-01,1.670784E-01,1.665219E-01,
1.660349E-01,1.656138E-01,1.652465E-01,1.649249E-01,1.646474E-01,
1.644072E-01,1.642024E-01,1.640284E-01,1.638813E-01,1.637560E-01,
1.636513E-01,1.635625E-01,1.634893E-01,1.634304E-01,1.633827E-01,
1.633430E-01,1.633104E-01,1.632844E-01,1.632638E-01,1.632450E-01,
1.632285E-01,1.632144E-01,1.631995E-01,1.631841E-01,1.631698E-01,
1.631576E-01,1.631456E-01,1.631335E-01,1.631227E-01,1.631120E-01,
1.631023E-01,1.630932E-01,1.630853E-01,1.630785E-01,1.630724E-01,
1.630675E-01,1.630627E-01,1.630592E-01,1.630557E-01,1.630531E-01,
1.630509E-01,1.630494E-01,1.630483E-01,1.630478E-01,1.630478E-01,
1.630482E-01,1.630490E-01,1.630502E-01,1.630518E-01,1.630538E-01,
1.630558E-01,1.630582E-01,1.630609E-01,1.630640E-01,1.630675E-01,
1.630710E-01,1.630751E-01,1.630796E-01,1.630840E-01,1.630888E-01,
1.630938E-01,1.630990E-01,1.631047E-01,1.631104E-01,1.631165E-01,
1.631230E-01,1.631297E-01,1.631366E-01,1.631440E-01,1.631513E-01,
1.631590E-01,1.631671E-01,1.631748E-01,1.631805E-01,1.631845E-01,
1.631879E-01,1.631909E-01,1.631937E-01,1.631963E-01,1.631986E-01,
1.632008E-01,1.632028E-01,1.632046E-01,1.632065E-01,1.632082E-01,
1.632099E-01,1.632113E-01,1.632128E-01,1.632143E-01,1.632156E-01,
1.632169E-01,1.632181E-01,1.632193E-01,1.632204E-01,1.632216E-01,
1.632226E-01,1.632238E-01,1.632247E-01,1.632256E-01,1.632265E-01,
1.632275E-01,1.632284E-01,1.632292E-01,1.632300E-01,1.632308E-01,
1.632316E-01,1.632323E-01,1.632330E-01,1.632339E-01,1.632345E-01,
1.632351E-01,1.632358E-01,1.632365E-01,1.632371E-01,1.632376E-01,
1.632382E-01,1.632388E-01,1.632394E-01,1.632399E-01,1.632404E-01,
1.632409E-01,1.632414E-01,1.632418E-01,1.632423E-01,1.632428E-01,
1.632432E-01,1.632436E-01,1.632440E-01,1.632443E-01,1.632447E-01,
1.632451E-01,1.632455E-01,1.632458E-01,1.632461E-01,1.632465E-01,
1.632467E-01,1.632470E-01,1.632473E-01,1.632476E-01,1.632478E-01,

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1.632481E-01,1.632484E-01,1.632486E-01,1.632488E-01,1.632489E-01,
1.632491E-01,1.632494E-01,1.632495E-01,1.632497E-01,1.632498E-01,
1.632500E-01,1.632501E-01,1.632502E-01,1.632503E-01,1.632505E-01,
1.632506E-01,1.632506E-01,1.632507E-01,1.632508E-01,1.632508E-01,
1.632509E-01,1.632509E-01,1.632510E-01,1.632510E-01,1.632510E-01,
1.632510E-01,1.632510E-01,1.631365E-01,1.631365E-01
POROSITY SURFACE #4; GAS GENERATION RATE #6.
PDATA (NSDATA =6,NTDATA=1:214,MKLOS =4)
1.013250E+05,1.037616E+05,1.064620E+05,1.361485E+05,1.737320E+05,
2.153770E+05,2.681425E+05,3.270940E+05,3.918626E+05,4.611288E+05,
5.325541E+05,6.089206E+05,6.881539E+05,7.693756E+05,8.549747E+05,
9.419661E+05,1.031590E+06,1.123621E+06,1.216973E+06,1.313244E+06,
1.410169E+06,1.508153E+06,1.607962E+06,1.808878E+06,2.011213E+06,
2.213233E+06,2.416201E+06,2.619227E+06,2.821798E+06,3.023611E+06,
3.224319E+06,3.423891E+06,3.622082E+06,3.818618E+06,4.013660E+06,
4.207126E+06,4.399073E+06,4.589644E+06,4.778817E+06,4.966654E+06,
5.153276E+06,5.338798E+06,5.523374E+06,5.707104E+06,5.890124E+06,
6.072539E+06,6.254260E+06,6.435841E+06,6.617137E+06,6.798209E+06,
6.979108E+06,7.159865E+06,7.340439E+06,7.520957E+06,7.701362E+06,
7.881659E+06,8.061889E+06,8.242039E+06,8.422087E+06,8.601988E+06,
8.781935E+06,8.961802E+06,9.141572E+06,9.321260E+06,9.500861E+06,
9.680365E+06,9.859708E+06,1.000411E+07,1.010313E+07,1.019254E+07,
1.028193E+07,1.037128E+07,1.046057E+07,1.054984E+07,1.063907E+07,
1.072825E+07,1.081738E+07,1.090646E+07,1.099549E+07,1.108442E+07,
1.117330E+07,1.126212E+07,1.135081E+07,1.143939E+07,1.152775E+07,
1.161575E+07,1.170421E+07,1.179267E+07,1.188087E+07,1.196889E+07,
1.205702E+07,1.214500E+07,1.223281E+07,1.232114E+07,1.240876E+07,
1.249643E+07,1.258439E+07,1.267274E+07,1.276090E+07,1.284874E+07,
1.293646E+07,1.302404E+07,1.311150E+07,1.319886E+07,1.328610E+07,
1.337323E+07,1.346024E+07,1.354718E+07,1.363401E+07,1.372075E+07,
1.380729E+07,1.389380E+07,1.398067E+07,1.406691E+07,1.415307E+07,
1.423909E+07,1.432502E+07,1.437689E+07,1.438511E+07,1.438289E+07,
1.438094E+07,1.437921E+07,1.437764E+07,1.437619E+07,1.437485E+07,
1.437362E+07,1.437247E+07,1.437139E+07,1.437034E+07,1.436935E+07,
1.436841E+07,1.436753E+07,1.436665E+07,1.436580E+07,1.436503E+07,
1.436426E+07,1.436351E+07,1.436278E+07,1.436205E+07,1.436137E+07,
1.436066E+07,1.435991E+07,1.435913E+07,1.435836E+07,1.435762E+07,
1.435690E+07,1.435617E+07,1.435548E+07,1.435481E+07,1.435414E+07,
1.435351E+07,1.435284E+07,1.435225E+07,1.435164E+07,1.435102E+07,
1.435039E+07,1.434979E+07,1.434920E+07,1.434862E+07,1.434802E+07,
1.434747E+07,1.434690E+07,1.434633E+07,1.434576E+07,1.434459E+07,

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1.434191E+07,1.434153E+07,1.434110E+07,1.434065E+07,1.434016E+07,
1.433967E+07,1.433918E+07,1.433871E+07,1.433825E+07,1.433780E+07,
1.433738E+07,1.433695E+07,1.433652E+07,1.433610E+07,1.433569E+07,
1.433531E+07,1.433491E+07,1.433451E+07,1.433414E+07,1.433378E+07,
1.433342E+07,1.433306E+07,1.433271E+07,1.433237E+07,1.433202E+07,
1.433168E+07,1.433134E+07,1.433102E+07,1.433071E+07,1.433039E+07,
1.433006E+07,1.432975E+07,1.432946E+07,1.432919E+07,1.432890E+07,
1.432860E+07,1.432832E+07,1.432805E+07,1.432779E+07,1.432751E+07,
1.432726E+07,1.432699E+07,1.432671E+07,1.432646E+07,1.432620E+07,
1.432595E+07,1.432569E+07,1.428634E+07,1.428634E+07

POROSITY SURFACE #3; GAS GENERATION RATE #6.

SDATA (NSDATA =6,NTDATA=1:214,MKLOS =4)

8.483495E-01,7.681744E-01,7.544597E-01,6.614296E-01,5.920096E-01,
5.305538E-01,4.801476E-01,4.370886E-01,4.009385E-01,3.773504E-01,
3.568268E-01,3.404598E-01,3.263779E-01,3.138956E-01,3.037175E-01,
2.942323E-01,2.860314E-01,2.786787E-01,2.717777E-01,2.659129E-01,
2.604211E-01,2.555460E-01,2.512794E-01,2.434133E-01,2.372162E-01,
2.322261E-01,2.280308E-01,2.245061E-01,2.215451E-01,2.190515E-01,
2.169568E-01,2.151892E-01,2.137052E-01,2.124746E-01,2.114482E-01,
2.106006E-01,2.099033E-01,2.093302E-01,2.088662E-01,2.084954E-01,
2.082025E-01,2.079741E-01,2.077979E-01,2.076644E-01,2.075655E-01,
2.074936E-01,2.074417E-01,2.074048E-01,2.073790E-01,2.073616E-01,
2.073504E-01,2.073439E-01,2.073414E-01,2.073421E-01,2.073459E-01,
2.073524E-01,2.073603E-01,2.073699E-01,2.073817E-01,2.073952E-01,
2.074084E-01,2.074228E-01,2.074389E-01,2.074564E-01,2.074750E-01,
2.074950E-01,2.075164E-01,2.075373E-01,2.075542E-01,2.075700E-01,
2.075861E-01,2.076025E-01,2.076195E-01,2.076370E-01,2.076550E-01,
2.076736E-01,2.076929E-01,2.077129E-01,2.077336E-01,2.077551E-01,
2.077778E-01,2.078013E-01,2.078270E-01,2.078540E-01,2.078847E-01,
2.079217E-01,2.079490E-01,2.079767E-01,2.080068E-01,2.080411E-01,
2.080732E-01,2.081072E-01,2.081433E-01,2.081706E-01,2.082092E-01,
2.082466E-01,2.082787E-01,2.083039E-01,2.083317E-01,2.083639E-01,
2.083983E-01,2.084342E-01,2.084717E-01,2.085105E-01,2.085503E-01,
2.085914E-01,2.086335E-01,2.086765E-01,2.087207E-01,2.087657E-01,
2.088118E-01,2.088588E-01,2.089070E-01,2.089558E-01,2.090054E-01,
2.090560E-01,2.091075E-01,2.091556E-01,2.091949E-01,2.092274E-01,
2.092559E-01,2.092813E-01,2.093043E-01,2.093256E-01,2.093451E-01,
2.093632E-01,2.093801E-01,2.093961E-01,2.094115E-01,2.094259E-01,
2.094396E-01,2.094527E-01,2.094655E-01,2.094779E-01,2.094894E-01,
2.095006E-01,2.095117E-01,2.095224E-01,2.095330E-01,2.095430E-01,
2.095536E-01,2.095645E-01,2.095760E-01,2.095873E-01,2.095983E-01,

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2.096087E-01, 2.096194E-01, 2.096296E-01, 2.096395E-01, 2.096492E-01,
2.096587E-01, 2.096685E-01, 2.096772E-01, 2.096862E-01, 2.096953E-01,
2.097046E-01, 2.097133E-01, 2.097221E-01, 2.097306E-01, 2.097394E-01,
2.097475E-01, 2.097560E-01, 2.097644E-01, 2.097728E-01, 2.097901E-01,
2.098295E-01, 2.098351E-01, 2.098413E-01, 2.098480E-01, 2.098552E-01,
2.098624E-01, 2.098696E-01, 2.098767E-01, 2.098834E-01, 2.098900E-01,
2.098962E-01, 2.099026E-01, 2.099089E-01, 2.099152E-01, 2.099211E-01,
2.099268E-01, 2.099326E-01, 2.099384E-01, 2.099440E-01, 2.099493E-01,
2.099547E-01, 2.099600E-01, 2.099650E-01, 2.099701E-01, 2.099752E-01,
2.099803E-01, 2.099852E-01, 2.099900E-01, 2.099946E-01, 2.099995E-01,
2.100042E-01, 2.100088E-01, 2.100130E-01, 2.100170E-01, 2.100213E-01,
2.100257E-01, 2.100299E-01, 2.100338E-01, 2.100377E-01, 2.100418E-01,
2.100456E-01, 2.100495E-01, 2.100535E-01, 2.100573E-01, 2.100612E-01,
2.100649E-01, 2.100686E-01, 2.106514E-01, 2.106514E-01

POROSITY SURFACE #4; GAS GENERATION RATE #7.

PDATA (NSDATA =7,NTDATA=1:214,MKLOS =4)

1.013250E+05, 1.043718E+05, 1.076808E+05, 1.455748E+05, 1.916487E+05,
2.425412E+05, 3.097650E+05, 3.818360E+05, 4.627055E+05, 5.478908E+05,
6.353438E+05, 7.291689E+05, 8.253129E+05, 9.246608E+05, 1.027507E+06,
1.131968E+06, 1.240430E+06, 1.350298E+06, 1.461671E+06, 1.575236E+06,
1.689529E+06, 1.805100E+06, 1.921634E+06, 2.155953E+06, 2.391338E+06,
2.627255E+06, 2.863102E+06, 3.097453E+06, 3.329035E+06, 3.558903E+06,
3.787157E+06, 4.013378E+06, 4.237323E+06, 4.459443E+06, 4.679750E+06,
4.898373E+06, 5.115349E+06, 5.330767E+06, 5.544825E+06, 5.757781E+06,
5.969940E+06, 6.181693E+06, 6.392880E+06, 6.603239E+06, 6.813165E+06,
7.022710E+06, 7.231764E+06, 7.440940E+06, 7.649995E+06, 7.858937E+06,
8.067774E+06, 8.276512E+06, 8.485088E+06, 8.693635E+06, 8.902084E+06,
9.110435E+06, 9.318680E+06, 9.526813E+06, 9.734812E+06, 9.942520E+06,
1.015008E+07, 1.035737E+07, 1.056456E+07, 1.077155E+07, 1.097836E+07,
1.118499E+07, 1.139132E+07, 1.155709E+07, 1.167047E+07, 1.177262E+07,
1.187543E+07, 1.197805E+07, 1.208046E+07, 1.218278E+07, 1.228499E+07,
1.238711E+07, 1.248913E+07, 1.259106E+07, 1.269287E+07, 1.279456E+07,
1.289617E+07, 1.299766E+07, 1.309906E+07, 1.320035E+07, 1.330154E+07,
1.340259E+07, 1.350354E+07, 1.360439E+07, 1.370504E+07, 1.380566E+07,
1.390616E+07, 1.400655E+07, 1.410678E+07, 1.420690E+07, 1.430689E+07,
1.440677E+07, 1.450650E+07, 1.460609E+07, 1.470555E+07, 1.480484E+07,
1.490401E+07, 1.500302E+07, 1.510187E+07, 1.520057E+07, 1.529912E+07,
1.539749E+07, 1.549567E+07, 1.559370E+07, 1.569153E+07, 1.578731E+07,
1.588202E+07, 1.597873E+07, 1.607510E+07, 1.617015E+07, 1.626484E+07,
1.635980E+07, 1.645473E+07, 1.651006E+07, 1.651618E+07, 1.651191E+07,
1.650780E+07, 1.650395E+07, 1.650034E+07, 1.649691E+07, 1.649369E+07,

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1.649064E+07, 1.648772E+07, 1.648492E+07, 1.648223E+07, 1.647964E+07,
1.647714E+07, 1.647473E+07, 1.647238E+07, 1.647009E+07, 1.646787E+07,
1.646572E+07, 1.646363E+07, 1.646158E+07, 1.645959E+07, 1.645764E+07,
1.645573E+07, 1.645386E+07, 1.645203E+07, 1.645023E+07, 1.644844E+07,
1.644669E+07, 1.644500E+07, 1.644333E+07, 1.644168E+07, 1.644008E+07,
1.643851E+07, 1.643697E+07, 1.643541E+07, 1.643391E+07, 1.643243E+07,
1.643101E+07, 1.642959E+07, 1.642818E+07, 1.642677E+07, 1.642539E+07,
1.642397E+07, 1.642262E+07, 1.642130E+07, 1.641989E+07, 1.641839E+07,
1.641705E+07, 1.641579E+07, 1.641448E+07, 1.641328E+07, 1.641203E+07,
1.641073E+07, 1.640949E+07, 1.640830E+07, 1.640710E+07, 1.640589E+07,
1.640467E+07, 1.640344E+07, 1.640218E+07, 1.640101E+07, 1.639986E+07,
1.639869E+07, 1.639755E+07, 1.639642E+07, 1.639527E+07, 1.639415E+07,
1.639297E+07, 1.639175E+07, 1.639062E+07, 1.638947E+07, 1.638838E+07,
1.638731E+07, 1.638623E+07, 1.638520E+07, 1.638415E+07, 1.638310E+07,
1.638203E+07, 1.638089E+07, 1.637979E+07, 1.637872E+07, 1.637768E+07,
1.637669E+07, 1.637571E+07, 1.637478E+07, 1.637375E+07, 1.637275E+07,
1.637179E+07, 1.637074E+07, 1.636975E+07, 1.636873E+07, 1.636778E+07,
1.636691E+07, 1.636612E+07, 1.608991E+07, 1.608991E+07

POROSITY SURFACE #3; GAS GENERATION RATE #7.

SDATA (NSDATA =7, NTDATA=1:214, MKLOS =4)

8.483495E-01, 7.680837E-01, 7.534831E-01, 6.635969E-01, 5.917762E-01,
5.305661E-01, 4.815979E-01, 4.380220E-01, 4.043772E-01, 3.798455E-01,
3.594839E-01, 3.442136E-01, 3.304213E-01, 3.186850E-01, 3.088574E-01,
2.997887E-01, 2.920576E-01, 2.850254E-01, 2.787129E-01, 2.732785E-01,
2.681828E-01, 2.637881E-01, 2.598454E-01, 2.528531E-01, 2.472896E-01,
2.426932E-01, 2.389054E-01, 2.358298E-01, 2.334026E-01, 2.314157E-01,
2.297767E-01, 2.284478E-01, 2.273896E-01, 2.265353E-01, 2.258532E-01,
2.253133E-01, 2.248940E-01, 2.245769E-01, 2.243411E-01, 2.241666E-01,
2.240356E-01, 2.239286E-01, 2.238489E-01, 2.238029E-01, 2.237748E-01,
2.237605E-01, 2.237543E-01, 2.237528E-01, 2.237550E-01, 2.237603E-01,
2.237682E-01, 2.237785E-01, 2.237908E-01, 2.238050E-01, 2.238210E-01,
2.238388E-01, 2.238582E-01, 2.238795E-01, 2.239030E-01, 2.239306E-01,
2.239619E-01, 2.239978E-01, 2.240344E-01, 2.240737E-01, 2.241152E-01,
2.241589E-01, 2.242057E-01, 2.242520E-01, 2.242944E-01, 2.243361E-01,
2.243643E-01, 2.243955E-01, 2.244298E-01, 2.244656E-01, 2.245029E-01,
2.245412E-01, 2.245807E-01, 2.246212E-01, 2.246629E-01, 2.247059E-01,
2.247499E-01, 2.247953E-01, 2.248417E-01, 2.248892E-01, 2.249378E-01,
2.249877E-01, 2.250382E-01, 2.250902E-01, 2.251430E-01, 2.251972E-01,
2.252526E-01, 2.253088E-01, 2.253665E-01, 2.254254E-01, 2.254858E-01,
2.255470E-01, 2.256096E-01, 2.256736E-01, 2.257388E-01, 2.258051E-01,
2.258728E-01, 2.259421E-01, 2.260130E-01, 2.260851E-01, 2.261585E-01,

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2.262336E-01, 2.263100E-01, 2.263882E-01, 2.264684E-01, 2.265770E-01,
2.266985E-01, 2.267906E-01, 2.268945E-01, 2.270071E-01, 2.271233E-01,
2.272340E-01, 2.273442E-01, 2.274569E-01, 2.275451E-01, 2.276041E-01,
2.276612E-01, 2.277146E-01, 2.277647E-01, 2.278124E-01, 2.278570E-01,
2.278996E-01, 2.279402E-01, 2.279791E-01, 2.280166E-01, 2.280525E-01,
2.280874E-01, 2.281211E-01, 2.281537E-01, 2.281857E-01, 2.282165E-01,
2.282465E-01, 2.282758E-01, 2.283043E-01, 2.283322E-01, 2.283594E-01,
2.283860E-01, 2.284120E-01, 2.284377E-01, 2.284627E-01, 2.284878E-01,
2.285122E-01, 2.285360E-01, 2.285593E-01, 2.285824E-01, 2.286049E-01,
2.286268E-01, 2.286484E-01, 2.286702E-01, 2.286912E-01, 2.287119E-01,
2.287318E-01, 2.287517E-01, 2.287714E-01, 2.287913E-01, 2.288105E-01,
2.288303E-01, 2.288493E-01, 2.288678E-01, 2.288876E-01, 2.289087E-01,
2.289275E-01, 2.289451E-01, 2.289635E-01, 2.289803E-01, 2.289979E-01,
2.290162E-01, 2.290336E-01, 2.290502E-01, 2.290671E-01, 2.290841E-01,
2.291013E-01, 2.291185E-01, 2.291362E-01, 2.291527E-01, 2.291688E-01,
2.291852E-01, 2.292014E-01, 2.292174E-01, 2.292335E-01, 2.292492E-01,
2.292658E-01, 2.292829E-01, 2.292988E-01, 2.293151E-01, 2.293303E-01,
2.293454E-01, 2.293606E-01, 2.293753E-01, 2.293899E-01, 2.294047E-01,
2.294199E-01, 2.294358E-01, 2.294514E-01, 2.294665E-01, 2.294811E-01,
2.294952E-01, 2.295090E-01, 2.295221E-01, 2.295366E-01, 2.295507E-01,
2.295642E-01, 2.295790E-01, 2.295932E-01, 2.296075E-01, 2.296208E-01,
2.296333E-01, 2.296443E-01, 2.336116E-01, 2.336116E-01

POROSITY SURFACE #4; GAS GENERATION RATE #8.

PDATA (NSDATA =8, NTDATA=1:214, MKLOS =4)

1.013250E+05, 1.049813E+05, 1.089282E+05, 1.533419E+05, 2.097246E+05,
2.721453E+05, 3.496942E+05, 4.370342E+05, 5.321045E+05, 6.333046E+05,
7.372072E+05, 8.466991E+05, 9.599410E+05, 1.075344E+06, 1.195860E+06,
1.317651E+06, 1.441751E+06, 1.568146E+06, 1.695703E+06, 1.825636E+06,
1.956078E+06, 2.087194E+06, 2.219225E+06, 2.483551E+06, 2.747981E+06,
3.011399E+06, 3.273454E+06, 3.533293E+06, 3.790754E+06, 4.045822E+06,
4.298462E+06, 4.548591E+06, 4.796305E+06, 5.041810E+06, 5.285151E+06,
5.526630E+06, 5.766527E+06, 6.005165E+06, 6.242781E+06, 6.479689E+06,
6.716097E+06, 6.952142E+06, 7.187935E+06, 7.423522E+06, 7.658970E+06,
7.894270E+06, 8.129143E+06, 8.364190E+06, 8.599112E+06, 8.833914E+06,
9.068593E+06, 9.303130E+06, 9.537271E+06, 9.771328E+06, 1.000534E+07,
1.023922E+07, 1.047284E+07, 1.070613E+07, 1.093929E+07, 1.117229E+07,
1.140513E+07, 1.163755E+07, 1.186954E+07, 1.210114E+07, 1.233235E+07,
1.256316E+07, 1.279349E+07, 1.297817E+07, 1.310428E+07, 1.321803E+07,
1.333181E+07, 1.344556E+07, 1.355920E+07, 1.367278E+07, 1.378627E+07,
1.389966E+07, 1.401291E+07, 1.412603E+07, 1.423900E+07, 1.435179E+07,
1.446445E+07, 1.457691E+07, 1.468905E+07, 1.479727E+07, 1.491026E+07,

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1.502292E+07,1.513528E+07,1.524725E+07,1.535786E+07,1.546849E+07,
1.557951E+07,1.568991E+07,1.579969E+07,1.590885E+07,1.601820E+07,
1.612787E+07,1.623741E+07,1.634621E+07,1.645435E+07,1.656181E+07,
1.666871E+07,1.677498E+07,1.688065E+07,1.698568E+07,1.709015E+07,
1.719404E+07,1.729722E+07,1.739981E+07,1.750174E+07,1.760291E+07,
1.770283E+07,1.780142E+07,1.789921E+07,1.799523E+07,1.809020E+07,
1.818388E+07,1.827615E+07,1.832459E+07,1.831849E+07,1.830080E+07,
1.828454E+07,1.826948E+07,1.825544E+07,1.824215E+07,1.822976E+07,
1.821804E+07,1.820692E+07,1.819631E+07,1.818617E+07,1.817645E+07,
1.816710E+07,1.815808E+07,1.814936E+07,1.814084E+07,1.813267E+07,
1.812472E+07,1.811700E+07,1.810946E+07,1.810211E+07,1.809494E+07,
1.808791E+07,1.808105E+07,1.807432E+07,1.806771E+07,1.806117E+07,
1.805482E+07,1.804857E+07,1.804243E+07,1.803639E+07,1.803041E+07,
1.802456E+07,1.801876E+07,1.801306E+07,1.800742E+07,1.800180E+07,
1.799630E+07,1.799089E+07,1.798551E+07,1.798021E+07,1.797497E+07,
1.796979E+07,1.796466E+07,1.795959E+07,1.795457E+07,1.794959E+07,
1.794463E+07,1.793975E+07,1.793494E+07,1.793015E+07,1.792542E+07,
1.792074E+07,1.791609E+07,1.791148E+07,1.790694E+07,1.790243E+07,
1.789791E+07,1.789348E+07,1.788910E+07,1.788474E+07,1.788043E+07,
1.787616E+07,1.787192E+07,1.786774E+07,1.786358E+07,1.785945E+07,
1.785537E+07,1.785128E+07,1.784727E+07,1.784329E+07,1.783935E+07,
1.783543E+07,1.783156E+07,1.782771E+07,1.782390E+07,1.782012E+07,
1.781636E+07,1.781261E+07,1.780894E+07,1.780530E+07,1.780168E+07,
1.779810E+07,1.779455E+07,1.779102E+07,1.778754E+07,1.778408E+07,
1.778065E+07,1.777724E+07,1.777384E+07,1.777051E+07,1.776719E+07,
1.776391E+07,1.776066E+07,1.682655E+07,1.682655E+07

POROSITY SURFACE #3; GAS GENERATION RATE #8.

SDATA (NSDATA =8,NTDATAB=1:214,MKLOS =4)

8.483495E-01,7.679683E-01,7.533363E-01,6.603640E-01,5.926789E-01,
5.323986E-01,4.829134E-01,4.410058E-01,4.050808E-01,3.826473E-01,
3.630153E-01,3.475672E-01,3.345024E-01,3.228274E-01,3.135687E-01,
3.049974E-01,2.976684E-01,2.912542E-01,2.852840E-01,2.802634E-01,
2.756223E-01,2.715046E-01,2.680433E-01,2.616855E-01,2.567487E-01,
2.527773E-01,2.495910E-01,2.470501E-01,2.450259E-01,2.434135E-01,
2.421369E-01,2.411419E-01,2.403765E-01,2.397955E-01,2.393693E-01,
2.390638E-01,2.388509E-01,2.387066E-01,2.386133E-01,2.385533E-01,
2.385161E-01,2.384938E-01,2.384816E-01,2.384768E-01,2.384773E-01,
2.384822E-01,2.384905E-01,2.385021E-01,2.385164E-01,2.385332E-01,
2.385525E-01,2.385746E-01,2.386035E-01,2.386350E-01,2.386660E-01,
2.386991E-01,2.387364E-01,2.387792E-01,2.388234E-01,2.388674E-01,
2.389145E-01,2.389685E-01,2.390292E-01,2.390954E-01,2.391665E-01,

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2.392426E-01,2.393238E-01,2.394043E-01,2.394742E-01,2.395381E-01,
2.396001E-01,2.396618E-01,2.397237E-01,2.397860E-01,2.398489E-01,
2.399128E-01,2.399779E-01,2.400442E-01,2.401118E-01,2.401810E-01,
2.402518E-01,2.403248E-01,2.404022E-01,2.405422E-01,2.406028E-01,
2.406678E-01,2.407360E-01,2.408098E-01,2.409026E-01,2.409952E-01,
2.410805E-01,2.411743E-01,2.412755E-01,2.413856E-01,2.414911E-01,
2.415904E-01,2.416902E-01,2.417997E-01,2.419177E-01,2.420434E-01,
2.421763E-01,2.423166E-01,2.424638E-01,2.426182E-01,2.427790E-01,
2.429460E-01,2.431203E-01,2.433014E-01,2.434898E-01,2.436865E-01,
2.438966E-01,2.441238E-01,2.443679E-01,2.446242E-01,2.448918E-01,
2.451738E-01,2.454724E-01,2.457703E-01,2.460395E-01,2.462786E-01,
2.464988E-01,2.467031E-01,2.468939E-01,2.470748E-01,2.472437E-01,
2.474036E-01,2.475556E-01,2.477007E-01,2.478396E-01,2.479728E-01,
2.481012E-01,2.482252E-01,2.483452E-01,2.484624E-01,2.485750E-01,
2.486847E-01,2.487913E-01,2.488954E-01,2.489970E-01,2.490962E-01,
2.491935E-01,2.492887E-01,2.493820E-01,2.494738E-01,2.495646E-01,
2.496529E-01,2.497397E-01,2.498253E-01,2.499095E-01,2.499928E-01,
2.500744E-01,2.501552E-01,2.502348E-01,2.503137E-01,2.503921E-01,
2.504693E-01,2.505451E-01,2.506203E-01,2.506945E-01,2.507680E-01,
2.508408E-01,2.509129E-01,2.509841E-01,2.510547E-01,2.511247E-01,
2.511946E-01,2.512632E-01,2.513311E-01,2.513984E-01,2.514652E-01,
2.515312E-01,2.515969E-01,2.516620E-01,2.517262E-01,2.517900E-01,
2.518538E-01,2.519165E-01,2.519787E-01,2.520404E-01,2.521016E-01,
2.521622E-01,2.522223E-01,2.522818E-01,2.523408E-01,2.523994E-01,
2.524575E-01,2.525156E-01,2.525727E-01,2.526293E-01,2.526855E-01,
2.527412E-01,2.527965E-01,2.528514E-01,2.529058E-01,2.529598E-01,
2.530133E-01,2.530668E-01,2.531194E-01,2.531715E-01,2.532232E-01,
2.532745E-01,2.533254E-01,2.533758E-01,2.534257E-01,2.534753E-01,
2.535244E-01,2.535733E-01,2.536221E-01,2.536700E-01,2.537176E-01,
2.537648E-01,2.538114E-01,2.679867E-01,2.679867E-01

POROSITY SURFACE #4; GAS GENERATION RATE #9.

PDATA (NSDATA =9,NTDATA=1:214,MKLOS =4)

1.013250E+05,1.061996E+05,1.116166E+05,1.716325E+05,2.453350E+05,
3.263810E+05,4.309130E+05,5.441849E+05,6.703624E+05,8.017092E+05,
9.356528E+05,1.076473E+06,1.220129E+06,1.366868E+06,1.517579E+06,
1.669778E+06,1.824989E+06,1.981220E+06,2.138349E+06,2.296473E+06,
2.454768E+06,2.613225E+06,2.771598E+06,3.087600E+06,3.401797E+06,
3.712535E+06,4.020255E+06,4.324479E+06,4.625526E+06,4.923169E+06,
5.217787E+06,5.509734E+06,5.799333E+06,6.087082E+06,6.373458E+06,
6.658916E+06,6.943759E+06,7.228205E+06,7.512365E+06,7.796292E+06,
8.080037E+06,8.363600E+06,8.647003E+06,8.930098E+06,9.213011E+06,

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9.495864E+06, 9.778156E+06, 1.006061E+07, 1.034298E+07, 1.062517E+07,
1.090692E+07, 1.118830E+07, 1.146924E+07, 1.174986E+07, 1.203002E+07,
1.230970E+07, 1.258881E+07, 1.286719E+07, 1.314491E+07, 1.342193E+07,
1.369836E+07, 1.397362E+07, 1.424908E+07, 1.452411E+07, 1.479804E+07,
1.507093E+07, 1.534002E+07, 1.555604E+07, 1.570385E+07, 1.583710E+07,
1.596997E+07, 1.610239E+07, 1.623423E+07, 1.636554E+07, 1.649619E+07,
1.662622E+07, 1.675560E+07, 1.688434E+07, 1.701245E+07, 1.713981E+07,
1.726645E+07, 1.739234E+07, 1.751738E+07, 1.764157E+07, 1.776407E+07,
1.788461E+07, 1.800387E+07, 1.812161E+07, 1.823745E+07, 1.835171E+07,
1.846438E+07, 1.857522E+07, 1.868428E+07, 1.879146E+07, 1.889661E+07,
1.899988E+07, 1.910110E+07, 1.919999E+07, 1.929681E+07, 1.939116E+07,
1.948290E+07, 1.957187E+07, 1.965783E+07, 1.974078E+07, 1.982072E+07,
1.989765E+07, 1.997136E+07, 2.004196E+07, 2.010952E+07, 2.017407E+07,
2.023554E+07, 2.029433E+07, 2.035050E+07, 2.040372E+07, 2.045466E+07,
2.050297E+07, 2.054875E+07, 2.054603E+07, 2.048604E+07, 2.041770E+07,
2.035503E+07, 2.029720E+07, 2.024353E+07, 2.019304E+07, 2.014623E+07,
2.010233E+07, 2.006100E+07, 2.002195E+07, 1.998492E+07, 1.994963E+07,
1.991612E+07, 1.988422E+07, 1.985373E+07, 1.982413E+07, 1.979598E+07,
1.976897E+07, 1.974279E+07, 1.971755E+07, 1.969322E+07, 1.966967E+07,
1.964683E+07, 1.962482E+07, 1.960325E+07, 1.958234E+07, 1.956179E+07,
1.954210E+07, 1.952282E+07, 1.950413E+07, 1.948583E+07, 1.946798E+07,
1.945057E+07, 1.943344E+07, 1.941694E+07, 1.940067E+07, 1.938466E+07,
1.936909E+07, 1.935391E+07, 1.933901E+07, 1.932438E+07, 1.931001E+07,
1.929590E+07, 1.928213E+07, 1.926862E+07, 1.925533E+07, 1.924226E+07,
1.922933E+07, 1.921674E+07, 1.920436E+07, 1.919222E+07, 1.918026E+07,
1.916845E+07, 1.915688E+07, 1.914548E+07, 1.913424E+07, 1.912320E+07,
1.911225E+07, 1.910157E+07, 1.909102E+07, 1.908064E+07, 1.907040E+07,
1.906030E+07, 1.905036E+07, 1.904055E+07, 1.903090E+07, 1.902136E+07,
1.901194E+07, 1.900257E+07, 1.899341E+07, 1.898440E+07, 1.897549E+07,
1.896669E+07, 1.895801E+07, 1.894943E+07, 1.894097E+07, 1.893263E+07,
1.892436E+07, 1.891612E+07, 1.890808E+07, 1.890013E+07, 1.889227E+07,
1.888451E+07, 1.887685E+07, 1.886926E+07, 1.886177E+07, 1.885436E+07,
1.884703E+07, 1.883979E+07, 1.883253E+07, 1.882545E+07, 1.881844E+07,
1.881149E+07, 1.880464E+07, 1.740963E+07, 1.740963E+07

POROSITY SURFACE #3; GAS GENERATION RATE #9.

SDATA (NSDATA =9,NTDATA=1:214,MKLOS =4)

8.483495E-01, 7.680336E-01, 7.543689E-01, 6.638804E-01, 5.939087E-01,
5.338273E-01, 4.863748E-01, 4.443563E-01, 4.103615E-01, 3.872913E-01,
3.683102E-01, 3.543246E-01, 3.420185E-01, 3.315559E-01, 3.230275E-01,
3.151969E-01, 3.086818E-01, 3.029075E-01, 2.977366E-01, 2.934887E-01,
2.895498E-01, 2.862068E-01, 2.833332E-01, 2.783191E-01, 2.744995E-01,

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2.715842E-01,2.693582E-01,2.676780E-01,2.664112E-01,2.654903E-01,
2.648328E-01,2.643782E-01,2.640789E-01,2.638908E-01,2.637775E-01,
2.637114E-01,2.636744E-01,2.636554E-01,2.636481E-01,2.636490E-01,
2.636562E-01,2.636683E-01,2.636849E-01,2.637093E-01,2.637384E-01,
2.637670E-01,2.637996E-01,2.638356E-01,2.638717E-01,2.639102E-01,
2.639576E-01,2.640113E-01,2.640705E-01,2.641362E-01,2.642090E-01,
2.642888E-01,2.643771E-01,2.644767E-01,2.645853E-01,2.647017E-01,
2.648266E-01,2.649686E-01,2.651018E-01,2.652375E-01,2.653878E-01,
2.655513E-01,2.657734E-01,2.659646E-01,2.661000E-01,2.662255E-01,
2.663554E-01,2.664907E-01,2.666324E-01,2.667816E-01,2.669390E-01,
2.671036E-01,2.672765E-01,2.674568E-01,2.676443E-01,2.678400E-01,
2.680448E-01,2.682584E-01,2.684817E-01,2.687149E-01,2.689706E-01,
2.692525E-01,2.695491E-01,2.698653E-01,2.702037E-01,2.705633E-01,
2.709417E-01,2.713423E-01,2.717636E-01,2.722081E-01,2.726769E-01,
2.731674E-01,2.736825E-01,2.742254E-01,2.747924E-01,2.753884E-01,
2.760163E-01,2.766777E-01,2.773756E-01,2.781100E-01,2.788810E-01,
2.796882E-01,2.805341E-01,2.814181E-01,2.823388E-01,2.832957E-01,
2.842883E-01,2.853140E-01,2.863805E-01,2.874719E-01,2.885898E-01,
2.897392E-01,2.909195E-01,2.920866E-01,2.931709E-01,2.941569E-01,
2.950670E-01,2.959119E-01,2.967002E-01,2.974457E-01,2.981404E-01,
2.987948E-01,2.994133E-01,3.000003E-01,3.005590E-01,3.010933E-01,
3.016025E-01,3.020888E-01,3.025552E-01,3.030093E-01,3.034422E-01,
3.038589E-01,3.042639E-01,3.046555E-01,3.050337E-01,3.054008E-01,
3.057576E-01,3.061024E-01,3.064409E-01,3.067698E-01,3.070939E-01,
3.074048E-01,3.077100E-01,3.080064E-01,3.082971E-01,3.085813E-01,
3.088590E-01,3.091325E-01,3.093966E-01,3.096576E-01,3.099146E-01,
3.101652E-01,3.104097E-01,3.106500E-01,3.108867E-01,3.111192E-01,
3.113478E-01,3.115713E-01,3.117910E-01,3.120072E-01,3.122204E-01,
3.124313E-01,3.126370E-01,3.128397E-01,3.130387E-01,3.132349E-01,
3.134289E-01,3.136192E-01,3.138069E-01,3.139922E-01,3.141746E-01,
3.143554E-01,3.145320E-01,3.147068E-01,3.148790E-01,3.150489E-01,
3.152169E-01,3.153823E-01,3.155455E-01,3.157065E-01,3.158656E-01,
3.160229E-01,3.161797E-01,3.163328E-01,3.164838E-01,3.166332E-01,
3.167809E-01,3.169267E-01,3.170711E-01,3.172135E-01,3.173540E-01,
3.174933E-01,3.176324E-01,3.177682E-01,3.179027E-01,3.180356E-01,
3.181669E-01,3.182966E-01,3.184255E-01,3.185525E-01,3.186785E-01,
3.188030E-01,3.189262E-01,3.190498E-01,3.191705E-01,3.192901E-01,
3.194087E-01,3.195256E-01,3.452785E-01,3.452785E-01
POROSITY SURFACE #4; GAS GENERATION RATE #10.
PDATA (NSDATA =10,NTDATA=1:214,MKLOS =4)
1.013250E+05,1.074180E+05,1.137721E+05,1.885482E+05,2.811374E+05,

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3.828126E+05, 5.103179E+05, 6.505580E+05, 8.048431E+05, 9.641940E+05,
1.126100E+06, 1.294307E+06, 1.466103E+06, 1.640818E+06, 1.819981E+06,
2.000168E+06, 2.181971E+06, 2.364194E+06, 2.546741E+06, 2.729412E+06,
2.911994E+06, 3.094364E+06, 3.275987E+06, 3.637529E+06, 3.994508E+06,
4.346783E+06, 4.695047E+06, 5.039146E+06, 5.379459E+06, 5.716282E+06,
6.050278E+06, 6.382280E+06, 6.713021E+06, 7.042989E+06, 7.372451E+06,
7.701587E+06, 8.030442E+06, 8.359080E+06, 8.687435E+06, 9.015474E+06,
9.343366E+06, 9.671064E+06, 9.998686E+06, 1.032614E+07, 1.065329E+07,
1.097998E+07, 1.130576E+07, 1.163153E+07, 1.195684E+07, 1.228143E+07,
1.260539E+07, 1.292859E+07, 1.325127E+07, 1.357294E+07, 1.389110E+07,
1.420987E+07, 1.452977E+07, 1.484867E+07, 1.516674E+07, 1.548363E+07,
1.579873E+07, 1.611147E+07, 1.642176E+07, 1.672945E+07, 1.703447E+07,
1.733670E+07, 1.763591E+07, 1.787069E+07, 1.802371E+07, 1.815920E+07,
1.829367E+07, 1.842655E+07, 1.855766E+07, 1.868673E+07, 1.881373E+07,
1.893867E+07, 1.906135E+07, 1.918148E+07, 1.929930E+07, 1.941432E+07,
1.952650E+07, 1.963565E+07, 1.974166E+07, 1.984383E+07, 1.994206E+07,
2.003665E+07, 2.012675E+07, 2.021329E+07, 2.029516E+07, 2.037304E+07,
2.044691E+07, 2.051638E+07, 2.058248E+07, 2.064476E+07, 2.070375E+07,
2.075961E+07, 2.081209E+07, 2.086198E+07, 2.090894E+07, 2.095298E+07,
2.099472E+07, 2.103398E+07, 2.107135E+07, 2.110670E+07, 2.114009E+07,
2.117193E+07, 2.120199E+07, 2.123054E+07, 2.125757E+07, 2.128314E+07,
2.130758E+07, 2.133104E+07, 2.135369E+07, 2.137503E+07, 2.139528E+07,
2.141436E+07, 2.143263E+07, 2.140176E+07, 2.131372E+07, 2.121992E+07,
2.113518E+07, 2.105810E+07, 2.098741E+07, 2.092154E+07, 2.086119E+07,
2.080513E+07, 2.075256E+07, 2.070316E+07, 2.065660E+07, 2.061248E+07,
2.057058E+07, 2.053095E+07, 2.049312E+07, 2.045658E+07, 2.042212E+07,
2.038882E+07, 2.035713E+07, 2.032644E+07, 2.029688E+07, 2.026818E+07,
2.024064E+07, 2.021396E+07, 2.018814E+07, 2.016303E+07, 2.013846E+07,
2.011489E+07, 2.009190E+07, 2.006956E+07, 2.004791E+07, 2.002664E+07,
2.000601E+07, 1.998576E+07, 1.996609E+07, 1.994686E+07, 1.992793E+07,
1.990954E+07, 1.989153E+07, 1.987405E+07, 1.985681E+07, 1.983994E+07,
1.982345E+07, 1.980737E+07, 1.979152E+07, 1.977599E+07, 1.976071E+07,
1.974562E+07, 1.973097E+07, 1.971656E+07, 1.970242E+07, 1.968853E+07,
1.967493E+07, 1.966152E+07, 1.964833E+07, 1.963537E+07, 1.962261E+07,
1.960994E+07, 1.959758E+07, 1.958542E+07, 1.957343E+07, 1.956167E+07,
1.955009E+07, 1.953867E+07, 1.952742E+07, 1.951633E+07, 1.950539E+07,
1.949459E+07, 1.948385E+07, 1.947340E+07, 1.946309E+07, 1.945289E+07,
1.944284E+07, 1.943291E+07, 1.942311E+07, 1.941345E+07, 1.940392E+07,
1.939450E+07, 1.938513E+07, 1.937595E+07, 1.936688E+07, 1.935793E+07,
1.934910E+07, 1.934038E+07, 1.933176E+07, 1.932323E+07, 1.931480E+07,
1.930647E+07, 1.929821E+07, 1.928999E+07, 1.928195E+07, 1.927401E+07,

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1.926614E+07,1.925839E+07,1.773312E+07,1.773312E+07
POROSITY SURFACE #3; GAS GENERATION RATE #10.
SDATA(NSDATA =10,NTDATA=1:214,MKLOS =4)
8.483495E-01,7.681255E-01,7.524542E-01,6.622762E-01,5.946153E-01,
5.356882E-01,4.890094E-01,4.483044E-01,4.141878E-01,3.927770E-01,
3.749908E-01,3.618225E-01,3.504490E-01,3.405533E-01,3.326676E-01,
3.254621E-01,3.195708E-01,3.145164E-01,3.099690E-01,3.063785E-01,
3.030539E-01,3.002129E-01,2.978681E-01,2.937815E-01,2.908741E-01,
2.887537E-01,2.872304E-01,2.861629E-01,2.854401E-01,2.849824E-01,
2.847118E-01,2.845611E-01,2.844797E-01,2.844383E-01,2.844200E-01,
2.844161E-01,2.844221E-01,2.844355E-01,2.844572E-01,2.844872E-01,
2.845198E-01,2.845558E-01,2.845918E-01,2.846299E-01,2.846744E-01,
2.847283E-01,2.847913E-01,2.848616E-01,2.849389E-01,2.850290E-01,
2.851288E-01,2.852403E-01,2.853556E-01,2.854888E-01,2.856879E-01,
2.858669E-01,2.860150E-01,2.861761E-01,2.863462E-01,2.865291E-01,
2.867393E-01,2.869835E-01,2.872616E-01,2.875741E-01,2.879207E-01,
2.883017E-01,2.887176E-01,2.891518E-01,2.895700E-01,2.899886E-01,
2.904171E-01,2.908650E-01,2.913333E-01,2.918276E-01,2.923479E-01,
2.928928E-01,2.934657E-01,2.940704E-01,2.947033E-01,2.953703E-01,
2.960734E-01,2.968145E-01,2.975950E-01,2.984249E-01,2.993057E-01,
3.002328E-01,3.012180E-01,3.022484E-01,3.033379E-01,3.044809E-01,
3.056752E-01,3.069270E-01,3.082205E-01,3.095638E-01,3.109486E-01,
3.123729E-01,3.138408E-01,3.153405E-01,3.168776E-01,3.184517E-01,
3.200551E-01,3.216903E-01,3.233484E-01,3.250320E-01,3.267403E-01,
3.284673E-01,3.302164E-01,3.319847E-01,3.337724E-01,3.355786E-01,
3.373963E-01,3.392269E-01,3.410783E-01,3.429337E-01,3.448030E-01,
3.466870E-01,3.485817E-01,3.504399E-01,3.521655E-01,3.537294E-01,
3.551541E-01,3.564602E-01,3.576666E-01,3.587980E-01,3.598409E-01,
3.608152E-01,3.617334E-01,3.626009E-01,3.634221E-01,3.642039E-01,
3.649493E-01,3.656572E-01,3.663356E-01,3.669931E-01,3.676156E-01,
3.682189E-01,3.687948E-01,3.693545E-01,3.698951E-01,3.704214E-01,
3.709281E-01,3.714200E-01,3.718974E-01,3.723629E-01,3.728195E-01,
3.732585E-01,3.736878E-01,3.741060E-01,3.745120E-01,3.749117E-01,
3.753005E-01,3.756825E-01,3.760545E-01,3.764190E-01,3.767785E-01,
3.771280E-01,3.774713E-01,3.778049E-01,3.781347E-01,3.784578E-01,
3.787743E-01,3.790835E-01,3.793886E-01,3.796881E-01,3.799833E-01,
3.802749E-01,3.805589E-01,3.808384E-01,3.811132E-01,3.813835E-01,
3.816484E-01,3.819102E-01,3.821679E-01,3.824214E-01,3.826713E-01,
3.829200E-01,3.831626E-01,3.834015E-01,3.836377E-01,3.838696E-01,
3.840982E-01,3.843239E-01,3.845464E-01,3.847660E-01,3.849830E-01,
3.851974E-01,3.854108E-01,3.856188E-01,3.858241E-01,3.860274E-01,

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3.862281E-01, 3.864263E-01, 3.866223E-01, 3.868158E-01, 3.870067E-01,
3.871956E-01, 3.873838E-01, 3.875685E-01, 3.877508E-01, 3.879312E-01,
3.881090E-01, 3.882851E-01, 3.884590E-01, 3.886312E-01, 3.888019E-01,
3.889704E-01, 3.891378E-01, 3.893045E-01, 3.894678E-01, 3.896290E-01,
3.897890E-01, 3.899466E-01, 4.236799E-01, 4.236799E-01

POROSITY SURFACE #4; GAS GENERATION RATE #11.

PDATA(NSDATA =11,NTDATA=1:214,MKLOS =4)

1.013250E+05, 1.086359E+05, 1.165871E+05, 2.058360E+05, 3.166507E+05,
4.382150E+05, 5.890103E+05, 7.555014E+05, 9.383270E+05, 1.126235E+06,
1.316657E+06, 1.513030E+06, 1.712366E+06, 1.913964E+06, 2.117813E+06,
2.322356E+06, 2.528242E+06, 2.733913E+06, 2.939536E+06, 3.144263E+06,
3.348586E+06, 3.552136E+06, 3.754167E+06, 4.155705E+06, 4.551236E+06,
4.941210E+06, 5.326665E+06, 5.707895E+06, 6.085630E+06, 6.460917E+06,
6.834721E+06, 7.207669E+06, 7.580081E+06, 7.952133E+06, 8.323809E+06,
8.695128E+06, 9.066237E+06, 9.437196E+06, 9.807923E+06, 1.017822E+07,
1.054821E+07, 1.091782E+07, 1.128702E+07, 1.165565E+07, 1.202371E+07,
1.239124E+07, 1.275757E+07, 1.312344E+07, 1.348836E+07, 1.385230E+07,
1.421518E+07, 1.457692E+07, 1.493728E+07, 1.529634E+07, 1.565337E+07,
1.600468E+07, 1.635575E+07, 1.670698E+07, 1.705504E+07, 1.739935E+07,
1.773997E+07, 1.807498E+07, 1.840275E+07, 1.872242E+07, 1.903327E+07,
1.933479E+07, 1.962564E+07, 1.983887E+07, 1.996269E+07, 2.006852E+07,
2.017271E+07, 2.027352E+07, 2.037032E+07, 2.046302E+07, 2.055139E+07,
2.063426E+07, 2.071323E+07, 2.078711E+07, 2.085657E+07, 2.092221E+07,
2.098365E+07, 2.104076E+07, 2.109499E+07, 2.114546E+07, 2.119276E+07,
2.123708E+07, 2.127890E+07, 2.131766E+07, 2.135476E+07, 2.139006E+07,
2.142238E+07, 2.145335E+07, 2.148276E+07, 2.151048E+07, 2.153699E+07,
2.156167E+07, 2.158526E+07, 2.160746E+07, 2.162887E+07, 2.164848E+07,
2.166872E+07, 2.168756E+07, 2.170507E+07, 2.172137E+07, 2.173726E+07,
2.175247E+07, 2.176757E+07, 2.178229E+07, 2.179602E+07, 2.180920E+07,
2.182182E+07, 2.183344E+07, 2.184531E+07, 2.185738E+07, 2.186894E+07,
2.187959E+07, 2.188951E+07, 2.185001E+07, 2.175285E+07, 2.165111E+07,
2.155923E+07, 2.147552E+07, 2.139940E+07, 2.132867E+07, 2.126367E+07,
2.120307E+07, 2.114659E+07, 2.109369E+07, 2.104374E+07, 2.099663E+07,
2.095212E+07, 2.090966E+07, 2.086913E+07, 2.082986E+07, 2.079255E+07,
2.075681E+07, 2.072258E+07, 2.068972E+07, 2.065795E+07, 2.062743E+07,
2.059761E+07, 2.056895E+07, 2.054131E+07, 2.051426E+07, 2.048782E+07,
2.046262E+07, 2.043814E+07, 2.041415E+07, 2.039085E+07, 2.036806E+07,
2.034595E+07, 2.032425E+07, 2.030334E+07, 2.028270E+07, 2.026237E+07,
2.024268E+07, 2.022344E+07, 2.020458E+07, 2.018632E+07, 2.016832E+07,
2.015071E+07, 2.013337E+07, 2.011642E+07, 2.009986E+07, 2.008361E+07,
2.006744E+07, 2.005178E+07, 2.003638E+07, 2.002127E+07, 2.000641E+07,

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1.999188E+07,1.997761E+07,1.996354E+07,1.994972E+07,1.993613E+07,
1.992258E+07,1.990944E+07,1.989650E+07,1.988377E+07,1.987124E+07,
1.985890E+07,1.984672E+07,1.983473E+07,1.982293E+07,1.981129E+07,
1.979983E+07,1.978840E+07,1.977724E+07,1.976625E+07,1.975539E+07,
1.974464E+07,1.973406E+07,1.972365E+07,1.971337E+07,1.970324E+07,
1.969320E+07,1.968319E+07,1.967346E+07,1.966383E+07,1.965431E+07,
1.964490E+07,1.963561E+07,1.962643E+07,1.961738E+07,1.960842E+07,
1.959955E+07,1.959082E+07,1.958206E+07,1.957352E+07,1.956505E+07,
1.955669E+07,1.954843E+07,1.792855E+07,1.792855E+07

POROSITY SURFACE #3; GAS GENERATION RATE #11.

SDATA(NSDATA =11,NTDATA=1:214,MKLOS =4)

8.483495E-01,7.680444E-01,7.537600E-01,6.626914E-01,5.956017E-01,
5.373901E-01,4.916968E-01,4.516874E-01,4.175932E-01,3.967207E-01,
3.794281E-01,3.668271E-01,3.561774E-01,3.470423E-01,3.401434E-01,
3.338707E-01,3.287197E-01,3.243698E-01,3.204762E-01,3.174932E-01,
3.147517E-01,3.124452E-01,3.106092E-01,3.074693E-01,3.053698E-01,
3.039394E-01,3.030070E-01,3.024305E-01,3.021050E-01,3.019349E-01,
3.018499E-01,3.018110E-01,3.017973E-01,3.017991E-01,3.018142E-01,
3.018410E-01,3.018722E-01,3.019062E-01,3.019447E-01,3.019929E-01,
3.020470E-01,3.021077E-01,3.021756E-01,3.022540E-01,3.023427E-01,
3.024390E-01,3.025470E-01,3.026705E-01,3.028088E-01,3.029615E-01,
3.031289E-01,3.033119E-01,3.035117E-01,3.037304E-01,3.039786E-01,
3.043246E-01,3.046612E-01,3.049800E-01,3.053428E-01,3.057550E-01,
3.062174E-01,3.067578E-01,3.074000E-01,3.081535E-01,3.090257E-01,
3.100197E-01,3.111514E-01,3.123801E-01,3.135601E-01,3.147105E-01,
3.158745E-01,3.170794E-01,3.183346E-01,3.196431E-01,3.210079E-01,
3.224471E-01,3.239359E-01,3.254935E-01,3.271099E-01,3.287748E-01,
3.304963E-01,3.322768E-01,3.340930E-01,3.359599E-01,3.378690E-01,
3.398169E-01,3.417965E-01,3.438186E-01,3.458580E-01,3.479220E-01,
3.500282E-01,3.521504E-01,3.542915E-01,3.564553E-01,3.586340E-01,
3.608381E-01,3.630557E-01,3.652920E-01,3.675369E-01,3.698076E-01,
3.720641E-01,3.743406E-01,3.766365E-01,3.789497E-01,3.812666E-01,
3.835923E-01,3.859158E-01,3.882436E-01,3.905863E-01,3.929358E-01,
3.952904E-01,3.976620E-01,4.000401E-01,4.023967E-01,4.047603E-01,
4.071375E-01,4.095267E-01,4.118613E-01,4.140280E-01,4.159821E-01,
4.177629E-01,4.193987E-01,4.208974E-01,4.222998E-01,4.235967E-01,
4.248129E-01,4.259529E-01,4.270263E-01,4.280448E-01,4.290099E-01,
4.299255E-01,4.308030E-01,4.316436E-01,4.324613E-01,4.332410E-01,
4.339904E-01,4.347109E-01,4.354048E-01,4.360776E-01,4.367259E-01,
4.373614E-01,4.379740E-01,4.385661E-01,4.391473E-01,4.397165E-01,
4.402610E-01,4.407907E-01,4.413114E-01,4.418183E-01,4.423150E-01,

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4.427982E-01,4.432734E-01,4.437321E-01,4.441859E-01,4.446337E-01,
4.450685E-01,4.454940E-01,4.459119E-01,4.463174E-01,4.467177E-01,
4.471099E-01,4.474971E-01,4.478760E-01,4.482468E-01,4.486116E-01,
4.489748E-01,4.493272E-01,4.496745E-01,4.500155E-01,4.503513E-01,
4.506802E-01,4.510040E-01,4.513234E-01,4.516377E-01,4.519471E-01,
4.522561E-01,4.525562E-01,4.528519E-01,4.531434E-01,4.534304E-01,
4.537136E-01,4.539936E-01,4.542696E-01,4.545415E-01,4.548096E-01,
4.550740E-01,4.553384E-01,4.555967E-01,4.558511E-01,4.561033E-01,
4.563528E-01,4.565987E-01,4.568408E-01,4.570803E-01,4.573167E-01,
4.575511E-01,4.577849E-01,4.580125E-01,4.582379E-01,4.584610E-01,
4.586817E-01,4.589000E-01,4.591158E-01,4.593287E-01,4.595395E-01,
4.597487E-01,4.599547E-01,4.601612E-01,4.603632E-01,4.605636E-01,
4.607614E-01,4.609570E-01,5.028421E-01,5.028421E-01

POROSITY SURFACE #4; GAS GENERATION RATE #12.

PDATA(NSDATA =12,NTDATA=1:214,MKLOS =4)

1.013250E+05,1.110729E+05,1.212889E+05,2.398930E+05,3.869243E+05,
5.475982E+05,7.427812E+05,9.578388E+05,1.190852E+06,1.432230E+06,
1.675361E+06,1.920285E+06,2.167012E+06,2.414901E+06,2.664132E+06,
2.913219E+06,3.161898E+06,3.409092E+06,3.655577E+06,3.899764E+06,
4.142703E+06,4.383623E+06,4.621958E+06,5.095351E+06,5.561169E+06,
6.021113E+06,6.477698E+06,6.932117E+06,7.385386E+06,7.837992E+06,
8.290098E+06,8.741821E+06,9.193109E+06,9.644017E+06,1.009453E+07,
1.054475E+07,1.099457E+07,1.144388E+07,1.189239E+07,1.234000E+07,
1.278667E+07,1.323228E+07,1.367666E+07,1.411968E+07,1.456121E+07,
1.500064E+07,1.543688E+07,1.587062E+07,1.629942E+07,1.672627E+07,
1.715239E+07,1.757390E+07,1.798832E+07,1.839432E+07,1.879048E+07,
1.917520E+07,1.954705E+07,1.990430E+07,2.024580E+07,2.056974E+07,
2.087310E+07,2.115269E+07,2.140704E+07,2.163485E+07,2.183697E+07,
2.201508E+07,2.217250E+07,2.223711E+07,2.221461E+07,2.218600E+07,
2.216793E+07,2.215568E+07,2.214868E+07,2.214608E+07,2.214582E+07,
2.214818E+07,2.215250E+07,2.215749E+07,2.216452E+07,2.217302E+07,
2.218046E+07,2.218923E+07,2.219918E+07,2.220859E+07,2.221707E+07,
2.222520E+07,2.223372E+07,2.224221E+07,2.225194E+07,2.226107E+07,
2.226833E+07,2.227670E+07,2.228562E+07,2.229323E+07,2.230048E+07,
2.230746E+07,2.231489E+07,2.232192E+07,2.232887E+07,2.233455E+07,
2.234020E+07,2.234507E+07,2.235012E+07,2.235598E+07,2.236127E+07,
2.236579E+07,2.236992E+07,2.237430E+07,2.237906E+07,2.238302E+07,
2.238664E+07,2.239014E+07,2.239318E+07,2.239647E+07,2.239989E+07,
2.240294E+07,2.240463E+07,2.235582E+07,2.224896E+07,2.213813E+07,
2.203736E+07,2.194580E+07,2.186319E+07,2.178623E+07,2.171555E+07,
2.164977E+07,2.158839E+07,2.153055E+07,2.147597E+07,2.142453E+07,

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2.137567E+07,2.132930E+07,2.128485E+07,2.124166E+07,2.120075E+07,
2.116172E+07,2.112423E+07,2.108825E+07,2.105328E+07,2.101961E+07,
2.098734E+07,2.095605E+07,2.092506E+07,2.089598E+07,2.086688E+07,
2.083925E+07,2.081246E+07,2.078626E+07,2.076064E+07,2.073610E+07,
2.071204E+07,2.068825E+07,2.066539E+07,2.064309E+07,2.062100E+07,
2.059966E+07,2.057896E+07,2.055862E+07,2.053859E+07,2.051915E+07,
2.050007E+07,2.048145E+07,2.046321E+07,2.044524E+07,2.042757E+07,
2.041011E+07,2.039313E+07,2.037655E+07,2.036023E+07,2.034417E+07,
2.032854E+07,2.031305E+07,2.029778E+07,2.028287E+07,2.026822E+07,
2.025361E+07,2.023934E+07,2.022540E+07,2.021173E+07,2.019814E+07,
2.018466E+07,2.017151E+07,2.015860E+07,2.014586E+07,2.013327E+07,
2.012081E+07,2.010847E+07,2.009645E+07,2.008452E+07,2.007285E+07,
2.006139E+07,2.004994E+07,2.003868E+07,2.002760E+07,2.001665E+07,
2.000584E+07,1.999501E+07,1.998451E+07,1.997411E+07,1.996386E+07,
1.995373E+07,1.994371E+07,1.993386E+07,1.992410E+07,1.991439E+07,
1.990485E+07,1.989544E+07,1.988602E+07,1.987681E+07,1.986767E+07,
1.985867E+07,1.984975E+07,1.810892E+07,1.810892E+07

POROSITY SURFACE #3; GAS GENERATION RATE #12.

SDATA (NSDATA =12,NTDATA=1:214,MKLOS =4)

8.483495E-01,7.682230E-01,7.527017E-01,6.629687E-01,5.980765E-01,
5.415387E-01,4.975783E-01,4.596760E-01,4.272471E-01,4.072321E-01,
3.905837E-01,3.793911E-01,3.702406E-01,3.624610E-01,3.567323E-01,
3.515795E-01,3.474783E-01,3.441497E-01,3.412214E-01,3.390752E-01,
3.371784E-01,3.356768E-01,3.345899E-01,3.328079E-01,3.318332E-01,
3.313166E-01,3.310736E-01,3.309677E-01,3.309283E-01,3.309221E-01,
3.309362E-01,3.309641E-01,3.310045E-01,3.310547E-01,3.311129E-01,
3.311760E-01,3.312455E-01,3.313251E-01,3.314208E-01,3.315331E-01,
3.316629E-01,3.318102E-01,3.319782E-01,3.321676E-01,3.323803E-01,
3.326271E-01,3.329165E-01,3.332548E-01,3.336763E-01,3.341162E-01,
3.345477E-01,3.350465E-01,3.356520E-01,3.363875E-01,3.372684E-01,
3.383154E-01,3.395455E-01,3.409810E-01,3.426333E-01,3.445235E-01,
3.467003E-01,3.492085E-01,3.520676E-01,3.552970E-01,3.588824E-01,
3.627989E-01,3.669941E-01,3.713761E-01,3.755070E-01,3.793832E-01,
3.830862E-01,3.866936E-01,3.902110E-01,3.936531E-01,3.970542E-01,
4.004076E-01,4.037242E-01,4.070274E-01,4.102910E-01,4.135240E-01,
4.167758E-01,4.199998E-01,4.231985E-01,4.264054E-01,4.296272E-01,
4.328533E-01,4.360684E-01,4.392825E-01,4.424664E-01,4.456625E-01,
4.488942E-01,4.521009E-01,4.552927E-01,4.585102E-01,4.617333E-01,
4.649596E-01,4.681747E-01,4.713957E-01,4.746165E-01,4.778617E-01,
4.811069E-01,4.843677E-01,4.876225E-01,4.908585E-01,4.941053E-01,
4.973677E-01,5.006364E-01,5.038993E-01,5.071524E-01,5.104225E-01,

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5.136958E-01,5.169731E-01,5.202782E-01,5.235562E-01,5.268301E-01,
5.301112E-01,5.334246E-01,5.366726E-01,5.396719E-01,5.423852E-01,
5.448765E-01,5.471598E-01,5.492366E-01,5.511858E-01,5.529879E-01,
5.546756E-01,5.562601E-01,5.577611E-01,5.591855E-01,5.605346E-01,
5.618218E-01,5.630488E-01,5.642304E-01,5.653829E-01,5.664790E-01,
5.675290E-01,5.685408E-01,5.695152E-01,5.704660E-01,5.713842E-01,
5.722671E-01,5.731254E-01,5.739784E-01,5.747812E-01,5.755867E-01,
5.763538E-01,5.770989E-01,5.778298E-01,5.785468E-01,5.792346E-01,
5.799107E-01,5.805809E-01,5.812262E-01,5.818572E-01,5.824836E-01,
5.830899E-01,5.836798E-01,5.842600E-01,5.848325E-01,5.853892E-01,
5.859371E-01,5.864724E-01,5.869976E-01,5.875160E-01,5.880268E-01,
5.885321E-01,5.890246E-01,5.895067E-01,5.899814E-01,5.904495E-01,
5.909058E-01,5.913587E-01,5.918056E-01,5.922430E-01,5.926732E-01,
5.931029E-01,5.935231E-01,5.939344E-01,5.943380E-01,5.947399E-01,
5.951391E-01,5.955291E-01,5.959122E-01,5.962912E-01,5.966658E-01,
5.970371E-01,5.974054E-01,5.977644E-01,5.981214E-01,5.984706E-01,
5.988142E-01,5.991581E-01,5.994964E-01,5.998300E-01,6.001598E-01,
6.004859E-01,6.008126E-01,6.011298E-01,6.014448E-01,6.017547E-01,
6.020615E-01,6.023659E-01,6.026650E-01,6.029620E-01,6.032576E-01,
6.035477E-01,6.038349E-01,6.041223E-01,6.044035E-01,6.046832E-01,
6.049588E-01,6.052319E-01,6.637407E-01,6.637407E-01

POROSITY SURFACE #4; GAS GENERATION RATE #13.

PDATA (NSDATA =13,NTDATA=1:214,MKLOS =4)

1.013250E+05,1.135109E+05,1.272430E+05,2.730583E+05,4.567553E+05,
6.569513E+05,8.924043E+05,1.153898E+06,1.431559E+06,1.724854E+06,
2.017248E+06,2.306836E+06,2.596449E+06,2.885971E+06,3.174599E+06,
3.462088E+06,3.747935E+06,4.031126E+06,4.313115E+06,4.591690E+06,
4.868325E+06,5.142798E+06,5.413986E+06,5.953619E+06,6.486585E+06,
7.016163E+06,7.545006E+06,8.073072E+06,8.600315E+06,9.126985E+06,
9.653167E+06,1.017904E+07,1.070447E+07,1.122931E+07,1.175334E+07,
1.227640E+07,1.279825E+07,1.331882E+07,1.383771E+07,1.435438E+07,
1.486840E+07,1.537960E+07,1.588763E+07,1.639030E+07,1.688967E+07,
1.738755E+07,1.787701E+07,1.835724E+07,1.882599E+07,1.928069E+07,
1.971901E+07,2.013883E+07,2.053818E+07,2.091312E+07,2.125897E+07,
2.157178E+07,2.184996E+07,2.209338E+07,2.230454E+07,2.248708E+07,
2.264416E+07,2.277852E+07,2.289461E+07,2.299428E+07,2.308070E+07,
2.315684E+07,2.322088E+07,2.320261E+07,2.310465E+07,2.301433E+07,
2.294379E+07,2.288996E+07,2.284840E+07,2.281536E+07,2.278955E+07,
2.276879E+07,2.275100E+07,2.273844E+07,2.272746E+07,2.271874E+07,
2.271242E+07,2.270695E+07,2.270209E+07,2.269881E+07,2.269719E+07,
2.269413E+07,2.269196E+07,2.269158E+07,2.269128E+07,2.269044E+07,

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2.268961E+07, 2.268875E+07, 2.268815E+07, 2.268768E+07, 2.268698E+07,
2.268675E+07, 2.268506E+07, 2.268391E+07, 2.268311E+07, 2.268252E+07,
2.268087E+07, 2.267908E+07, 2.267713E+07, 2.267467E+07, 2.267255E+07,
2.267014E+07, 2.266696E+07, 2.266374E+07, 2.266067E+07, 2.265781E+07,
2.265456E+07, 2.265110E+07, 2.264752E+07, 2.264360E+07, 2.263961E+07,
2.263531E+07, 2.263096E+07, 2.257535E+07, 2.246027E+07, 2.234216E+07,
2.223589E+07, 2.213972E+07, 2.205185E+07, 2.196978E+07, 2.189444E+07,
2.182460E+07, 2.175940E+07, 2.169809E+07, 2.164003E+07, 2.158524E+07,
2.153331E+07, 2.148376E+07, 2.143694E+07, 2.139149E+07, 2.134843E+07,
2.130718E+07, 2.126757E+07, 2.122885E+07, 2.119199E+07, 2.115661E+07,
2.112166E+07, 2.108878E+07, 2.105644E+07, 2.102521E+07, 2.099464E+07,
2.096519E+07, 2.093635E+07, 2.090865E+07, 2.088192E+07, 2.085570E+07,
2.082988E+07, 2.080520E+07, 2.078127E+07, 2.075771E+07, 2.073431E+07,
2.071179E+07, 2.069004E+07, 2.066834E+07, 2.064746E+07, 2.062688E+07,
2.060697E+07, 2.058735E+07, 2.056821E+07, 2.054934E+07, 2.053088E+07,
2.051259E+07, 2.049498E+07, 2.047769E+07, 2.046057E+07, 2.044385E+07,
2.042755E+07, 2.041146E+07, 2.039571E+07, 2.038020E+07, 2.036492E+07,
2.034969E+07, 2.033490E+07, 2.032045E+07, 2.030620E+07, 2.029221E+07,
2.027840E+07, 2.026481E+07, 2.025143E+07, 2.023823E+07, 2.022526E+07,
2.021252E+07, 2.019975E+07, 2.018727E+07, 2.017498E+07, 2.016285E+07,
2.015090E+07, 2.013916E+07, 2.012760E+07, 2.011617E+07, 2.010491E+07,
2.009375E+07, 2.008263E+07, 2.007171E+07, 2.006089E+07, 2.005030E+07,
2.003987E+07, 2.002950E+07, 2.001932E+07, 2.000923E+07, 1.999929E+07,
1.998947E+07, 1.997979E+07, 1.997004E+07, 1.996055E+07, 1.995120E+07,
1.994190E+07, 1.993274E+07, 1.813986E+07, 1.813986E+07

POROSITY SURFACE #3; GAS GENERATION RATE #13.

SDATA (NSDATA =13, NTDATA=1:214, MKLOS =4)

8.483495E-01, 7.682490E-01, 7.554958E-01, 6.621399E-01, 5.999427E-01,
5.453771E-01, 5.029163E-01, 4.674858E-01, 4.364200E-01, 4.172156E-01,
4.011800E-01, 3.909041E-01, 3.830592E-01, 3.764068E-01, 3.717471E-01,
3.676792E-01, 3.644778E-01, 3.620491E-01, 3.599483E-01, 3.584940E-01,
3.573005E-01, 3.563910E-01, 3.558511E-01, 3.549922E-01, 3.546712E-01,
3.545476E-01, 3.545022E-01, 3.544967E-01, 3.545273E-01, 3.545767E-01,
3.546383E-01, 3.547049E-01, 3.547792E-01, 3.548655E-01, 3.549681E-01,
3.550908E-01, 3.552366E-01, 3.554060E-01, 3.556058E-01, 3.558462E-01,
3.561339E-01, 3.564675E-01, 3.568516E-01, 3.573285E-01, 3.578494E-01,
3.583698E-01, 3.590173E-01, 3.598251E-01, 3.608122E-01, 3.620160E-01,
3.634675E-01, 3.651922E-01, 3.672110E-01, 3.695882E-01, 3.723925E-01,
3.756842E-01, 3.794854E-01, 3.837960E-01, 3.885767E-01, 3.937677E-01,
3.993278E-01, 4.052167E-01, 4.113652E-01, 4.177510E-01, 4.243259E-01,
4.310435E-01, 4.379434E-01, 4.448272E-01, 4.512258E-01, 4.570874E-01,

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4.625949E-01,4.677937E-01,4.727605E-01,4.775681E-01,4.822361E-01,
4.868063E-01,4.913202E-01,4.957271E-01,5.001039E-01,5.044332E-01,
5.087130E-01,5.129760E-01,5.172272E-01,5.214439E-01,5.256227E-01,
5.298363E-01,5.340287E-01,5.381803E-01,5.423264E-01,5.464896E-01,
5.506528E-01,5.548169E-01,5.589738E-01,5.631288E-01,5.672898E-01,
5.714393E-01,5.756261E-01,5.797996E-01,5.839647E-01,5.881228E-01,
5.923104E-01,5.965027E-01,6.006996E-01,6.049107E-01,6.091140E-01,
6.133256E-01,6.175578E-01,6.217938E-01,6.260270E-01,6.302554E-01,
6.344920E-01,6.387382E-01,6.430115E-01,6.472711E-01,6.515338E-01,
6.558060E-01,6.600827E-01,6.642840E-01,6.682149E-01,6.717622E-01,
6.749869E-01,6.779321E-01,6.806456E-01,6.831995E-01,6.855606E-01,
6.877647E-01,6.898349E-01,6.917932E-01,6.936576E-01,6.954266E-01,
6.971115E-01,6.987267E-01,7.002602E-01,7.017553E-01,7.031774E-01,
7.045451E-01,7.058634E-01,7.071572E-01,7.083930E-01,7.095831E-01,
7.107628E-01,7.118763E-01,7.129752E-01,7.140390E-01,7.150837E-01,
7.160933E-01,7.170847E-01,7.180387E-01,7.189624E-01,7.198707E-01,
7.207676E-01,7.216267E-01,7.224617E-01,7.232859E-01,7.241062E-01,
7.248972E-01,7.256631E-01,7.264287E-01,7.271668E-01,7.278964E-01,
7.286028E-01,7.293006E-01,7.299828E-01,7.306567E-01,7.313167E-01,
7.319720E-01,7.326036E-01,7.332253E-01,7.338419E-01,7.344452E-01,
7.350342E-01,7.356165E-01,7.361878E-01,7.367509E-01,7.373062E-01,
7.378602E-01,7.383999E-01,7.389273E-01,7.394491E-01,7.399611E-01,
7.404674E-01,7.409668E-01,7.414588E-01,7.419449E-01,7.424226E-01,
7.428931E-01,7.433652E-01,7.438269E-01,7.442823E-01,7.447322E-01,
7.451764E-01,7.456129E-01,7.460434E-01,7.464693E-01,7.468896E-01,
7.473067E-01,7.477227E-01,7.481317E-01,7.485371E-01,7.489342E-01,
7.493262E-01,7.497161E-01,7.500990E-01,7.504793E-01,7.508541E-01,
7.512251E-01,7.515908E-01,7.519591E-01,7.523186E-01,7.526734E-01,
7.530259E-01,7.533738E-01,8.282532E-01,8.282532E-01

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11.3 Appendix C: Sample Output File

Below is listed an example BRAGFLO ASCII .OUT file. This file is given here for illustrative purposes only and is not the output file resulting from the input file given in Subsection 11.1, Appendix A. The output resulting from the input file given in Subsection 11.1, Appendix A. would be too long to list here.

```
*****  
** Beginning of BRAGFLO      Version: 6.0      Revised: 01/15/07      **  
** Begun on: 02/14/07 at 09:14:28  Run on: TDN   - ALPHA AXP OpenVMS V8.2 **  
*****
```

```
BBBBBB  RRRRRR   AAAAA  GGGGG  FFFFFFFF LL      OOOOO  
BB  BB  RR  RR  AA  AA  GG  GG  FF      LL      OO  OO  
BB  BB  RR  RR  AA  AA  GG      FF      LL      OO  OO  
BBBBBB  RRRRRR  AAAAAA  GG      FFFFF  LL      OO  OO  
BB  BB  RRRRR  AA  AA  GG  GGG  FF      LL      OO  OO  
BB  BB  RR  RR  AA  AA  GG  GG  FF      LL      OO  OO  
BBBBBB  RR  RR  AA  AA  GGGGG  FF      LLLLLL  OOOOO
```

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Ali A. Shinta, API
John Wormeck, Ecodynamics

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```
**QA**      -- QA info for:
PREBRAG     -- program name;
6.00        -- PREBRAG version number;
09/09/99    -- PREBRAG revision date;
09/09/99    -- PREBRAG run date;
12:12:12    -- PREBRAG run time.
```

Number of file names to follow = 5

```
*****
Input File Name:
PAA: [ANALYSIS.BF.QB0600.ES45.TEST1]BF2_QB0600_TEST1.INP;2
*****
```

```
*****
Closure Input File Name:
PAA: [ANALYSIS.BF.QB0600.ES45.TEST1]BF2_CLOSURE.DAT;1
*****
```

```
*****
ASCII Output File Name:
PAA: [ANALYSIS.BF.QB0600.ES45.TEST1]BF2_QB0600_ES45_TEST1.OUT;1
*****
```

```
*****
ASCII Summary File Name:
PAA: [ANALYSIS.BF.QB0600.ES45.TEST1]BF2_QB0600_ES45_TEST1.SUM;1
*****
```

```
*****
Binary Output File Name:
PAA: [ANALYSIS.BF.QB0600.ES45.TEST1]BF2_QB0600_ES45_TEST1.BIN;1
*****
```

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Simulation title:
BF2_TEST1.INP: PRESSURE BUILDUP TEST WITH RADIAL GRID

Size parameters: NX, NY, NZ
50 1 1

Number of grid blocks = 50

Model Type (MODTYPE) = 1-Dimensional

Parameters for adjusting DELT:
Number of times to fix DELT (NDTFIX) = 1
TIMEDTFIX = Time for fixing DELT, s
DTFIX = DELT to be used when TIMEDTFIX is exceeded, s
K TIMEDTFIX(K) DTFIX(K)
1 5.000000E+03 1.000000E+01

UNITS used in input:
SI

UNITS used in output:
SI

Start time of simulation (START) = 0.00000E+00 s
End time for simulation (FINISH) = 1.00000E+04 s
Max no. time steps allowed (MAXITF) = 100
Initial time step (DELTA) = 1.00000E+01 s
Minimum time step allowed (DELTMIN) = 9.99990E+00 s
Maximum time step allowed (DELTMAX) = 1.00000E+04 s
Max fractional increase in time step allowed (DTIMEMAX) = 1.30000E+00
Flag for auto time step control (0=No,1=Yes) (ITIMECNTRL) = 1
Switch from relative to absolute change
in variable for determining time step size (TSWITCH) = 1.00000E-02

ASCII print control type (IPRTYPEASC) = 0
Binary print control type (IPRTYPEBIN) = 0
Restart print control type (IPRTPERST) = 0

ASCII output timestep interval (IPRNTASC) = 1
Binary output timestep interval (IPRNTBIN) = 200
Restart output timestep interval (IPRNRST) = 200

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**** Variable Output Flags ****
 0 = Do NOT Print to Designated Output File
 1 = DO Print to Designated Output File

I	ASC	BIN	Variable	Description	Units
1	1	1	PO	Brine pressure	Pa
2	1	0	PG	Gas pressure	Pa
3	0	0	POTO	Brine rho*g*potentiometric head	Pa
4	0	0	POTG	Gas rho*g*potentiometric head	Pa
5	0	0	PBUB	Brine bubble pressure	Pa
6	0	0	PHI	Porosity	dimensionless
7	1	0	RKO	Relative permeability to brine	dimensionless
8	1	0	RKG	Relative permeability to gas	dimensionless
9	0	0	RHOB	Brine density	kg/m ³
10	0	0	RHOG	Gas density	kg/m ³
11	0	0	PERMBX	Permeability to brine, x-direction	m ²
12	0	0	PERMBY	Permeability to brine, y-direction	m ²
13	0	0	PERMBZ	Permeability to brine, z-direction	m ²
14	0	0	PERMGX	Permeability to gas, x-direction	m ²
15	0	0	PERMGY	Permeability to gas, y-direction	m ²
16	0	0	PERMGZ	Permeability to gas, z-direction	m ²
17	1	1	SO	Brine saturation	fraction void volume
18	1	1	SG	Gas saturation	fraction void volume
19	0	0	COO	Brine component of brine phase	mass fr brine phase
20	0	0	CGO	Gas component of brine phase	mass fr brine phase
21	0	0	QOREFAVE	Time-average well brine flow rate	m ³ /s (ref conds)
22	0	0	QGREFAVE	Time-average well gas flow rate	m ³ /s (ref conds)
23	0	0	QOCUM	Cumulative well brine flow	m ³ (ref conds)
24	0	0	QGCUM	Cumulative well gas flow	m ³ (ref conds)
25	0	0	VODAVEI	Time-avg brine Darcy velocity, x-dir	m/s
26	0	0	VODAVEJ	Time-avg brine Darcy velocity, y-dir	m/s
27	0	0	VODAVEK	Time-avg brine Darcy velocity, z-dir	m/s
28	0	0	VGDAVEI	Time-avg gas Darcy velocity, x-dir	m/s
29	0	0	VGDAVEJ	Time-avg gas Darcy velocity, y-dir	m/s
30	0	0	VGDAVEK	Time-avg gas Darcy velocity, z-dir	m/s
31	0	0	QODAVEI	Time-avg interblock brine flow, x-dir	m ³ /s (@ ref conds)
32	0	0	QODAVEJ	Time-avg interblock brine flow, y-dir	m ³ /s (@ ref conds)
33	0	0	QODAVEK	Time-avg interblock brine flow, z-dir	m ³ /s (@ ref conds)
34	0	0	QGDAVEI	Time-avg interblock gas flow, x-dir	m ³ /s (@ ref conds)
35	0	0	QGDAVEJ	Time-avg interblock gas flow, y-dir	m ³ /s (@ ref conds)
36	0	0	QGDAVEK	Time-avg interblock gas flow, z-dir	m ³ /s (@ ref conds)
37	0	0	BRNBALREL	Relative Brine mass balance	dimensionless
38	0	0	GASBALREL	Relative Gas mass balance	dimensionless
39	0	0	RXNR (I,J,K,1)	Inundated corrosion rate	mol/s
40	0	0	RXNR (I,J,K,2)	Humid corrosion rate	mol/s
41	0	0	RXNR (I,J,K,3)	Inundated biodegradation rate	mol/s
42	0	0	RXNR (I,J,K,4)	Humid biodegradation rate	mol/s
43	0	0	RXNR (I,J,K,5)	Fe(OH)2 sulfidation rate	mol/s

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44	0	0	RXNR(I,J,K,6)	Fe sulfidation rate	mol/s
45	0	0	RXNR(I,J,K,7)	MgO hydration rate	mol/s
46	0	0	RXNR(I,J,K,8)	Mg(OH)2 carbonation rate	mol/s
47	0	0	RXNR(I,J,K,9)	MgO carbonation rate	mol/s
48	0	0	QR(I,J,K,1)	H2 generation rate -- simple model	kg/(s*m^3)
49	0	0	QR(I,J,K,2)	Brine consumption rate -- simple model	kg/(s*m^3)
50	0	0	QR(I,J,K,3)	Fe consumption rate -- simple model	kg/(s*m^3)
51	0	0	QR(I,J,K,4)	C6-H10-O5 consumption rate -- simple model	kg/(s*m^3)
52	0	0	QR(I,J,K,5)	Fe(OH)2 generation rate -- simple model	kg/(s*m^3)
53	0	0	QR(I,J,K,6)	FeS generation rate -- simple model	kg/(s*m^3)
54	0	0	QR(I,J,K,7)	MgO generation rate -- simple model	kg/(s*m^3)
55	0	0	QR(I,J,K,8)	Mg(OH)2 generation rate -- simple model	kg/(s*m^3)
56	0	0	QR(I,J,K,9)	MgCO3 generation rate -- simple model	kg/(s*m^3)
57	0	0	CONCFE(I,J,K,1)	Fe concentration -- simple model	kg/m^3
58	0	0	CONCBIO	C6-H10-O5 concentration -- simple model	kg/m^3
59	0	0	CONCFE(I,J,K,2)	Fe(OH)2 concentration -- simple model	kg/m^3
60	0	0	CONCFE(I,J,K,3)	FeS concentration -- simple model	kg/m^3
61	0	0	CONCMG(I,J,K,1)	MgO concentration -- simple model	kg/m^3
62	0	0	CONCMG(I,J,K,2)	Mg(OH)2 concentration -- simple model	kg/m^3
63	0	0	CONCMG(I,J,K,3)	MgCO3 concentration -- simple model	kg/m^3
64	0	0	CONCST	Salt concentration -- simple model	kg/m^3
65	0	0	PORSOLID	Volume fraction of generated solids	dimensionless
66	0	0	GENRAT(1,I,J,K)	H2 generation rate -- reaction path model	kg/(s*m^3)
67	0	0	GENRAT(2,I,J,K)	CO2 generation rate -- reaction path model	kg/(s*m^3)
68	0	0	GENRAT(3,I,J,K)	CH4 generation rate -- reaction path model	kg/(s*m^3)
69	0	0	GENRAT(4,I,J,K)	N2 generation rate -- reaction path model	kg/(s*m^3)
70	0	0	GENRAT(5,I,J,K)	H2S generation rate -- reaction path model	kg/(s*m^3)
71	0	0	GENRAT(6,I,J,K)	O2 generation rate -- reaction path model	kg/(s*m^3)
72	0	0	GENRAT(7,I,J,K)	H2O generation rate -- reaction path model	kg/(s*m^3)
73	0	0	GENRAT(8,I,J,K)	H2SO4 generation rate -- reaction path model	kg/(s*m^3)
74	0	0	GENRAT(9,I,J,K)	HNO3 generation rate -- reaction path model	kg/(s*m^3)
75	0	0	GENRAT(10,I,J,K)	C6-H10-O5 consumption rate -- reaction path model	kg/(s*m^3)
76	0	0	GENRAT(11,I,J,K)	Fe consumption rate -- reaction path model	kg/(s*m^3)
77	0	0	GENRAT(12,I,J,K)	FeS2_F generation rate -- reaction path model	kg/(s*m^3)
78	0	0	GENRAT(13,I,J,K)	FeS2_O generation rate -- reaction path model	kg/(s*m^3)
79	0	0	GENRAT(14,I,J,K)	FeCO3_F generation rate -- reaction path model	kg/(s*m^3)
80	0	0	GENRAT(15,I,J,K)	FeCO3_O generation rate -- reaction path model	kg/(s*m^3)
81	0	0	GENRAT(16,I,J,K)	Fe(OH)2 generation rate -- reaction path model	kg/(s*m^3)
82	0	0	GENRAT(17,I,J,K)	FeO(OH) generation rate -- reaction path model	kg/(s*m^3)
83	0	0	GENRAT(18,I,J,K)	Fe3O4 generation rate -- reaction path model	kg/(s*m^3)
84	0	0	GENRAT(19,I,J,K)	FeS generation rate -- reaction path model	kg/(s*m^3)
85	0	0	GENRAT(20,I,J,K)	CaO generation rate -- reaction path model	kg/(s*m^3)
86	0	0	GENRAT(21,I,J,K)	Ca(OH)2 generation rate -- reaction path model	kg/(s*m^3)
87	0	0	GENRAT(22,I,J,K)	CaCO3 generation rate -- reaction path model	kg/(s*m^3)
88	0	0	GENRAT(23,I,J,K)	H2 generation rate -- radiolysis	kg/(s*m^3)
89	0	0	CONCRXN(1,I,J,K)	H2 concentration -- reaction path model	kg/m^3
90	0	0	CONCRXN(2,I,J,K)	CO2 concentration -- reaction path model	kg/m^3
91	0	0	CONCRXN(3,I,J,K)	CH4 concentration -- reaction path model	kg/m^3
92	0	0	CONCRXN(4,I,J,K)	N2 concentration -- reaction path model	kg/m^3
93	0	0	CONCRXN(5,I,J,K)	H2S concentration -- reaction path model	kg/m^3
94	0	0	CONCRXN(6,I,J,K)	O2 concentration -- reaction path model	kg/m^3

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95	0	0	CONCRXN(7,I,J,K)	H2O concentration -- reaction path model	kg/m ³
96	0	0	CONCRXN(8,I,J,K)	H2SO4 concentration -- reaction path model	kg/m ³
97	0	0	CONCRXN(9,I,J,K)	HNO3 concentration -- reaction path model	kg/m ³
98	0	0	CONCRXN(10,I,J,K)	C6-H10-O5 concentration -- reaction path model	kg/m ³
99	0	0	CONCRXN(11,I,J,K)	Fe concentration -- reaction path model	kg/m ³
100	0	0	CONCRXN(12,I,J,K)	FeS2_F concentration -- reaction path model	kg/m ³
101	0	0	CONCRXN(13,I,J,K)	FeS2_O concentration -- reaction path model	kg/m ³
102	0	0	CONCRXN(14,I,J,K)	FeCO3_F concentration -- reaction path model	kg/m ³
103	0	0	CONCRXN(15,I,J,K)	FeCO3_O concentration -- reaction path model	kg/m ³
104	0	0	CONCRXN(16,I,J,K)	Fe(OH)2 concentration -- reaction path model	kg/m ³
105	0	0	CONCRXN(17,I,J,K)	FeO(OH) concentration -- reaction path model	kg/m ³
106	0	0	CONCRXN(18,I,J,K)	Fe3O4 concentration -- reaction path model	kg/m ³
107	0	0	CONCRXN(19,I,J,K)	FeS concentration -- reaction path model	kg/m ³
108	0	0	CONCRXN(20,I,J,K)	CaO concentration -- reaction path model	kg/m ³
109	0	0	CONCRXN(21,I,J,K)	Ca(OH)2 concentration -- reaction path model	kg/m ³
110	0	0	CONCRXN(22,I,J,K)	CaCO3 concentration -- reaction path model	kg/m ³
111	0	0	CONCRXN(23,I,J,K)	H2 concentration -- radiolysis	kg/m ³
112	0	0	H2OFLOWIN	Water inflow rate	kg/s
113	0	0	B_MASS_CUM(1)	Total isotope mass from Waste Region 1	kg
114	0	0	B_CONC_CUM(1)	Total isotope conc from Waste Region 1	kg/m ³
115	0	0	S_MASS_CUM(1)	Total solid isotope mass from Waste Region 1	kg
116	0	0	B_MASS_CUM(2)	Total isotope mass from Waste Region 2	kg
117	0	0	B_CONC_CUM(2)	Total isotope conc from Waste Region 2	kg/m ³
118	0	0	S_MASS_CUM(2)	Total solid isotope mass from Waste Region 2	kg
119	0	0	B_MASS(1,1)	Mass of isotope 1 from Waste Region 1	kg
120	0	0	B_MASS(1,2)	Mass of isotope 1 from Waste Region 2	kg
121	0	0	B_CONC(1,1)	Conc of isotope 1 from Waste Region 1	kg/m ³
122	0	0	B_CONC(1,2)	Conc of isotope 1 from Waste Region 2	kg/m ³
123	0	0	S_MASS(1,1)	Solid mass of isotope 1 from Waste Region 1	kg
124	0	0	S_MASS(1,2)	Solid mass of isotope 1 from Waste Region 2	kg

Number of variables to be printed as History Variables (NHIV) = 0
 NOTE: History variables printed only to Binary output file.

Monitor key parameters (MONITOR): T
 Number of Monitor Blocks (NMON) = 1
 I-index of grid block 1 to be monitored (IMONITOR) = 1
 J-index of grid block 1 to be monitored (JMONITOR) = 1
 K-index of grid block 1 to be monitored (KMONITOR) = 1

Geometry Flags -- Specifies how block thicknesses are to be read.
 IDXFLAG = 1
 IDYFLAG = 0
 IDZFLAG = 1
 IDEPTHFLAG = 0

Grid block dimensions in I-direction, m
 1.000000E-02 1.300000E-02 1.690000E-02 2.197000E-02 2.856100E-02
 3.712929E-02 4.826808E-02 6.274850E-02 8.157305E-02 1.060450E-01

Information Only

```

1.378584E-01 1.792160E-01 2.329807E-01 3.028749E-01 3.937374E-01
5.118586E-01 6.654161E-01 8.650409E-01 1.124553E+00 1.461919E+00
1.900495E+00 2.470643E+00 3.211836E+00 4.175386E+00 5.428001E+00
7.056402E+00 9.173322E+00 1.192532E+01 1.550291E+01 2.015379E+01
2.619992E+01 3.405989E+01 4.427786E+01 5.756122E+01 7.482958E+01
9.727845E+01 1.264620E+02 1.644006E+02 2.137207E+02 2.778369E+02
3.611880E+02 4.695444E+02 6.104077E+02 7.935300E+02 1.031589E+03
1.341066E+03 1.743385E+03 2.266401E+03 2.946321E+03 3.830217E+03
  
```

Incremental grid block dimension in J-direction (DYCONST) = 1.000000E+00 m

Grid block dimensions in K-direction, m

```

3.141593E-02 1.036726E-01 1.976062E-01 3.197199E-01 4.784677E-01
6.848398E-01 9.531236E-01 1.301892E+00 1.755292E+00 2.344711E+00
3.110957E+00 4.107075E+00 5.402029E+00 7.085469E+00 9.273942E+00
1.211896E+01 1.581747E+01 2.062555E+01 2.687604E+01 3.500168E+01
4.556502E+01 5.929735E+01 7.714938E+01 1.003570E+02 1.305270E+02
1.697479E+02 2.207350E+02 2.870184E+02 3.731867E+02 4.852056E+02
6.308300E+02 8.201418E+02 1.066247E+03 1.386184E+03 1.802102E+03
2.342795E+03 3.045697E+03 3.959469E+03 5.147372E+03 6.691646E+03
8.699202E+03 1.130903E+04 1.470179E+04 1.911240E+04 2.484618E+04
3.230009E+04 4.199018E+04 5.458730E+04 7.096354E+04 9.225267E+04
  
```

Constant elevation to grid block centers (DEPTHCONST) = 1.000000E+01 m

Number of times to specify well conditions (NWELLTIMES) = 2

```

-----
WELLTIME = Time when conditions first become valid, s
NWELLS = Number of grid blocks containing wells
NWELLSPERGRID = Number of wells in grid block
IWELLNODE = I-index of grid block
JWELLNODE = J-index of grid block
KWELLNODE = K-index of grid block
IWELL = Well block number for grid block
        (IWELLNODE, JWELLNODE, KWELLNODE)
WELLTYPE = Type of well:
           INJP = Pressure-controlled injection
           INJQ = Flow-rate-controlled injection
           PROD = Production
           NONE = None of above (initialized)
QGWELL = Gas flow rate, kg/s
QOWELL = Brine flow rate, kg/s
PIWELL = Injectivity or productivity index, m^3
PW = Well bore pressure, Pa
  
```

```

-----
I  WELLTIME(I)  NWELLS(I)
1  0.000000E+00  1
  
```

```

           IWELL JWELL KWELL NWELLS-  WELL
          J  NODE  NODE  NODE PERGRID  K  TYPE  QGWELL  QOWELL  PIWELL  PW
  
```

Information Only


```
1 1 1 1 1
2 5.000000E+03 0
1 'INJQ' 0.000000E+00 -1.233000E+01 1.000000E+00 1.000000E+05

Dirichlet BCs to be specified? (T/F) (DIRICHLET) = F
Number of grid blocks where Dirichlet BCs specified (NO_DIRGRID) = 0

SATLIMIT and DEPLIMIT for 2 equations:
SATLIMIT = 1.000E-03
DEPLIMIT(1) = 1.000E-01
DEPLIMIT(2) = -1.000E+07 Pa

Variable change allowed to keep same time step (DELTADEPNORM):
DELTADEPNORM(1) = 6.000E-01
DELTADEPNORM(2) = 1.000E+06 Pa

Max variable change allowed over time step (DDEPMAX):
DDEPMAX(1) = 1.000E+00
DDEPMAX(2) = 1.000E+07 Pa

NORMAL Newton-Raphson convergence criteria (EPSNORM):
EPSNORM(1) = 7.000E+00
EPSNORM(2) = 1.000E-07

LOOSE Newton-Raphson convergence criteria (EPSLOOSE):
EPSLOOSE(1) = 7.000E+00
EPSLOOSE(2) = 1.000E-07

NORMAL Min. value of RHS function vector below which
convergence is accepted regardless of EPS (FTOLNORM):
FTOLNORM(1) = 1.000E-06
FTOLNORM(2) = 1.000E-06

LOOSE Min. value of RHS function vector below which
convergence is accepted regardless of EPS (FTOLLOOSE):
FTOLLOOSE(1) = 1.000E-06
FTOLLOOSE(2) = 1.000E-06

Convergence criteria for gas component transport:
EPGAS(1) = -1.000E-05
EPGAS(2) = 1.000E-05
EPGAS(3) = 1.000E-05
EPGAS(4) = 1.000E-05

Solver to be used (CHSOLVER): LU

Newton-Raphson control parameters:
Maximum number of Newton-Raphson iterations (ITMAX) = 40
Maximum number of interval halvings
if Newton-Raphson encounters errors (IRESETMAX) = 40
Interval frequency for updating Jacobian (IJACINPUT) = 1
```

Information Only

Scaling of matrix to be done before solution (LSCALE) = F
 Pressure scaling factor (P_SCALE) = 1.000E+07
 Variable switching allowed (LVARSWTCH) = F
 Upstream weighting update frequency for relative permeabilities (IUPRPFLAG) = 40
 Upstream weighting update frequency for mass fractions (IUPMFFLAG) = 40
 Timestep reduction factor if error occurs (DELTFACTOR) = 5.000E-01
 Transmissivity averaging method (ITRAVE) = 1
 Mass fraction averaging method (IMFRAVE) = 0

Jacobian reevaluation control parameters:
 Number of time step reductions allowed before Jacobian starts to be reevaluated every IJACMINth iteration (IJACSWITCH) = 40
 New number of iterations allowed before Jacobian is reevaluated (IJACMIN) = 40
 Number of time steps IJACMIN is in effect after violation of IJACSWITCH (IJACRESE) = 40
 Upstream weighting update frequency for relative permeabilities while IJACMIN is in effect (IUPRPLOOSE) = 40
 Upstream weighting update frequency for dissolved gas while IJACMIN is in effect (IUPMFLOOSE) = 40

Relative change in variable for Jacobian element derivative calculations (DH):
 DH(1) = 1.000E-08
 DH(2) = 1.000E-08

Minimum variable change allowed for Jacobian element derivative calculations (HMIN):
 HMIN(1) = 1.000E-09
 HMIN(2) = 1.000E-02 Pa

Number of times to specify material grid (NMATTIMES) = 1

Material time number = 1 Starting at time = 0.000000E+00 s

Layer 1
 1
 1 1 1 1 1 1 1 1 1

Material type number and name of material:
 1 ROCK

Special material index numbers:
 Number of waste regions (NWST) = 0
 Initial waste matl index nos. (MAT_WASTEI) =
 Final waste matl index numbers (MAT_WASTE) =

Number of MAT_DRZ regions (NDRZ) = 0
 Material type index for DRZ before
 IC's are reset (MAT_DRZ) =
 Material type index for DRZ after
 IC's are reset (MAT_DRZNEW) =
 Number of material regions
 where IC's will be reset (NMATRESET) = 0
 Material type indexes of material regions
 where IC's will be reset (MATRESET) =
 Borehole matl index number (MAT_BOREHOLE) = 0

Initial Conditions reset parameters:
 Time when IC's are reset (TIMEICRESET) = 0.00000E+00 s
 Startup Initial Conditions will be used
 instead of Input IC's for the Cavities
 [0=No, 1=Yes] (ICWASTE) = 0
 Uniform Cavity Region
 Uniform Cavity Region

 Material properties:

XLAMDA = Brooks-Corey parameter "lambda,"
 for calculating relative permeability
 SBR = Residual brine saturation
 SGR = Residual gas saturation
 XKX = X-direction permeability, m²
 YKY = Y-direction permeability, m²
 ZKZ = Z-direction permeability, m²
 PORROCKMAT = Rock porosity
 CROCK = Rock compressibility, 1/Pa
 SBMIN = Min brine satn at which Pc will be
 computed using char curve params
 POMIN = Min brine pressure used to adjust cap
 pressure when variable model used, Pa
 PCMAX = Max Pc that can be used, Pa
 PCTA = Constant in threshold cap press (PCT) correlation, Pa
 PCTEXP = Exponent in PCT correlation:
 PCT = PCTA*PERMBX**PCTEXP
 KRP = Relative permeability model number
 KPC = Capillary pressure model number
 KPT = Threshold capillary pressure (PCT) flag:
 0 = PCT constant
 1 = PCT function of dynamic permeability

 I XLAMDA SBR SGR XKX YKY ZKZ PORREFROCK CROCK SBMIN POMIN PCMAX PCTA PCTEXP KRP KPC KPT

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1 7.00E-01 2.00E-01 0.00E+00 1.80E-11 1.80E-11 1.80E-11 1.00E-01 0.00E+00 2.00E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00 3 1 0
TOL = 1.0000E-02
SOCEFFMIN = 1.0000E-03

Fracture model will be used? (K FRACTURE): F

Klinkenberg effect will be included? (KLINK): F

Constants :
Gravity constant (GSTD) = 9.79000E+00 m/s²
Gas constant (R) = 8.31451E+00 J/(mol*K)

Reference conditions:
Reference temperature (TREF) = 3.00000E+02 K
Reference pressure (PREF) = 1.01325E+05 Pa

Brine salinity (SALT) = 2.9600E+01 wt %
Brine density at ref. conditions (DENOSC) = 1.2300E+03 kg/m³
Gas-free (=0) or gas-sat'd brine (=1) (KGSAT) = 0
Dissolved gas (=1) or no dissolved gas (=0) (IDGAS) = 0
Brine compressibility (BRCOMP) = 2.5000E-10 1/Pa
Salt Molecular Weight (WMSALT) = 5.8442E-02 kg/mol
Water Molecular Weight (WMSALT) = 1.8015E-02 kg/mol

Brine viscosity (VISO) = 1.8000E-03 Pa*s
Gas viscosity (VISG) = 8.9200E-06 Pa*s

Flag for calculating gas density (INTERPDENG):
INTERPDENG = 1: Interpolate from table with RKS EOS.

Gas parameters:
Gas mole fraction (YGAS)
H2: 1.000E+00 CO2: 0.000E+00
CH4: 0.000E+00 N2: 0.000E+00
H2S: 0.000E+00 O2: 0.000E+00
Gas component molecular weights (WMGAS) kg/mol
H2: 2.016E-03 CO2: 4.401E-02
CH4: 1.604E-02 N2: 2.801E-02
H2S: 3.408E-02 O2: 3.200E-02
Number of gases actually used (NGAS) = 1
Gas number used if NGAS=1;
(1=H2, 2=CO2, 3=CH4, 4=N2
5=H2S, 6=O2) (NGAS1) = 1

Additional RKS EOS Gas parameters:
Gas component Critical Temperatures (TC) K
H2: 4.360E+01 CO2: 3.041E+02
CH4: 1.906E+02 N2: 1.262E+02
H2S: 3.736E+02 O2: 1.548E+02

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Gas component Critical Pressures (PC) Pa
H2: 2.047E+06 CO2: 7.376E+06
CH4: 4.617E+06 N2: 3.394E+06
H2S: 9.007E+06 O2: 5.080E+06
Gas component Acentric Factors (ACEN)
H2: 0.000E+00 CO2: 2.310E-01
CH4: 1.000E-02 N2: 4.500E-02
H2S: 1.000E-01 O2: 1.900E-02

Additional RKS EOS Gas parameters:
H2 Special Critical Temperatures (TCH2) K
H2: 4.360E+01
H2 Special Critical Pressures (PCH2) Pa
H2: 2.047E+06
H2 Special Molecular Weight (WMH2) Pa
H2: 2.016E-03

Additional RKS EOS Constants:
OMEGAA Constant (OMEGAA) 4.275E-01
OMEGAB Constant (OMEGAB) 8.664E-02

Binary Interaction Parameters for RKS EOS:
H2 interaction with
H2: 0.000E+00 CO2: -3.426E-01
CH4: -2.220E-02 N2: 9.780E-02
H2S: 0.000E+00 O2: 0.000E+00
CO2 interaction with
H2: -3.426E-01 CO2: 0.000E+00
CH4: 9.330E-02 N2: -3.150E-02
H2S: 9.890E-02 O2: 0.000E+00
CH4 interaction with
H2: -2.220E-02 CO2: 9.330E-02
CH4: 0.000E+00 N2: 2.780E-02
H2S: 8.500E-02 O2: 0.000E+00
N2 interaction with
H2: 9.780E-02 CO2: -3.150E-02
CH4: 2.780E-02 N2: 0.000E+00
H2S: 1.696E-01 O2: -7.800E-03
H2S interaction with
H2: 0.000E+00 CO2: 9.890E-02
CH4: 8.500E-02 N2: 1.696E-01
H2S: 0.000E+00 O2: 0.000E+00
O2 interaction with
H2: 0.000E+00 CO2: 0.000E+00
CH4: 0.000E+00 N2: -7.800E-03
H2S: 0.000E+00 O2: 0.000E+00

Gas generation model (IGASVAR) = 1
Original model: Zeroth-order corrosion & biodegradation.

Information Only

Intrinsic reaction rate constants? (LINTRIN): F

Reaction rate constants (RK):

Corrosion reaction rate constant = 0.000000E+00 mol Fe/(s*m³)
Biodegradation reaction rate constant = 0.000000E+00 mol cell/(s*m³)

Factor for humid reaction rate constants (HF):

Corrosion reaction = 1.000000E+00
Biodegradation reaction = 1.000000E+00

MgO hydration reaction rate constants:

Inundated reaction (BRUCITEI) = 0.000000E+00 mol MgO/(s*m³)
Humid reaction (BRUCITEH) = 0.000000E+00 mol MgO/(s*m³)

Saturation cutoff value (SOCMIN): 0.000000E+00

Stoichiometric coeff's for Rxn 1:

H2 coefficient = 0.000000E+00
H2O coefficient = 0.000000E+00
Fe coefficient = 0.000000E+00
Bio coefficient = 0.000000E+00
Fe(OH)2 coefficient = 0.000000E+00
FeS coefficient = 0.000000E+00
MgO coefficient = 0.000000E+00
Mg(OH)2 coefficient = 0.000000E+00
MgCO3 coefficient = 0.000000E+00

Stoichiometric coeff's for Rxn 2:

H2 coefficient = 0.000000E+00
H2O coefficient = 0.000000E+00
Fe coefficient = 0.000000E+00
Bio coefficient = 0.000000E+00
Fe(OH)2 coefficient = 0.000000E+00
FeS coefficient = 0.000000E+00
MgO coefficient = 0.000000E+00
Mg(OH)2 coefficient = 0.000000E+00
MgCO3 coefficient = 0.000000E+00

Stoichiometric coeff's for Rxn 3:

H2 coefficient = 0.000000E+00
H2O coefficient = 0.000000E+00
Fe coefficient = 0.000000E+00
Bio coefficient = 0.000000E+00
Fe(OH)2 coefficient = 0.000000E+00
FeS coefficient = 0.000000E+00
MgO coefficient = 0.000000E+00
Mg(OH)2 coefficient = 0.000000E+00
MgCO3 coefficient = 0.000000E+00

Stoichiometric coeff's for Rxn 4:

Information Only

H2 coefficient = 0.000000E+00
H2O coefficient = 0.000000E+00
Fe coefficient = 0.000000E+00
Bio coefficient = 0.000000E+00
Fe(OH)2 coefficient = 0.000000E+00
FeS coefficient = 0.000000E+00
MgO coefficient = 0.000000E+00
Mg(OH)2 coefficient = 0.000000E+00
MgCO3 coefficient = 0.000000E+00

Stoichiometric coeff's for Rxn 5:

H2 coefficient = 0.000000E+00
H2O coefficient = 0.000000E+00
Fe coefficient = 0.000000E+00
Bio coefficient = 0.000000E+00
Fe(OH)2 coefficient = 0.000000E+00
FeS coefficient = 0.000000E+00
MgO coefficient = 0.000000E+00
Mg(OH)2 coefficient = 0.000000E+00
MgCO3 coefficient = 0.000000E+00

Stoichiometric coeff's for Rxn 6:

H2 coefficient = 0.000000E+00
H2O coefficient = 0.000000E+00
Fe coefficient = 0.000000E+00
Bio coefficient = 0.000000E+00
Fe(OH)2 coefficient = 0.000000E+00
FeS coefficient = 0.000000E+00
MgO coefficient = 0.000000E+00
Mg(OH)2 coefficient = 0.000000E+00
MgCO3 coefficient = 0.000000E+00

Stoichiometric coeff's for Rxn 7:

H2 coefficient = 0.000000E+00
H2O coefficient = 0.000000E+00
Fe coefficient = 0.000000E+00
Bio coefficient = 0.000000E+00
Fe(OH)2 coefficient = 0.000000E+00
FeS coefficient = 0.000000E+00
MgO coefficient = 0.000000E+00
Mg(OH)2 coefficient = 0.000000E+00
MgCO3 coefficient = 0.000000E+00

Wicking term (SATWICK) = 0.000000E+00
Humid rates to be smoothed? (LARXN) = F
Concentration rates to be smoothed? (LARXN2) = F
Humid rate smoothing factor (ALPHARXN) = 5.000000E+01

Molecular weights (WM):

H2: 2.0159E-03 kg/mol
H2O: 1.8015E-02 kg/mol

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Fe: 5.5847E-02 kg/mol
Bio: 2.7023E-02 kg/mol

Molecular weights (WM):
Fe(OH)2: 8.9862E-02 kg/mol
FeS: 8.7900E-02 kg/mol
MgO: 4.0304E-02 kg/mol
Mg(OH)2: 5.8320E-02 kg/mol
MgCO3: 8.4314E-02 kg/mol

Densities (DEN(1-4)):
Fe: 7.8700E+03 kg/m3
Fe(OH)2: 3.4000E+03 kg/m3
FeS: 4.7000E+03 kg/m3
Bio: 1.1000E+03 kg/m3

Densities (DEN(5-8)):
MgO: 3.6000E+03 kg/m3
Mg(OH)2: 2.3700E+03 kg/m3
MgCO3: 3.0500E+03 kg/m3
SALT: 2.1700E+03 kg/m3

Will creep closure be used (CLOSURE): F

Radionuclide decay will be calculated? (LRADDK): F

Solute transport will be calculated? (LTRANS): F
Solute radiolysis will be calculated? (LRADLSIS): F

Decay has been turned off (LRADDK changed to F),
since neither transport nor radiolysis is on:
(LTRANS = LRADLSIS = F)

Will gas component transport be calculated? (LRXGAST): F

Total mesh volume = 8.654445E+08 m³
Total waste volume = 0.000000E+00 m³
Density of initial brine at ref cond = 1.230000E+03 kg/m³
Density of initial gas at ref cond = 8.184076E-02 kg/m³
Mass fraction of initial brine in brine phase at ref. cond = 1.000000E+00
Mass fraction of initial gas in brine phase at ref. cond = 0.000000E+00
Original brine in place at ref. cond = 8.675888E+07 m³
Original brine in place = 1.067134E+11 kg
Original gas in place at ref. cond = 8.073260E+01 m³
Original gas in place = 6.607218E+00 kg

Number of element variables printed to ASCII output = 6

Information Only

Number of global variables printed to ASCII output = 10

No.	CAMCON Vbl Name	Element Variable Description	Units Label	Factor	Units Conv
1	PRESBRIN	Brine pressure	Pa	1.000000E+00	
2	PRESGAS	Gas pressure	Pa	1.000000E+00	
7	RELPERMB	Relative permeability to brine	dimensionless	1.000000E+00	
8	RELPERMG	Relative permeability to gas	dimensionless	1.000000E+00	
17	SATBRINE	Brine saturation	fraction void volume	1.000000E+00	
18	SATGAS	Gas saturation	fraction void volume	1.000000E+00	

No.	CAMCON Vbl Name	Global Variable Description	Units Label	Factor	Units Conv
1	BRNMBCUM	Cumulative brine mass balance	dimensionless	1.000000E+00	
2	GASMBCUM	Cumulative gas mass balance	dimensionless	1.000000E+00	
3	BRNMBMAX	Maximum brine mass balance	dimensionless	1.000000E+00	
4	GASMBMAX	Maximum gas mass balance	dimensionless	1.000000E+00	
5	IBRNMBMX	I-index, location of maximum brine mass balance	dimensionless	1.000000E+00	
6	JBRNMBMX	J-index, location of maximum brine mass balance	dimensionless	1.000000E+00	
7	KBRNMBMX	K-index, location of maximum brine mass balance	dimensionless	1.000000E+00	
8	IGASMBMX	I-index, location of maximum gas mass balance	dimensionless	1.000000E+00	
9	JGASMBMX	J-index, location of maximum gas mass balance	dimensionless	1.000000E+00	
10	KGASMBMX	K-index, location of maximum gas mass balance	dimensionless	1.000000E+00	

Grid block dimensions

Grid block dimensions in X-direction

Layer	m									
1	1.00000E-02	1.30000E-02	1.69000E-02	2.19700E-02	2.85610E-02	3.71293E-02	4.82681E-02	6.27485E-02	8.15730E-02	1.06045E-01
	1.37858E-01	1.79216E-01	2.32981E-01	3.02875E-01	3.93737E-01	5.11859E-01	6.65416E-01	8.65041E-01	1.12455E+00	1.46192E+00
	1.90050E+00	2.47064E+00	3.21184E+00	4.17539E+00	5.42800E+00	7.05640E+00	9.17332E+00	1.19253E+01	1.55029E+01	2.01538E+01
	2.61999E+01	3.40599E+01	4.42779E+01	5.75612E+01	7.48296E+01	9.72785E+01	1.26462E+02	1.64401E+02	2.13721E+02	2.77837E+02
	3.61188E+02	4.69544E+02	6.10408E+02	7.93530E+02	1.03159E+03	1.34107E+03	1.74338E+03	2.26640E+03	2.94632E+03	3.83022E+03

Grid block dimensions in Y-direction

Layer	m									
1	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

Grid block dimensions in Z-direction

Layer	m									
1	3.14159E-02	1.03673E-01	1.97606E-01	3.19720E-01	4.78468E-01	6.84840E-01	9.53124E-01	1.30189E+00	1.75529E+00	2.34471E+00
	3.11096E+00	4.10708E+00	5.40203E+00	7.08547E+00	9.27394E+00	1.21190E+01	1.58175E+01	2.06256E+01	2.68760E+01	3.50017E+01
	4.55650E+01	5.92974E+01	7.71494E+01	1.00357E+02	1.30527E+02	1.69748E+02	2.20735E+02	2.87018E+02	3.73187E+02	4.85206E+02

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6.30830E+02	8.20142E+02	1.06625E+03	1.38618E+03	1.80210E+03	2.34280E+03	3.04570E+03	3.95947E+03	5.14737E+03	6.69165E+03
8.69920E+03	1.13090E+04	1.47018E+04	1.91124E+04	2.48462E+04	3.23001E+04	4.19902E+04	5.45873E+04	7.09635E+04	9.22527E+04

Grid Block Volumes

m^3

Layer	1																		
1	3.14159E-04	1.34774E-03	3.33954E-03	7.02425E-03	1.36655E-02	2.54276E-02	4.60054E-02	8.16918E-02	1.43185E-01	2.48645E-01									
	4.28872E-01	7.36054E-01	1.25857E+00	2.14601E+00	3.65150E+00	6.20319E+00	1.05252E+01	1.78419E+01	3.02235E+01	5.11696E+01									
	8.65961E+01	1.46503E+02	2.47791E+02	4.19029E+02	7.08501E+02	1.19781E+03	2.02487E+03	3.42279E+03	5.78548E+03	9.77873E+03									
	1.65277E+04	2.79339E+04	4.72111E+04	7.97904E+04	1.34851E+05	2.27903E+05	3.85165E+05	6.50939E+05	1.10010E+06	1.85919E+06									
	3.14205E+06	5.31009E+06	8.97409E+06	1.51663E+07	2.56310E+07	4.33166E+07	7.32050E+07	1.23717E+08	2.09081E+08	3.53348E+08									

 Elapsed Time
 0.000000E+00 sec = 0.000000E+00 day = 0.000000E+00 yr
 DELT
 0.000000E+00 sec = 0.000000E+00 day = 0.000000E+00 yr
 Time Step Number = 0
 Total Newton-Raphson Iterations = 0
 Avg Newton-Raphson Iterations/Time Step = 0.000
 CPU Time (this time step) = 0.00 sec = 0.00000 hr
 CPU Time (total for run) = 0.00 sec = 0.00000 hr

Cumulative Mass Balance
 Brine: 0.000000E+00
 Gas: 0.000000E+00

Maximum Relative Mass Balance (Current Time Step)
 Brine: 0.000000E+00 at (I,J,K) = 0 0 0
 Gas: 0.000000E+00 at (I,J,K) = 0 0 0

 Brine pressure Pa
 Layer 1
 1 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07
 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07
 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07
 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07

 Gas pressure Pa
 Layer 1
 1 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07
 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07
 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07
 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07 1.00000E+07

 Relative permeability to brine dimensionless
 Layer 1
 1 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00
 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00 1.00000E+00

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1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

Relative permeability to gas dimensionless
Layer 1

1	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24
	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24
	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24
	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24
	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24

Brine saturation fraction void volume
Layer 1

1	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

Gas saturation fraction void volume
Layer 1

1	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08
	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08
	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08
	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08
	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08

Date: 02/14/07 Time: 09:14:28 CPU Time: 0 0: 0: 0.03 (0.03 sec) ASCII
Time Step No. = 0 Elapsed Time = 0.000000E+00 days
Date: 02/14/07 Time: 09:14:28 CPU Time: 0 0: 0: 0.03 (0.03 sec) Binary

Elapsed Time
1.000000E+01 sec = 1.157407E-04 day = 3.168876E-07 yr
DELT
1.000000E+01 sec = 1.157407E-04 day = 3.168876E-07 yr
Time Step Number = 1
Total Newton-Raphson Iterations = 3
Avg Newton-Raphson Iterations/Time Step = 3.000
CPU Time (this time step) = 0.03 sec = 0.00001 hr
CPU Time (total for run) = 0.03 sec = 0.00001 hr

Cumulative Mass Balance
Brine: -2.556405E-19
Gas: -4.876697E-20

Maximum Relative Mass Balance (Current Time Step)

Brine: 7.403527E-12 at (I,J,K) = 1 1 1
 Gas: 9.317929E-15 at (I,J,K) = 1 1 1

Brine pressure		Pa								
Layer 1										
1	8.44724E+06	8.66917E+06	8.77466E+06	8.85180E+06	8.91602E+06	8.97299E+06	9.02543E+06	9.07485E+06	9.12220E+06	9.16805E+06
	9.21282E+06	9.25680E+06	9.30017E+06	9.34309E+06	9.38565E+06	9.42794E+06	9.47000E+06	9.51185E+06	9.55349E+06	9.59491E+06
	9.63605E+06	9.67680E+06	9.71703E+06	9.75650E+06	9.79488E+06	9.83173E+06	9.86648E+06	9.89841E+06	9.92673E+06	9.95063E+06
	9.96952E+06	9.98318E+06	9.99196E+06	9.99680E+06	9.99899E+06	9.99976E+06	9.99996E+06	1.00000E+07	1.00000E+07	1.00000E+07
	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07

Gas pressure		Pa								
Layer 1										
1	8.44724E+06	8.66917E+06	8.77466E+06	8.85180E+06	8.91602E+06	8.97299E+06	9.02543E+06	9.07485E+06	9.12220E+06	9.16805E+06
	9.21282E+06	9.25680E+06	9.30017E+06	9.34309E+06	9.38565E+06	9.42794E+06	9.47000E+06	9.51185E+06	9.55349E+06	9.59491E+06
	9.63605E+06	9.67680E+06	9.71703E+06	9.75650E+06	9.79488E+06	9.83173E+06	9.86648E+06	9.89841E+06	9.92673E+06	9.95063E+06
	9.96952E+06	9.98318E+06	9.99196E+06	9.99680E+06	9.99899E+06	9.99976E+06	9.99996E+06	1.00000E+07	1.00000E+07	1.00000E+07
	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07	1.00000E+07

Relative permeability to brine		dimensionless								
Layer 1										
1	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

Relative permeability to gas		dimensionless								
Layer 1										
1	1.21748E-23	1.13059E-23	1.09225E-23	1.06533E-23	1.04361E-23	1.02484E-23	1.00798E-23	9.92423E-24	9.77834E-24	9.63981E-24
	9.50714E-24	9.37926E-24	9.25542E-24	9.13508E-24	9.01783E-24	8.90338E-24	8.79152E-24	8.68212E-24	8.57510E-24	8.47045E-24
	8.36824E-24	8.26863E-24	8.17191E-24	8.07852E-24	7.98909E-24	7.90449E-24	7.82585E-24	7.75453E-24	7.69204E-24	7.63981E-24
	7.59888E-24	7.56948E-24	7.55066E-24	7.54031E-24	7.53564E-24	7.53400E-24	7.53357E-24	7.53349E-24	7.53348E-24	7.53348E-24
	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24	7.53348E-24

Brine saturation		fraction void volume								
Layer 1										
1	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

Gas saturation		fraction void volume								
Layer 1										
1	1.17351E-08	1.14491E-08	1.13181E-08	1.12244E-08	1.11476E-08	1.10804E-08	1.10192E-08	1.09623E-08	1.09083E-08	1.08565E-08
	1.08065E-08	1.07578E-08	1.07103E-08	1.06636E-08	1.06178E-08	1.05727E-08	1.05282E-08	1.04844E-08	1.04411E-08	1.03985E-08
	1.03565E-08	1.03152E-08	1.02749E-08	1.02356E-08	1.01977E-08	1.01615E-08	1.01277E-08	1.00969E-08	1.00697E-08	1.00468E-08
	1.00289E-08	1.00159E-08	1.00076E-08	1.00030E-08	1.00010E-08	1.00002E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08
	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08	1.00000E-08

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Date: 02/14/07 Time: 09:14:28 CPU Time: 0 0: 0: 0.14 (0.14 sec) ASCII
 Time Step No. = 41 Elapsed Time = 1.140010E-01 days
 Date: 02/14/07 Time: 09:14:28 CPU Time: 0 0: 0: 0.14 (0.14 sec) Binary

```
*****
Elapsed Time
1.000000E+04 sec = 1.157407E-01 day = 3.168876E-04 yr
DELT
1.503141E+02 sec = 1.739746E-03 day = 4.763268E-06 yr
Time Step Number = 42
Total Newton-Raphson Iterations = 87
Avg Newton-Raphson Iterations/Time Step = 2.071
CPU Time (this time step) = 0.00 sec = 0.00000 hr
CPU Time (total for run) = 0.14 sec = 0.00004 hr
*****
```

Cumulative Mass Balance
 Brine: -1.710337E-17
 Gas: -9.620979E-17

Maximum Relative Mass Balance (Current Time Step)
 Brine: -3.207471E-10 at (I,J,K) = 1 1 1
 Gas: -2.971335E-12 at (I,J,K) = 1 1 1

Brine pressure Pa

Layer 1

1	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06
	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06
	9.94280E+06	9.94280E+06	9.94281E+06	9.94281E+06	9.94281E+06	9.94281E+06	9.94281E+06	9.94282E+06	9.94282E+06	9.94284E+06
	9.94286E+06	9.94290E+06	9.94297E+06	9.94308E+06	9.94327E+06	9.94359E+06	9.94413E+06	9.94503E+06	9.94651E+06	9.94891E+06
	9.95271E+06	9.95844E+06	9.96648E+06	9.97645E+06	9.98665E+06	9.99446E+06	9.99848E+06	9.99975E+06	9.99998E+06	1.00000E+07

Gas pressure Pa

Layer 1

1	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06
	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06	9.94280E+06
	9.94280E+06	9.94280E+06	9.94281E+06	9.94281E+06	9.94281E+06	9.94281E+06	9.94281E+06	9.94282E+06	9.94282E+06	9.94284E+06
	9.94286E+06	9.94290E+06	9.94297E+06	9.94308E+06	9.94327E+06	9.94359E+06	9.94413E+06	9.94503E+06	9.94651E+06	9.94891E+06
	9.95271E+06	9.95844E+06	9.96648E+06	9.97645E+06	9.98665E+06	9.99446E+06	9.99848E+06	9.99975E+06	9.99998E+06	1.00000E+07

Relative permeability to brine dimensionless

Layer 1

1	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

Relative permeability to gas dimensionless

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Layer	1									
1	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24
	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24	7.65686E-24
	7.65686E-24	7.65686E-24	7.65685E-24	7.65685E-24	7.65685E-24	7.65685E-24	7.65684E-24	7.65683E-24	7.65681E-24	7.65678E-24
	7.65673E-24	7.65664E-24	7.65650E-24	7.65625E-24	7.65583E-24	7.65514E-24	7.65396E-24	7.65201E-24	7.64879E-24	7.64356E-24
	7.63530E-24	7.62285E-24	7.60545E-24	7.58394E-24	7.56204E-24	7.54531E-24	7.53672E-24	7.53402E-24	7.53353E-24	7.53348E-24

Brine saturation	fraction void volume									
Layer	1									
1	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00
	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00	1.00000E+00

Gas saturation	fraction void volume									
Layer	1									
1	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08
	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08
	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08	1.00543E-08
	1.00542E-08	1.00542E-08	1.00541E-08	1.00540E-08	1.00538E-08	1.00535E-08	1.00530E-08	1.00522E-08	1.00508E-08	1.00485E-08
	1.00449E-08	1.00394E-08	1.00317E-08	1.00223E-08	1.00126E-08	1.00052E-08	1.00014E-08	1.00002E-08	1.00000E-08	1.00000E-08

Date: 02/14/07 Time: 09:14:28 CPU Time: 0 0: 0: 0.14 (0.14 sec) ASCII

Time Step No. = 42 Elapsed Time = 1.157407E-01 days
Date: 02/14/07 Time: 09:14:28 CPU Time: 0 0: 0: 0.14 (0.14 sec) Binary

* End of BRAGFLO Version: 6.0 Revised: 01/15/07 *
* Completed: 02/14/07 at 09:14:28 Run on: TDN - ALPHA AXP OpenVMS V8.2 *

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11.4 Appendix D: Functionality Not Tested

For BRAGFLO Version 6.02, the following features will not be tested at this time because they will not be used as part of the WIPP compliance calculations:

- 1) Radionuclide transport. BRAGFLO is no longer used for transport calculations. The nuclide transport code NUTS (Gilkey, 2006b) has been developed for use in WIPP compliance calculations.
- 2) Gas dissolution. Dissolution of gas in brine may be simulated using either Henry's law for a single gas or bubble point tracking. The brine may be specified as initially gas-free or fully gas-saturated. This feature will not be used in the WIPP compliance calculations.
- 3) Numerous options are available for inputting the description of the mesh. Because only a couple of these are regularly used, the only ones that will be tested now will be those that will be used in the WIPP compliance calculations and in test cases for testing other features. Certain little-used options for inputting the mesh are not tested. For parameter IDZFLAG, which specifies how Δz is input, options 2, 3, and 4 are not tested. (IDZFLAG options that are tested include 0 and 1.) For parameter IDEPTHFLAG, which specifies how the grid block elevations are input, options 1, 2, 3, 4, 5, 6, and -1 are not tested. (IDEPTHFLAG options that are tested include 0, -2, -3, and 7.) All available options for parameters IDXFLAG and IDYFLAG, which specify how Δx and Δy are input, are tested.
- 4) Reaction path gas generation model. This model has been neither fully developed nor implemented and is not available for the WIPP compliance calculations.
- 5) Multicomponent gas transport. Without a source of multiple gas components (*i. e.*, the reaction path model), there is little point in tracking multiple gas components; this will not be done in the WIPP compliance calculations.
- 6) Three-dimensional calculations. Although BRAGFLO is a fully 3-D code, time and resource constraints currently preclude doing any 3-D calculations for WIPP compliance.
- 7) Three earlier creep closure surfaces. Creep closure data used for preliminary performance assessments have been retained in BRAGFLO to enable these calculations to be reproduced.
- 8) Alternative equation solvers. In addition to the original LU solver, BRAGFLO also has a Linpack LU solver and a point-SOR iterative solver. The Linpack LU solver offers no advantages over the original LU solver, except for certain debugging capabilities. Because it has been coded very inefficiently, nearly doubling the memory required by BRAGFLO when it is used, it has been disabled in version 4.00. The point-SOR solver is inadequate for use in the compliance calculations. An iterative multigrid solver was installed in BRAGFLO and was not successful in solving WIPP compliance calculations.

- 9) Capillary pressure treatment. An option in BRAGFLO allows the maximum capillary pressure to vary automatically. This model is experimental, has not been well-tested, and will not be used in the WIPP compliance calculations.
- 10) Numerical control parameters. The experience gained over several years of using BRAGFLO (WIPP PA 1992a) has shown what values of the various control parameters will enable BRAGFLO to run successfully. Test cases show that these values are being used as intended in the code.
- 11) Multicomponent gas properties. BRAGFLO is capable of calculating gas properties using either the ideal gas law or the Redlich-Kwong-Soave equation of state. Properties can be calculated for either pure gases or for mixtures of any of the following six gases: H₂, CO₂, CH₄, N₂, O₂, and H₂S. Because the WIPP compliance calculations will use pure hydrogen and the Redlich-Kwong-Soave equation of state, the calculation of mixture properties and use of the ideal gas law are not tested.
- 12) Restart capability. This feature is used only for debugging and will not be used for the WIPP compliance calculations.
- 13) Relative permeability and capillary pressure models. BRAGFLO currently has 12 relative permeability and capillary pressure models available. Only four of these are expected to be used for the WIPP compliance calculations, KRP = 1 (van Genuchten-Parker model) and 4 (modified Brooks-Corey model), KRP = 11 (linear model see Subsection 4.9), KRP=12 (second modified Brooks-Corey model, see Subsection 4.9) ; these will be tested for software QA. Three others (KRP = 5, 9, and 10) are used in QA testing, so these will also be tested. None of the other five models will be tested at this time.
- 14) Radiolysis (the radiolytic breakdown of water into hydrogen and oxygen) may be calculated. The initial inventory of radionuclides in the waste is input, and BRAGFLO calculates the decay of this inventory over time, along with the amount of water that is decomposed and the amount of gas generated. This feature will not be used in the WIPP compliance calculations and will not be tested now.
- 15) Certain little-used options for inputting the mesh are not tested. For parameter IDZFLAG, which specifies how Δz is input, options 2, 3, and 4 are not tested. (IDZFLAG options that are tested include 0 and 1.) For parameter IDEPTHFLAG, which specifies how the grid block elevations are input, options 1, 2, 3, 4, 5, 6, and -1 are not tested. (IDEPHFLAG options that are tested include 0, -2, -3, and 7.) All available options for parameters IDXFLAG and IDYFLAG, which specify how Δx and Δy are input, are tested.
- 16) Permeability versus porosity models for closure materials. Currently there are two models which are included, but are not used in the WIPP compliance calculations and will not be tested.
- 17) A fracture model which effectively holds the pressure constant during fracturing is included, but is not used in the WIPP compliance calculations and will not be tested.

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- 18) The option to limit the increase in porosity during a calculation is included, but is not used in the WIPP compliance calculations and will not be tested.

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