
**Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant**

Appendix BRAGFLO



**United States Department of Energy
Waste Isolation Pilot Plant**

**Carlsbad Area Office
Carlsbad, New Mexico**

WIPP PA User's Manual for BRAGFLO



ERRATA

All references to rock compressibility in the BRAGFLO appendix are synonymous with definitions of pore compressibility or formation compressibility.



WIPP PA

User's Manual

for

BRAGFLO, Version 4.00



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Acronyms

BRAGFLO.....	Brine And Gas FLOW
CCA	Compliance Certification Application
DEC	Digital Electronic Corporation
DOE.....	U.S. Department of Energy
DRZ	Disturbed Rock Zone
PA	Performance Assessment
PREBRAG.....	Preprocessor for BRAGFLO
QA.....	Quality Assurance
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, as used in the 1996 WIPP PA calculation. As such, it describes the code's purpose and function, 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 Number: 4.00 2/9/96
Platform: FORTRAN 77 for OpenVMS AXP, ver 6.1, on DEC Alpha

The previous version of BRAGFLO was Version 3.62ZO, 9/8/95.

The previous version of the User's Manual was WPO # 24179, Version 1.00, dated 10/3/95.

1.2 Points of Contact

1.2.1 Code Sponsor

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2.0 FUNCTIONAL REQUIREMENTS

- 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, and the concentration of biodegradables.
- R.6 Parameters are input that control 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. Only two solvers are currently available, the original LU decomposition solver and the point successive overrelaxation (SOR) solver, and only the original LU decomposition solver will be used 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 permeabilities, reference condition porosities, and compressibilities. Also specified are the relative permeability and capillary pressure model to be used for each material.
- R.8 Relative permeabilities and capillary pressure are calculated for each material using one of several available models. The compliance calculations will use either a modified Brooks-Corey model or a van Genuchten/Parker model. Some of the QA 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.
- 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. The WIPP compliance calculations will use a single pure gas, H_2 .
- R.13 Two chemical reactions are modeled in BRAGFLO: anoxic corrosion of iron and microbial degradation of cellulose. Both of these reactions produce gas (H_2) and consume brine according to specified stoichiometry. Reaction rates are specified for brine-inundated conditions and for humid conditions.
- 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. BRAGFLO version 4.00 uses a "porosity surface" for the waste that is similar to that used in version 3.62ZO, but based on improved models of creep closure and new results from SANCHO simulations.
- 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 that are completed 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 downhole pressure wells.
- R.17 BRAGFLO simulates flow through heterogeneous as well as homogeneous porous media.

3.0 REQUIRED USER TRAINING AND/OR BACKGROUND

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

- Open VMS
- Digital Command Language
- Sandia's CAMDAT database.

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, the DOE uses the two-phase flow code BRAGFLO to simulate gas and brine flow as well as to incorporate the effects of disposal room consolidation and closure, gas generation, and interbed fracture 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).

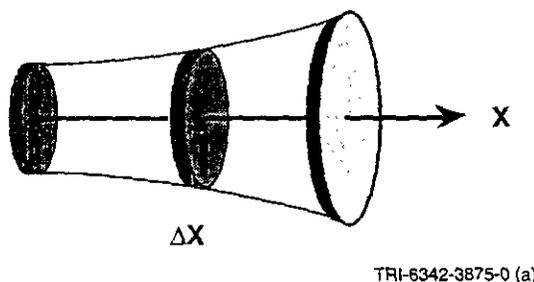


Figure 1. One dimensional reservoir with area-normal-to-flow as a function of x .

We 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 ; $\text{Area} = A(x)$. 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]
- $\rho =$ fluid density [m/l^3]
- $q =$ mass flow rate [m/t]
- $v =$ flow velocity [l/t]
- $\phi =$ porosity [pore volume/bulk volume]
- $A =$ normal cross-section area [l^2]

where the generic units are:

- $m =$ mass
- $l =$ length
- $t =$ time.

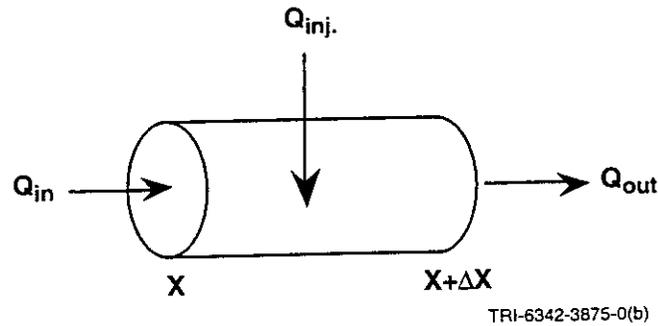


Figure 2. Element of volume of length Δx .

The mass rate and volume rate of flow are related by $q = \rho Q$.

The sign convention on Q_{inj} is

- $Q_{inj} > 0$, injection,
- $Q_{inj} < 0$, production.

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

Mass balance requires that

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

where

$$q_{inj} = \text{mass injection rate/unit volume.}$$

Now

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

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

and

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

The mass balance is then

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

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

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

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

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

4.2 Darcy's Law

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

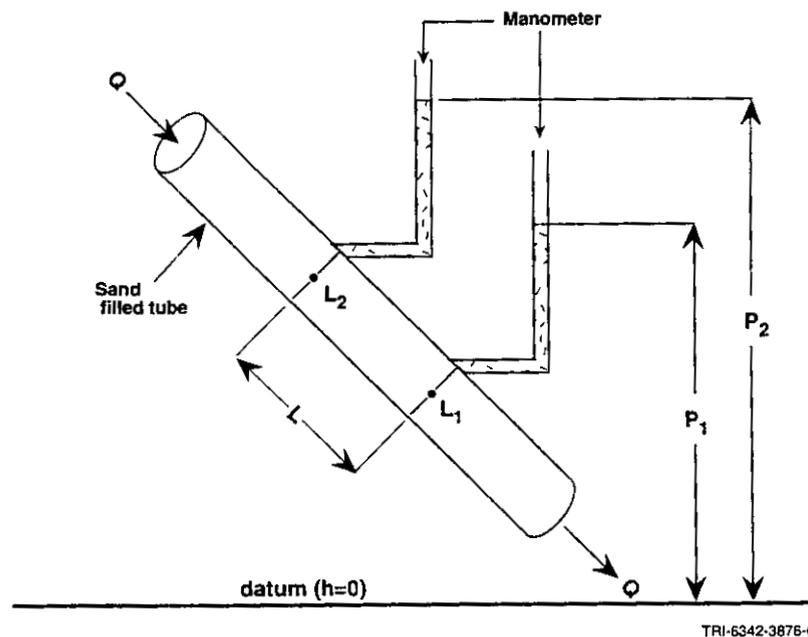


Figure 3. Experiment for illustration of Darcy's Law.

In Figure 3, Q is volume flow rate [l^3/t] and positive distance is measured from L_2 to L_1 . Potential is measured as

$$\Phi = p + \rho gh$$

where depth, h, is measured positive upward from a reference datum and gravity acts downward. For example, a fluid in gravity equilibrium, $\Phi = \text{constant}$, exhibits a pressure increase with decrease in depth.

Darcy observed that

$$Q > 0, \text{ if } \Phi_2 > \Phi_1$$

$$Q < 0, \text{ if } \Phi_2 < \Phi_1$$

$$Q = 0, \text{ if } \Phi_2 = \Phi_1.$$

The implication is that flow is in the direction of decreasing potential. Next, Darcy observed that if $\Phi_2 - \Phi_1$ is doubled, Q is doubled. Thus

$$Q \approx \Phi_2 - \Phi_1 \text{ (}\approx \text{ is read proportional to)}$$

Also, if L is doubled, Q is halved. Thus

$$Q \approx \frac{\Phi_2 - \Phi_1}{L}$$

If cross-sectional area is doubled, Q is doubled. Thus

$$Q \approx \frac{A(\Phi_2 - \Phi_1)}{L}$$

If the fluid is changed (different viscosity), then

$$Q \approx \frac{A(\Phi_2 - \Phi_1)}{\mu L}$$

Finally,



$$Q = \frac{kA(\Phi_2 - \Phi_1)}{\mu L}$$

where the constant of proportion, k, is called the absolute permeability of the media. The differ-

ential form of Darcy's Law is obtained when $L \rightarrow 0$,

$$Q = \frac{-kA \, d\Phi}{\mu \, dx}$$

The negative sign in Darcy's Law indicates flow is in the direction of decreasing potential.

The units used in BRAGFLO are

$$Q = \text{m}^3/\text{s}$$

$$A = \text{m}^2$$

$$\mu = \text{Pa}\cdot\text{s}$$

$$\frac{d\Phi}{dx} = \frac{\text{Pa}}{\text{m}}$$

The units for permeability are

$$k = \left[\frac{\text{m}^3}{\text{s}} \right] [\text{Pa}\cdot\text{s}] \left[\frac{1}{\text{m}^2} \right] \left[\frac{\text{m}}{\text{Pa}} \right] = \text{m}^2.$$

Velocity is given by

$$v = \frac{Q}{A} = -\frac{k \, d\Phi}{\mu \, dx}$$

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



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

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 m^3 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.

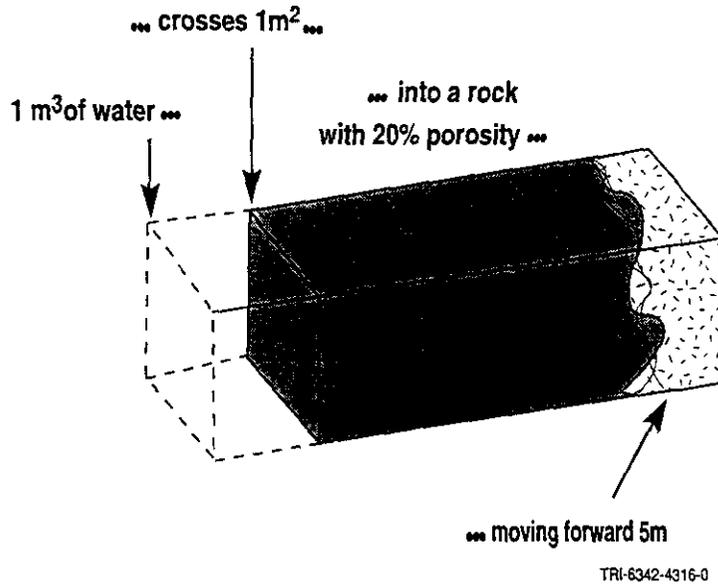


Figure 4. Bulk volume vs. Porous Media Displacement.

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 permeabilities 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.

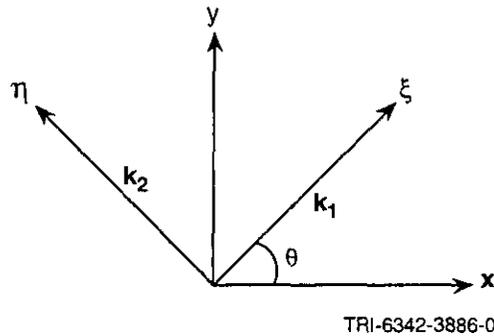


Figure 5. Permeability with anisotropic values k_1 and k_2 in direction ξ and η

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

$$x = \xi \cos \theta - \eta \sin \theta.$$

$$y = \xi \sin \theta + \eta \cos \theta.$$

If \hat{i}_ξ and \hat{i}_η represent the unit vectors in the ξ, η directions, respectively, then the Darcy velocity vector is

$$\hat{v} = -\frac{k_1}{\mu} \frac{\partial \Phi}{\partial \xi} \hat{i}_\xi - \frac{k_2}{\mu} \frac{\partial \Phi}{\partial \eta} \hat{i}_\eta.$$

The coordinate transformation maps the unit vectors into

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

and

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

The chain rule gives

$$\frac{\partial \Phi}{\partial \xi} = \cos \theta \frac{\partial \Phi}{\partial x} + \sin \theta \frac{\partial \Phi}{\partial y}$$

and

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

Then the Darcy velocity is

$$\hat{v} = \frac{-k_1}{\mu} \left(\cos\theta \frac{\partial\Phi}{\partial x} + \sin\theta \frac{\partial\Phi}{\partial y} \right) (\cos\theta \hat{i}_x + \sin\theta \hat{i}_y) + \frac{-k_2}{\mu} \left(-\sin\theta \frac{\partial\Phi}{\partial x} + \cos\theta \frac{\partial\Phi}{\partial y} \right) (-\sin\theta \hat{i}_x + \cos\theta \hat{i}_y).$$

The vector components of the Darcy velocity are

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

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

The dependence of the Darcy velocity components on pressure gradients in both x and y direction 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

$$v_x = \frac{-k_x}{\mu} \frac{\partial\Phi}{\partial x} \quad \text{and} \quad v_y = \frac{-k_y}{\mu} \frac{\partial\Phi}{\partial y}.$$

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



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

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

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

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

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

$$\frac{\partial}{\partial x} \left(\frac{\alpha \rho k_x}{\mu} \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\alpha \rho k_y}{\mu} \frac{\partial \Phi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\alpha \rho k_z}{\mu} \frac{\partial \Phi}{\partial z} \right) + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \Phi \rho)$$

4.4 Equation of State

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

$$\frac{\partial}{\partial x} \left(\frac{\alpha \rho k_x}{\mu} \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\alpha \rho k_y}{\mu} \frac{\partial \Phi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\alpha \rho k_z}{\mu} \frac{\partial \Phi}{\partial z} \right) + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \Phi \rho)$$

This equation has two dependent variables, pressure, p, and density, ρ . Independent variables are space (x, y, and 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:

$$\frac{d\rho}{d\rho} = c\rho,$$

where c is fluid compressibility.

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

$$\rho = \rho_0 \exp(c(p - p_0))$$

where ρ_0 is density at reference pressure p_0 . This is the equation BRAGFLO uses to evaluate brine density.

Recall

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$$

and if x is close to zero

$$e^x \cong 1 + x.$$

Therefore, if $c(p - p_0)$ is relatively small, then

$$\rho \cong \rho_0(1 + c(p - p_0)).$$

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

$$\rho = \rho(p, T)$$

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



$$\phi = \phi_0 \exp(c_r(p - p_0))$$

where ϕ_0 is the porosity at reference pressure p_0 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. Nonlinearity 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,

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

the material balance equation (PDE) requires:

initial conditions:

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

and

boundary conditions:

$$p(0,t) = g_0(t), \quad p(L,t) = g_L(t), \quad t \geq 0$$

or

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

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 $\frac{\partial p}{\partial x} = 0$ 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_0

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f^{(2)}(x_0)}{2!}(x - x_0)^2 + \dots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}$$

where ξ is the interval between x and x_0 . Thus

$$f(x) = p(x) + R_n(x, x_0)$$

or

$$f(x) - p(x) = R_n(x, x_0).$$

If $f^{(n+1)}$ is continuous on some interval $[a, b]$ containing x, x_0 , then $f^{(n+1)}$ is bounded,

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

and

$$|f(x) - p(x)| \leq C|x - x_0|^{n+1}.$$

Therefore, as $x \rightarrow x_0$, the error goes to zero like $(x - x_0)^{n+1}$. Consider the following derivative approximations. First order forward difference requires the Taylor formula:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + R_2(x, x_0)$$

Let $x = x_0 + h$, then



$$\left| \frac{f(x_0 + h) - f(x_0)}{h} - f'(x_0) \right| = \left| \frac{R_2(x, x_0)}{h} \right| \leq \frac{Ch^2}{h} = Ch.$$

The difference approximation

$$f'(x_0) \cong \frac{f(x_0 + h) - f(x_0)}{h}$$

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

Second order central approximation:

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{f^{(2)}(x_0)}{2!}h^2 + R_3(x_0, x_0 + h)$$
$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{f^{(2)}(x_0)}{2!}h^2 + R_3(x_0, x_0 - h)$$

where subtraction yields

$$f(x_0 + h) - f(x_0 - h) = 2hf'(x_0) + R_3(x_0, x_0 + h) - R_3(x_0, x_0 - h).$$

This is rearranged to give:

$$\frac{f(x_0 + h) - f(x_0 - h)}{2h} - f'(x_0) = \frac{R_3(x_0, x_0 + h) - R_3(x_0, x_0 - h)}{2h}$$

which produces the estimate

$$\left| \frac{f(x_0 + h) - f(x_0 - h)}{2h} - f'(x_0) \right| \leq \frac{Ch^3}{h} = Ch^2.$$

Therefore, the difference approximation $\frac{f(x_0 + h) - f(x_0 - h)}{h}$ is a second order approximation to $f'(x_0)$.

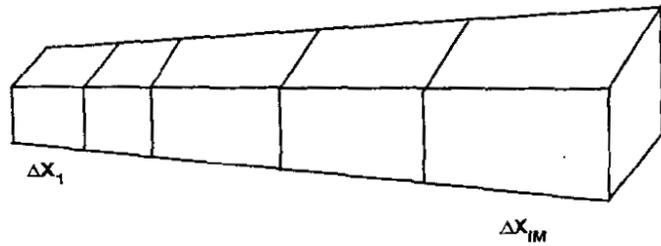
Consider discretization of the one-dimensional material balance equation:

$$\frac{\partial}{\partial x} \left(\frac{\alpha k \rho}{\mu} \frac{\partial p}{\partial x} \right) + \alpha q_{inj} = \frac{\partial}{\partial t} (\alpha \phi \rho),$$

where we assume the gradient of the depth is zero.

Space discretization requires the partition of the interval $[0, L]$ into IM subintervals with length Δx_i , $i=1, 2, \dots, IM$.

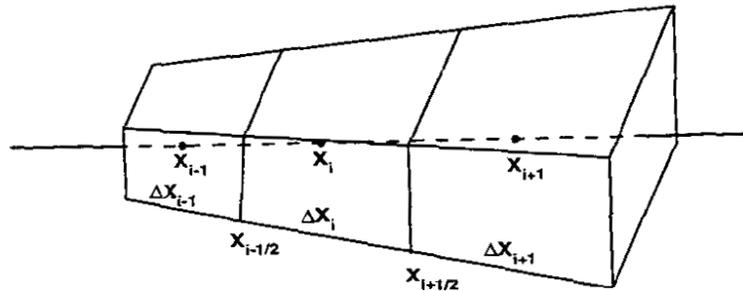




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Figure 6. Partition interval $[0, L]$ into IM subintervals.

Consider an arbitrary grid block i and its neighbors $i-1$, $i+1$ as shown in Figure 7.



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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,

$$x_{i-1/2} = x_{i-1} + \Delta x_{i-1/2}$$

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

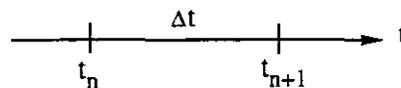
$$\frac{\partial}{\partial x} \left(\frac{\alpha k \rho}{\mu} \frac{\partial p}{\partial x} \right) \cong \frac{\left(\frac{\alpha k \rho}{\mu} \frac{\partial p}{\partial x} \right)_{i+1/2} - \left(\frac{\alpha k \rho}{\mu} \frac{\partial p}{\partial x} \right)_{i-1/2}}{\Delta x_i}$$

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

$$\left(\frac{\alpha k \rho}{\mu} \frac{\partial p}{\partial x} \right)_{i-1/2} = \left(\frac{\alpha k \rho}{\mu} \right)_{i-1/2} \frac{p_i - p_{i-1}}{x_i - x_{i-1}}$$

A similar expression exists at $i + 1/2$. If the gridding is nonuniform 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

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



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

$$\frac{(\alpha\phi\rho)_i^{n+1} - (\alpha\phi\rho)_i^n}{\Delta t} - \frac{1}{\Delta x_i} \left(\frac{(\alpha k \rho)}{\mu} \right)_{i+1/2} \frac{p_{i+1} - p_i}{x_{i+1} - x_i} + \frac{1}{\Delta x_i} \left(\frac{(\alpha k \rho)}{\mu} \right)_{i-1/2} \frac{p_i - p_{i-1}}{x_i - x_{i-1}} - \alpha_i (q_{inj})_i = 0,$$

$i = 1, 2, \dots, IM.$

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 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 interblock flux coefficients at $\pm 1/2$ will be discussed in Subsection 4.8, on Two Phase Flow.

4.6 Newton-Raphson Method for Solution of Nonlinear Algebraic Equations

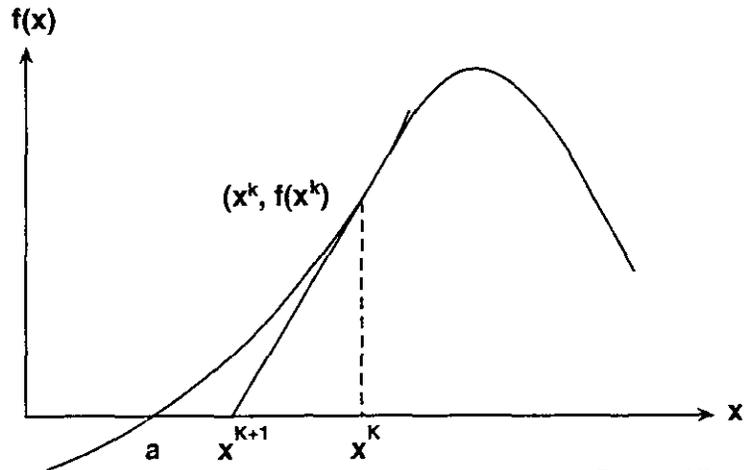


Figure 8. Newton-Raphson method.

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 :

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

Replace the nonlinear root problem with the linear approximation:

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

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

$$\delta x^k = x^{k+1} - x^k$$



Then

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

and

$$x^{k+1} = x^k + \delta x^k.$$

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 (NLS) in n unknowns:

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

In vector notation, the system is written

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

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

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



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

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

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

Replace the system of nonlinear equations

$$\begin{aligned}f_1(x_1, x_2) &= 0 \\f_2(x_1, x_2) &= 0\end{aligned}$$

by the linear system

$$\begin{aligned}\frac{\partial f_1}{\partial x_1}(\hat{x}^k)(x_1^{k+1} - x_1^k) + \frac{\partial f_1}{\partial x_2}(\hat{x}^k)(x_2^{k+1} - x_2^k) &= -f_1(\hat{x}^k) \\ \frac{\partial f_2}{\partial x_1}(\hat{x}^k)(x_1^{k+1} - x_1^k) + \frac{\partial f_2}{\partial x_2}(\hat{x}^k)(x_2^{k+1} - x_2^k) &= -f_2(\hat{x}^k)\end{aligned}$$

Define the change in iterate values

$$\begin{aligned}\delta x_1 &= x_1^{k+1} - x_1^k \\ \delta x_2 &= x_2^{k+1} - x_2^k.\end{aligned}$$

Then the above linear system is written

$$\begin{aligned}\frac{\partial f_1}{\partial x_1}(\hat{x}^k)\delta x_1 + \frac{\partial f_1}{\partial x_2}(\hat{x}^k)\delta x_2 &= -f_1(\hat{x}^k) \\ \frac{\partial f_2}{\partial x_1}(\hat{x}^k)\delta x_1 + \frac{\partial f_2}{\partial x_2}(\hat{x}^k)\delta x_2 &= -f_2(\hat{x}^k)\end{aligned}$$

The coefficient matrix

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



is called the Jacobian matrix for the nonlinear system.

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

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

or

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

and

$$\hat{x}^{k+1} = \hat{x}^k + \delta \hat{x}.$$

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

$$J(\hat{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\hat{x}) & \dots & \frac{\partial f_1}{\partial x_n}(\hat{x}) \\ \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1}(\hat{x}) & \dots & \frac{\partial f_n}{\partial x_n}(\hat{x}) \end{pmatrix}$$

or

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

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

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



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

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

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 4.10), 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

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

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

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

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

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

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 Section 7.2.6 for input parameters that specify when convergence has been obtained or that affect the rate of convergence.

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

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

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

4.7 Discretization in Two-Dimensions

Consider the two dimensional flow equation

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

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

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

A typical two dimensional grid is shown in Figure 9.

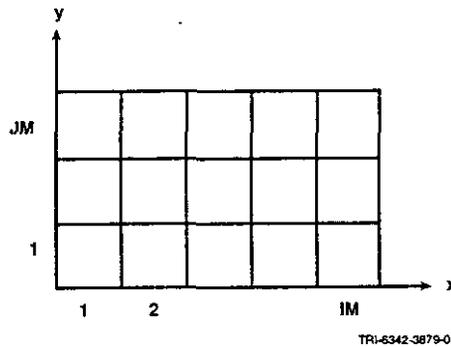


Figure 9. 2-dimensional grid.

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.

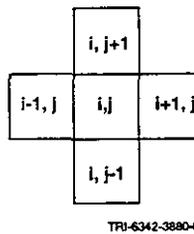


Figure 10. Computational molecule (or stencil).

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

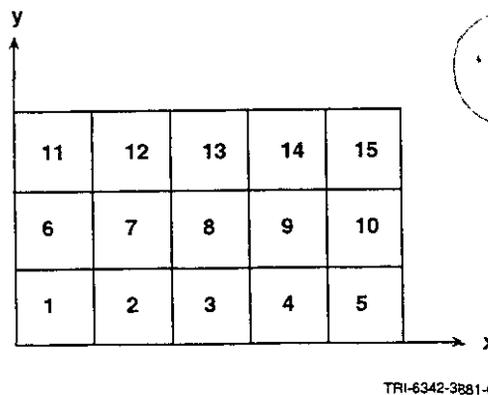
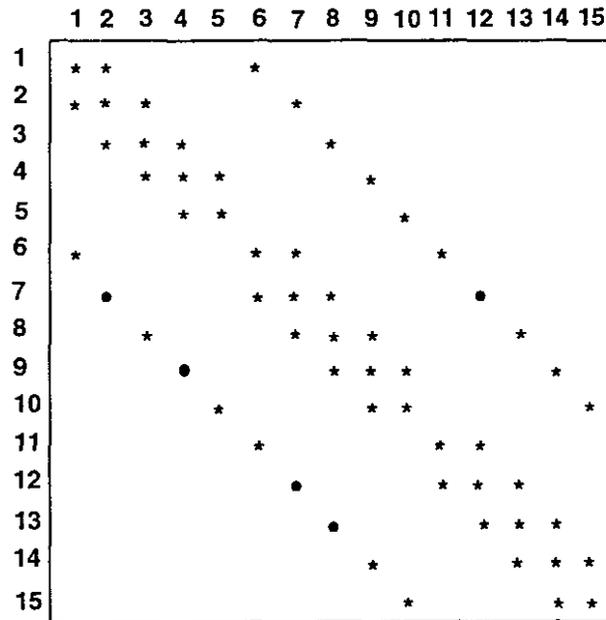


Figure 11. Sequential indexing of equations.

Then the Jacobian matrix has the structure shown in Figure 12 where * entries are the only non-zero values.

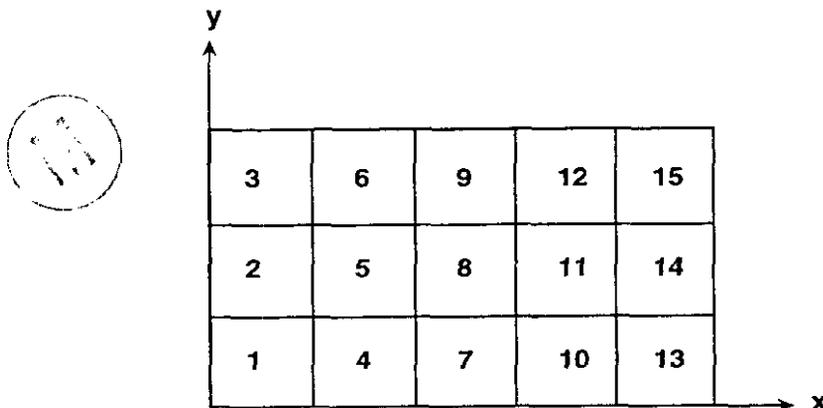


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Figure 12. Jacobian matrix.

This is said to have penta-diagonal band structure, with bandwidth = $IBW = 2 * IM + 1$ (for the example, $IBW=11$).

Suppose the grid is indexed as in Figure 13.



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Figure 13. A different sequential indexing.

Then $IBW = 2 * JM + 1$ (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

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

Storage requirements are as follows:

$$\begin{aligned} \text{Full matrix storage} &= (IM * JM)^2 \text{ words of memory} \\ \text{Band matrix storage} &= IM * JM * IBW \text{ words of memory} \end{aligned}$$

If $IM \leq JM$ then

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

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 multiplications/divisions.

Banded structure:

$$\text{multiplication/division} \cong NEQ * IB * IB \text{ where } IB \text{ is the half bandwidth,}$$

$$IB = \min (IM, JM).$$

Full matrix:

$$\text{multiplication/division} \cong 1/3 NEQ^3$$



A typical performance assessment grid is

$$\begin{aligned} \text{IM} &= 33 \\ \text{JM} &= 31 \\ \text{NEQ} &= 31(33) = 1023 \\ \text{IBW} &= 2(31) + 1 = 63 \\ \text{IB} &= 31 \end{aligned}$$

Computational effort

$$\begin{aligned} \text{banded matrix structure} &= 1023 (31 * 31) = 983,103 \\ \text{full matrix structure} &= 1/3 (1023)^3 \approx 3.57 \text{ E8.} \end{aligned}$$

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 $\text{NEQ} * \text{IB} * \text{IB}$ 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 phase. 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

$$\begin{aligned} S_w &= \text{water saturation} \\ S_g &= \text{gas saturation} \end{aligned}$$



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

$$S_w + S_g = 1.$$

Capillary pressure is defined by

$$P_c = P_g - P_w = P_c(S_w)$$

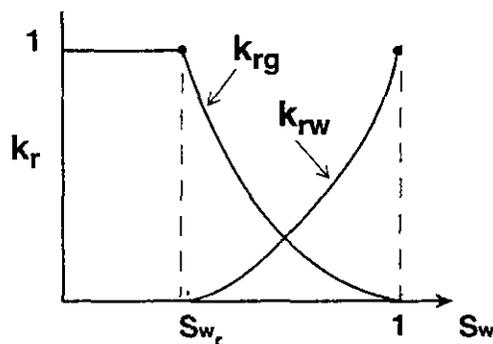
For a water wetting phase, $p_c \geq 0$.

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

$$k_{r1} = \frac{k_l}{k}$$

where k is the formation or absolute permeability, k_l is the effective permeability of phase l , and k_{r1} is the relative permeability of phase l . 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.



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Figure 14. Typical relative permeability curve.

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

$$\hat{q}_i = -\frac{kk_{rj}\rho}{\mu} \nabla\Phi.$$

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:

$$\nabla \cdot \left[\frac{\alpha\rho_g[k]k_{rg}}{\mu_g} \nabla(p_g + \rho_g gh) \right] + \alpha q_g + \alpha q_{rg} = \alpha \frac{\partial(\phi\rho_g S_g)}{\partial t}$$

Brine Mass Balance:

$$\nabla \cdot \left[\frac{\alpha\rho_w[k]k_{rw}}{\mu_w} \nabla(p_w + \rho_w gh) \right] + \alpha q_w + \alpha q_{rw} = \alpha \frac{\partial(\phi\rho_w S_w)}{\partial t}$$

Saturation Constraint:

$$S_g + S_w = 1$$

Capillary Pressure Constraint:



$$p_c = p_g - p_w$$

Additional terms include

- q_{rg} = 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 either one, two or three dimensions and then a discretization of the gas and brine mass balance equation 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

$$\begin{aligned} & \frac{1}{\Delta x_i} \left\{ \frac{1}{x_{i+1} - x_i} \left[\frac{\alpha \rho_g k_x k_{rg}}{\mu_g} \right]_{i+1/2,j}^{n+1} (\Phi_{\delta_{i+1,j}}^{n+1} - \Phi_{\delta_{i,j}}^{n+1}) - \frac{1}{x_i - x_{i-1}} \left[\frac{\alpha \rho_g k_x k_{rg}}{\mu_g} \right]_{i-1/2,j}^{n+1} (\Phi_{\delta_{i,j}}^{n+1} - \Phi_{\delta_{i-1,j}}^{n+1}) \right\} \\ & + \frac{1}{\Delta y_j} \left\{ \frac{1}{y_{j+1} - y_j} \left[\frac{\alpha \rho_g k_y k_{rg}}{\mu_g} \right]_{i,j+1/2}^{n+1} (\Phi_{\delta_{i,j+1}}^{n+1} - \Phi_{\delta_{i,j}}^{n+1}) - \frac{1}{y_j - y_{j-1}} \left[\frac{\alpha \rho_g k_y k_{rg}}{\mu_g} \right]_{i,j-1/2}^{n+1} (\Phi_{\delta_{i,j}}^{n+1} - \Phi_{\delta_{i,j-1}}^{n+1}) \right\} \\ & + \alpha_{ij} q_{g,i,j}^{n+1} + \alpha_{ij} q_{rg,i,j}^{n+1} - \frac{(\alpha \phi \rho_g S_g)_{i,j}^{n+1} - (\alpha \phi \rho_g S_g)_{i,j}^n}{\Delta t} = 0. \end{aligned}$$

A similar equation for the brine mass balance is obtained by replacing the gas subscript with the brine subscript. The superscript n refers to the time level t_n at which the solution is known and the superscript n+1 refers to the time level t_{n+1} at which the solution is to be computed. Note that the flux and rate terms are evaluated at time level n+1. Therefore, the formulation is fully implicit.

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_b . Consequently, at each time step it is necessary to solve $2 * NX * NY$ equations, where NX, NY are the number of grid blocks in the x,y direction, respectively, for $2 * NX * NY$ unknowns.

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 $NGB = NX * NY$. 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 |
| . | |
| . | |
| . | |
| $2 * NGB - 1$ | gas equation in grid block NGB |
| $2 * NGB$ | 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 * NGB-1	gas saturation in grid block NGB
2 * 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 penta diagonal structure and the resulting linear system in the Newton-Raphson iteration step can be represented as follows



The block vectors in the equation vector are

$$G_{\ell} = \begin{pmatrix} F_1(i,j) \\ F_2(i,j) \end{pmatrix}.$$

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 interblock 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 interblock flow terms.

Consider the following term in the brine equation for flow in the x-direction between grid blocks i and $i+1$:

$$\frac{1}{\Delta x_i(x_{i+1} - x_i)} \left(\frac{\alpha \rho_w k_x k_{rw}}{\mu_w} \right)_{i+1/2} (\Phi_{wi+1} - \Phi_{wi}).$$

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

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

or

$$H = \frac{2a_1a_2}{a_1 + a_2}.$$

Further, the weighted harmonic average of a_1 , a_2 is

$$\frac{1}{H} = \frac{w_1}{a_1} + \frac{w_2}{a_2}$$

or

$$H = \frac{a_1 a_2}{w_2 a_1 + w_1 a_2},$$

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

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

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

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

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 gravity potential

$$\bar{q}_{i+1/2} = \tau_{i+1/2} \frac{p_{i+1} - p_i}{x_{i+1} - x_i}$$

or

$$\bar{q}_{i+1/2} = \tau_{i+1/2} \frac{p_{i+1} - p_i}{1/2(\Delta x_i + \Delta x_{i+1})}$$

This yields

$$p_{i+1} - p_i = \frac{\bar{q}_{i+1/2} \frac{1}{2}(\Delta x_i + \Delta x_{i+1})}{\tau_{i+1/2}}$$



Similarly,

$$q_{i+1/2}^- = \tau_i \frac{(p_{i+1/2} - p_i)}{\frac{1}{2} \Delta x_i}$$

$$q_{i+1/2}^+ = \tau_{i+1} \frac{(p_{i+1} - p_{i+1/2})}{\frac{1}{2} \Delta x_{i+1}}$$

Pressure drop is then written as

$$P_{i+1} - P_i = P_{i+1} - P_{i+1/2} + (P_{i+1/2} - P_i)$$

Then

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

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

$$\tau_{i+1/2} = \frac{\tau_i \tau_{i+1}}{\frac{\Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}} \tau_i + \frac{\Delta x_i}{\Delta x_i + \Delta x_{i+1}} \tau_{i+1}}$$

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

One further modification is made in the interblock term

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

The harmonic averaging is used to evaluate

$$\left(\frac{\alpha \rho_w k_x}{\mu_w} \right)_{i+1/2}$$

However, the interblock relative permeability is evaluated by upstream weighting:



$$(k_{rw})_{i+1/2} = k_{rw_{i+1}}, P_{wi} < P_{w_{i+1}} \\ = k_{rw_i}, \text{ otherwise.}$$

This treatment of the interblock flow term is justified by the following process typical in performance assessment analysis. Assume gas is generated and is displacing water from the left to the right as in Figure 15. At the gas front, the gas potential 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 interblock

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.

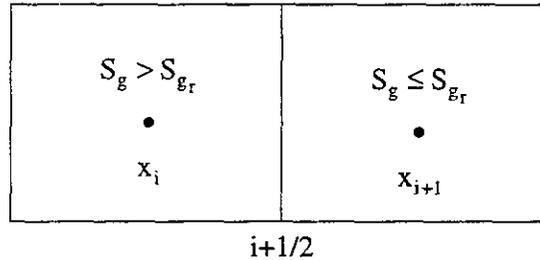


Figure 15. Gas Displacement Front.

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

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

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

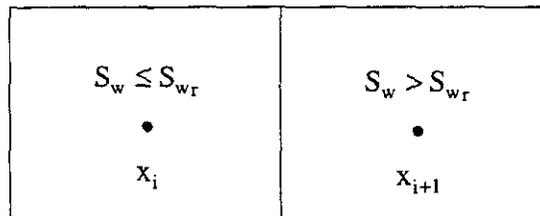


Figure 16. Displacement of Immobile Water.

with potential satisfying $\Phi_{w_i} > \Phi_{w_{i+1}}$. The potential tries to move water from i to $i+1$ block. Since $k_{rw_i} = 0$ and $k_{rw_{i+1}} > 0$, the interblock 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 interblock 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, 1992). Choice of the characteristic curves is controlled by input directives.

The van Genuchten-Parker model determines

Capillary Pressure

$$P_c = P_o(S_e^{-1/m} - 1)^{1-m}$$

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

Relative Permeabilities

$$k_{rw} = S_e^{1/2} \left[1 - (1 - S_e^{1/m})^m \right]^2$$
$$k_{rg} = (1 - S_e)^{1/2} (1 - S_e^{1/m})^{2m}$$

where the effective saturation is

$$S_e = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}$$

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

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

$$m = \frac{\lambda}{1 + \lambda}$$

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

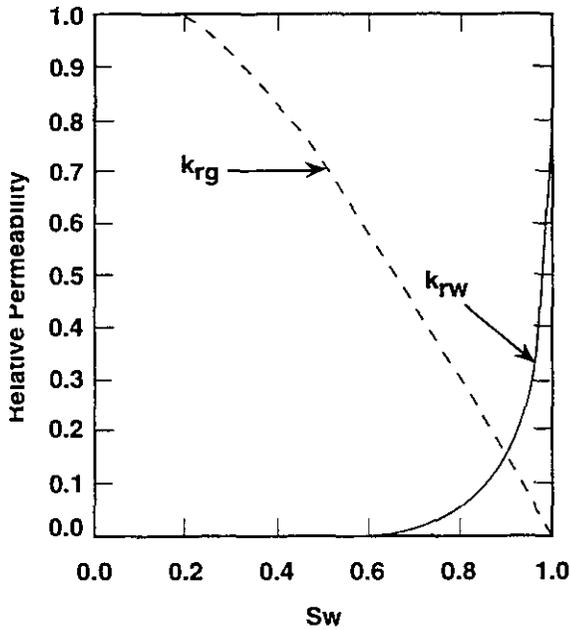
$$\lambda = 0.7 \quad (m = 0.41)$$
$$S_{wr} = 0.2.$$

The original Brooks-Corey model determines

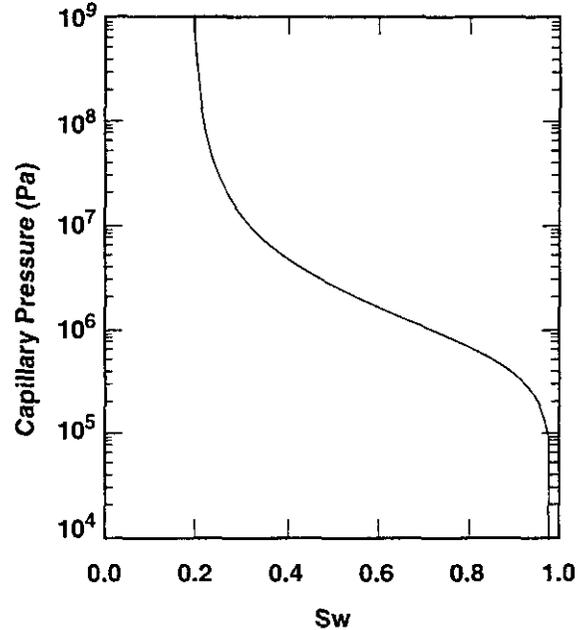
Capillary Pressure

$$P_c = P_t / S_e^{1/\lambda}$$





TRI-6342-3873-0(a)



TRI-6342-3873-1(b)

Figure 17. Relative Permeabilities for van Genuchten-Parker Model (left plot) and Capillary Pressure for van Genuchten-Parker Model (right plot).

Relative Permeabilities

$$k_{rw} = S_e^{(2+3\lambda)/\lambda}$$

$$k_{rg} = (1 - S_e)^2 (1 - S_e^{(2+\lambda)/\lambda})$$

where $S_e = (S_w - S_{wr}) / (1 - S_{wr})$, 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

$$\lambda = 0.7$$

$$S_{wr} = 0.2$$

$$P_t = 1.E6.$$



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

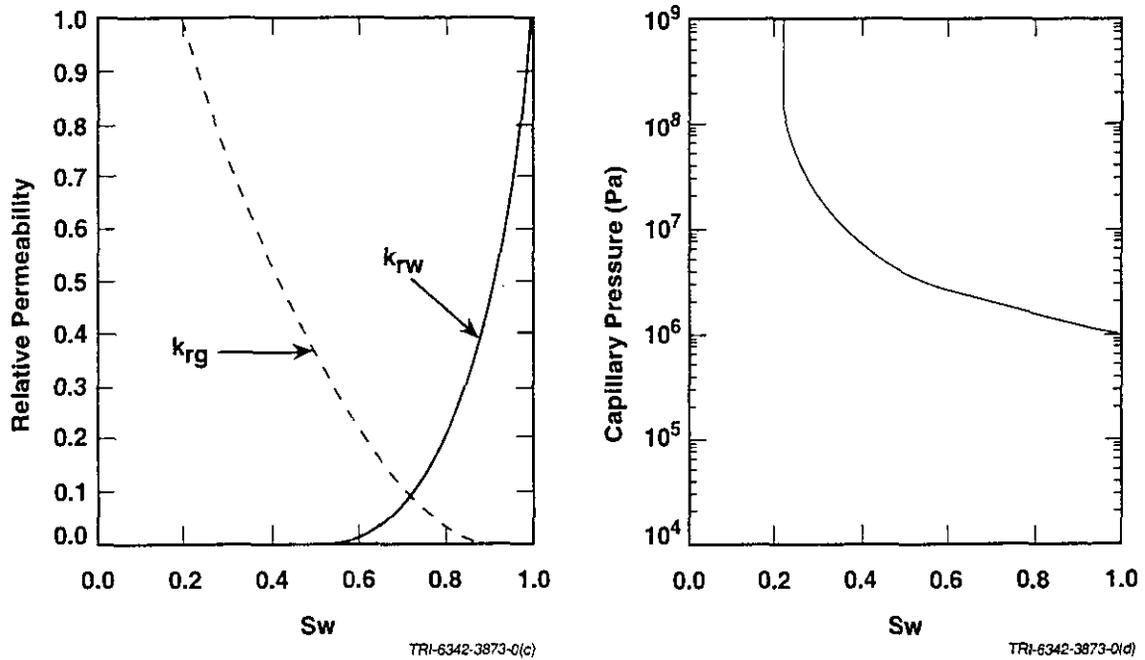


Figure 18. Relative Permeabilities for Original Brooks-Corey Model (left plot) and Capillary Pressure for Original Brooks-Corey Model (right plot).

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

$$S_e = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}$$

where S_{gr} is residual gas saturation.

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

$$\begin{aligned} \lambda &= 0.7 \\ S_{wr} &= 0.2 \\ S_{gr} &= 0.2 \\ P_t &= 1.E6. \end{aligned}$$

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 $S_w = 1 - S_{gr}$.

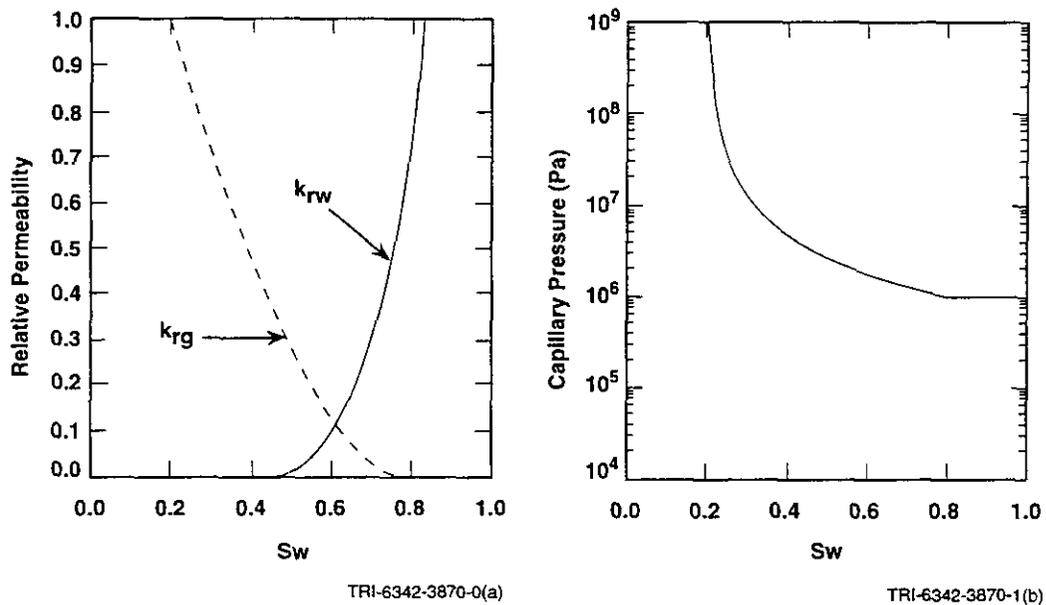


Figure 19. Relative Permeabilities for Modified Brooks-Corey Model (left plot) and Capillary Pressure for Modified Brooks-Corey Model (right plot).

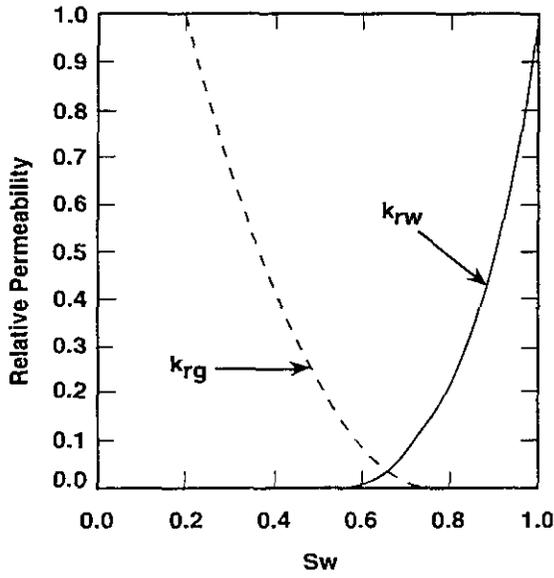
The second modified Brooks-Corey model uses residual gas saturation to calculate effective saturation only for the gas phase. This treatment results in the characteristic curves shown in Figure 20.

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 $P_c = P_t$.

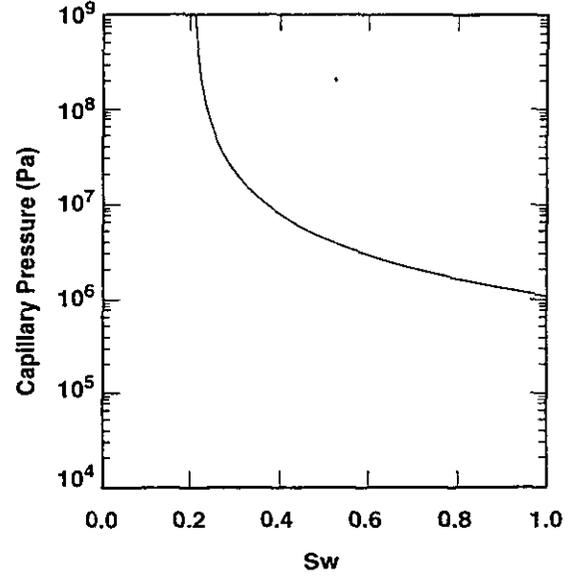
For both the van Genuchten-Parker and the Brooks-Corey model, the capillary pressure function is unbounded from the right ($S_w = S_{wr}^+$). An option is available which truncates the capillary pressure function at the PCMAX value. The capillary pressure curve with this option and PCMAX = 1.E8 is shown 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.

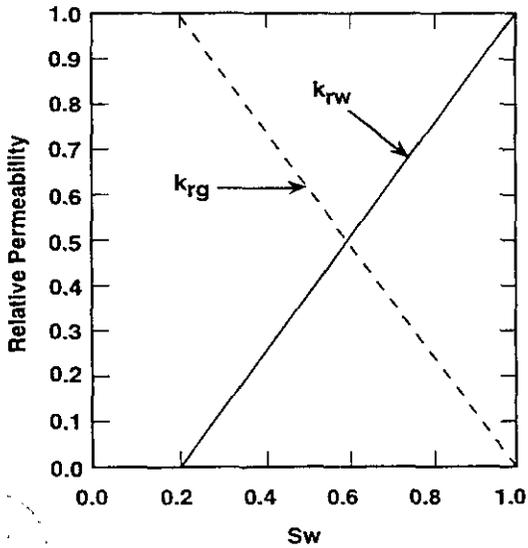


TRI-6342-3870-0(c)

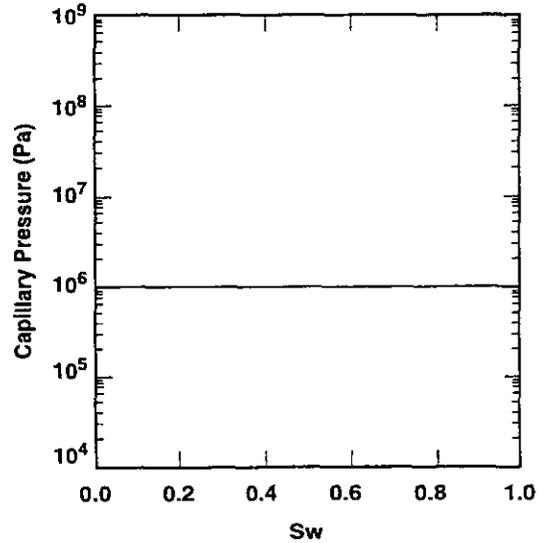


TRI-6342-3870-1(d)

Figure 20. Relative Permeabilities for Second Modified Brooks-Corey Model (left plot) and Capillary Pressure for Second Modified Brooks-Corey Model (right plot).



TRI-6342-3871-0(a)



TRI-6342-3871-0(b)

Figure 21. Relative Permeabilities for Linear Model (left plot) and Capillary Pressure for Linear Model (right plot).

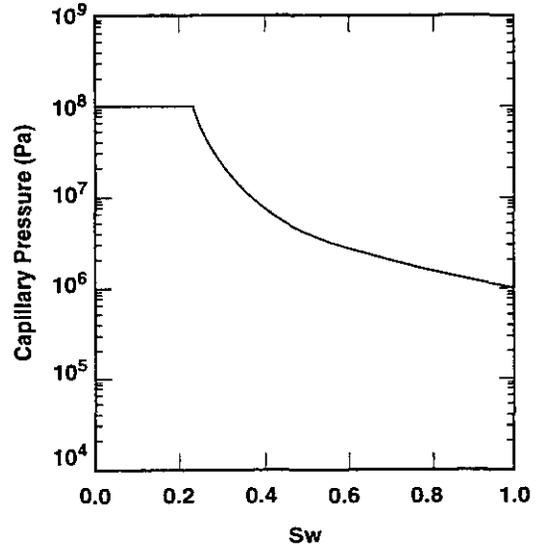
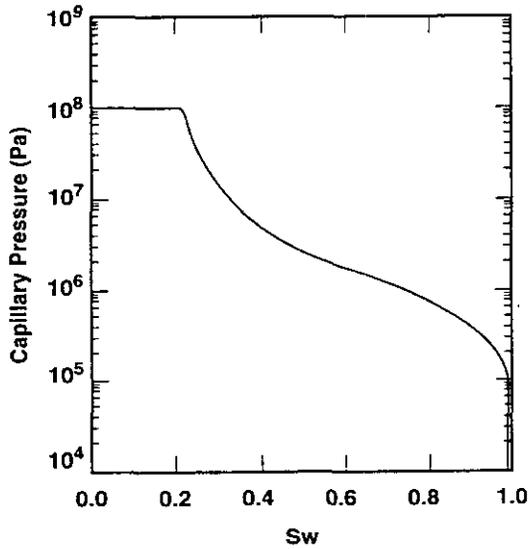


Figure 22. Capillary Pressure for van Genuchten-Parker Model PCMAX=1.0E+08 (left plot) and Capillary Pressure for Original Brooks-Corey Model PCMAX=1.0E+08 (right plot).

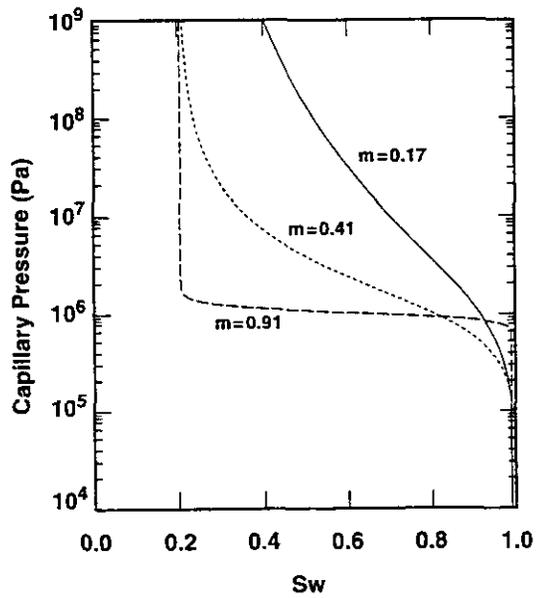
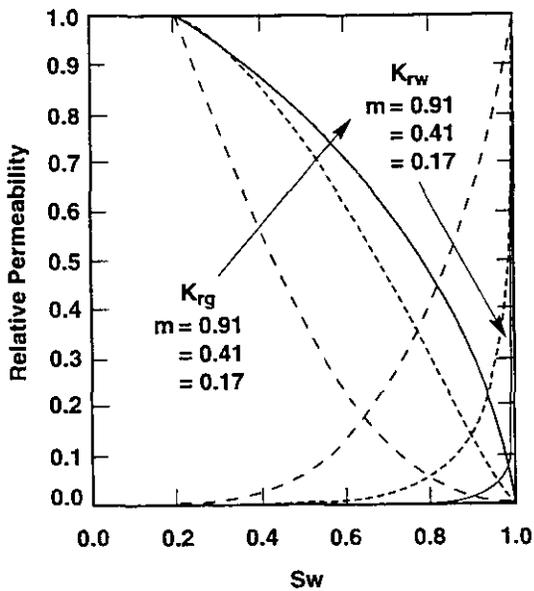


Figure 23. Relative Permeabilities for van Genuchten-Parker Model, effect of parameter m (left plot) and Capillary Pressure for van Genuchten-Parker Model, effect of parameter m (right plot).

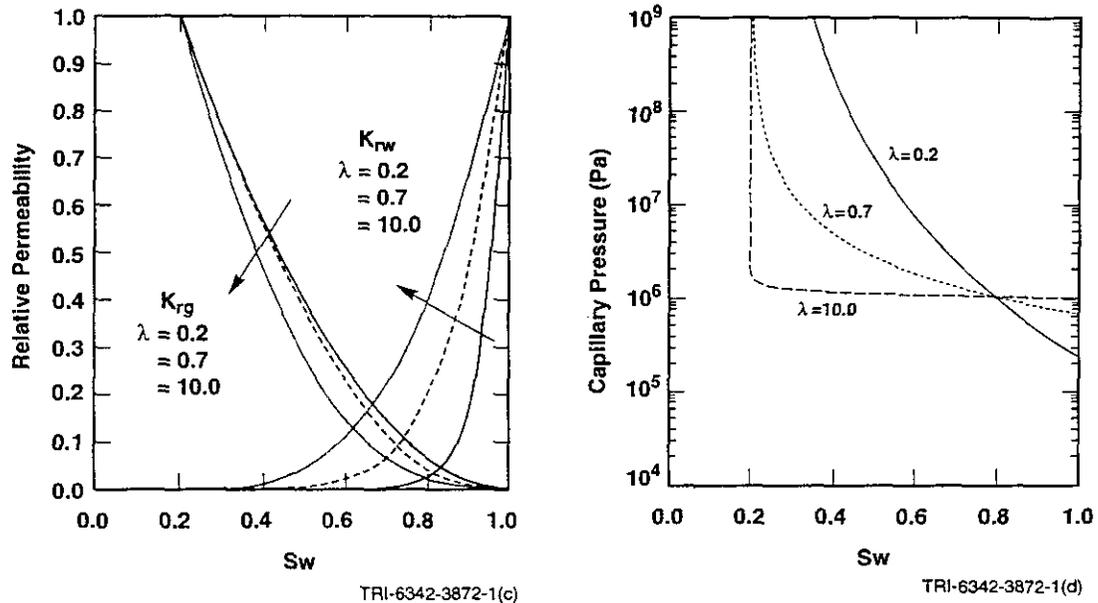


Figure 24. Relative Permeabilities for Brooks-Corey Model effect of pore size distribution parameter (left plot) and Capillary Pressure for Brooks-Corey Model effect of pore size distribution parameter (right plot).

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

$$C = \frac{1}{\phi} \frac{d\phi}{dp}$$

where

- C = rock compressibility,
- ϕ = porosity,
- p = pore pressure.

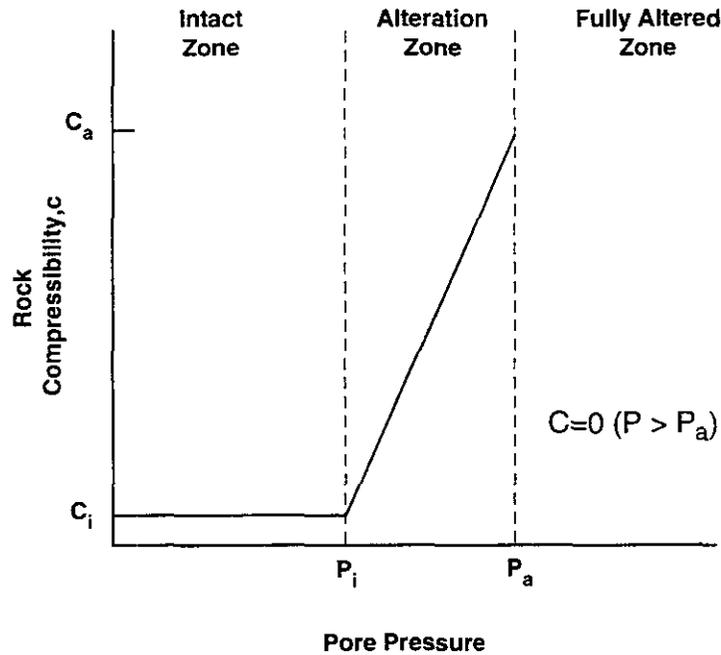
For constant compressibility, porosity can be expressed as a function of pressure

$$\phi = \phi_0 \exp(C(p - p_0))$$

where

$$\phi_0 = \text{porosity at reference pressure } p_0.$$

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 $C = 0$.



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Figure 25. Pressure dependent compressibility.

The porosity can now be computed from the compressibility definition giving for $p \leq p_i$

$$\phi = \phi_0 \exp(C_i(p - p_0)) \quad (A)$$

for $p_i < p \leq p_a$

$$\phi = \phi_o \exp \left\{ C_i (p - p_o) + \frac{(C_a - C_i) (p - p_i)^2}{(p_a - p_i) 2} \right\} \quad (B)$$

for $p \geq p_a$

$$\phi = \phi_a \quad (C)$$

BRAGFLO input requires the pressures p_i and p_a and the porosity at the fully altered conditions, ϕ_a . From this information, the fully altered compressibility, C_a , is determined from equation (B) as

$$C_a = C_i \left[1 - 2 \frac{(p_a - p_o)}{p_a - p_i} \right] + \frac{2}{(p_a - p_i)} \ln \left(\frac{\phi_a}{\phi_o} \right)$$

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

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

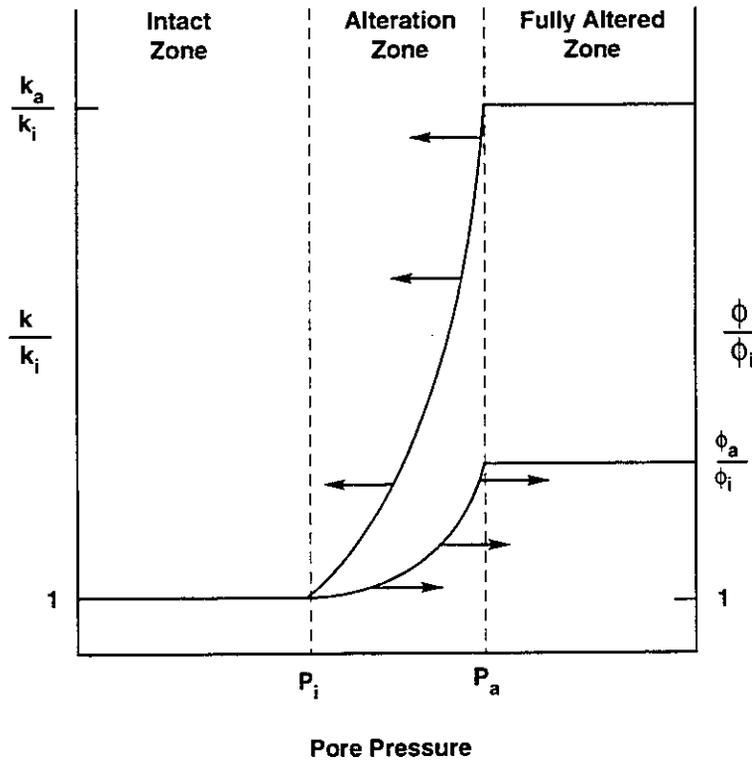
where

- 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.





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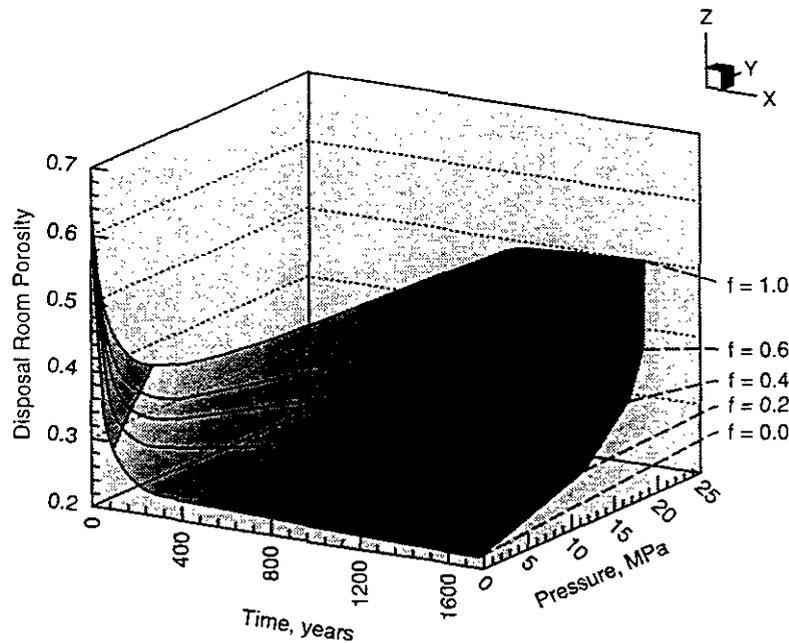
Figure 26. Pressure dependent porosity and permeability.

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.



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 (Butcher et al., 1995), 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.



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

The surface is generated by a family of five 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 . BRAGFLO uses a volumetric average pressure over the waste and time to interpolate the surface in Figure 27 for the average waste porosity.

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, 1992). 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

$$k_g = k_w (1 + b k_w^{-a} / p)$$

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 $b = 0.98$.

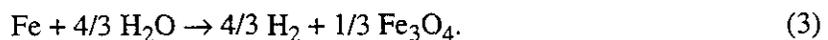
4.13 Gas Generation Model

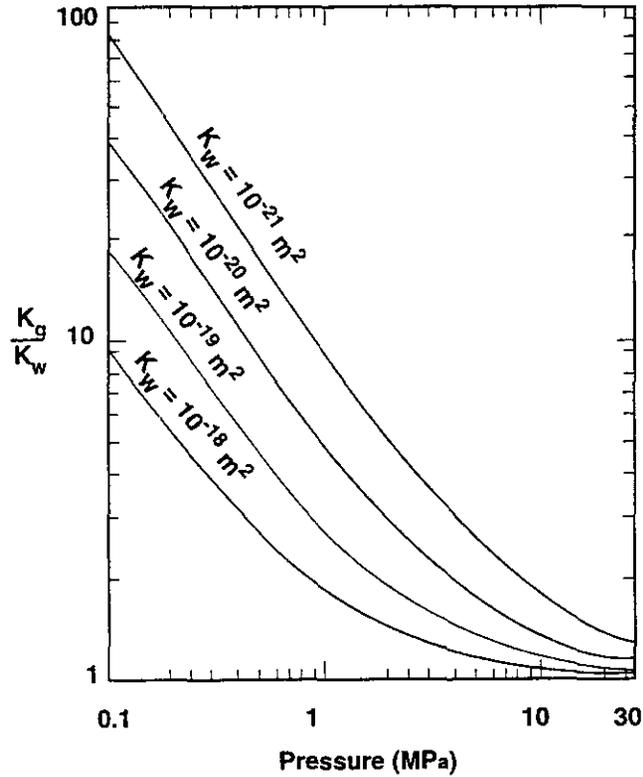
Within BRAGFLO there are chemical reactions with the effect of consuming brine and generating gas. One reaction represents the corrosion of the waste containers. A second reaction models the microbial consumption of cellulose material.

Two possible anoxic reactions are used to describe the corrosion when waste drums are exposed to brine:



If the equations are normalized to unit mole of iron, then equation (2) is written



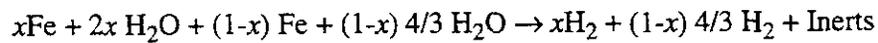


TRI-6342-3885-0

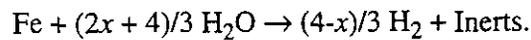


Figure 28. Increase in gas phase permeability due to Klinkenberg effect.

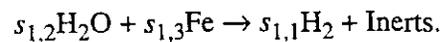
In the performance assessment of the WIPP site, a weighted average of the above two reactions is assumed



where weighting factor x satisfies $0 \leq x \leq 1$. This is written for a unit mole of iron as



From input (line 9.8), the corrosion stoichiometry is described by



The PA calculations sample x from a uniform distribution on the interval $[0,1]$ and compute stoichiometric coefficients

$$\begin{aligned} s_{1,1} &= (4-x)/3 && \text{[mol H}_2\text{/mol Fe]} \\ s_{1,2} &= (2x+4)/3 && \text{[mol H}_2\text{O/mol Fe]} \\ s_{1,3} &= 1.0 && \text{[mol Fe/mol Fe].} \end{aligned}$$

In order to account for the material balance of brine and gas, the rate of reaction must be specified. BRAGFLO assumes all 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

$$\begin{aligned} \text{RK}(1) &= \text{brine inundated corrosion reaction rate [mol Fe/m}^3\text{/s]}, \\ \text{HF}(1) &= \text{factor multiplying RK}(1) \text{ to get humid corrosion reaction rate.} \end{aligned}$$

We introduce the notation

$$\begin{aligned} K_{CI} &= \text{RK}(1), \text{ inundated reaction rate,} \\ K_{CH} &= \text{HF}(1) * \text{RK}(1), \text{ humid reaction rate.} \end{aligned}$$

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, S_g . Thus the effective corrosion reaction rate becomes

$$K_C = K_{CI} S_w + K_{CH} S_g.$$

The rate of H_2 production by corrosion per unit volume of panel is

$$q_{\text{CH}_2} = K_C s_{1,1} M_{\text{H}_2}$$



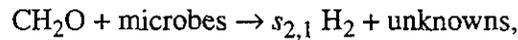
where M_{H_2} = molecular weight of H_2 [kg/mol].

The rate of brine consumption by corrosion per unit volume of panel is

$$q_{\text{CH}_2\text{O}} = K_C s_{1,2} M_{\text{H}_2\text{O}}$$

where $M_{\text{H}_2\text{O}}$ = molecular weight of H_2O [kg/mol].

In BRAGFLO the biodegradation reaction assumes microbial consumption of cellulose (CH_2O) with hydrogen gas as a product



where

$s_{2,1}$ = stoichiometric coefficient, [mol H_2 /mol CH_2O]

PA samples on $s_{2,1}$ as uniform distribution on the interval [0, 5/3]. The stoichiometric coefficients for the biodegradation reaction are read on input as

$s_{2,1}$	=	(sampled)	[mol H_2 /mol CH_2O]
$s_{2,2}$	=	moles $\text{H}_2\text{O} = 0.0$	[mol H_2O /mol CH_2O]
$s_{2,3}$	=	moles $\text{CH}_2\text{O} = 1.0$	[mol CH_2O /mol CH_2O].

Reaction rates for biodegradation are analogous to the 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 [mol CH_2O /m³/s]
HF(2) = factor multiplying RK(2) to get humid biodegradation rate.

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

Another gas generation model, the reaction path model, was planned and implementation had begun. 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 multicomponent gas transport scheme (see Sections 7.2.2, 7.2.9, and 7.2.12), but the reaction path model itself has not been implemented.

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 roundoff 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 roundoff 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 has been used exclusively and is strongly recommended. It has been found from experience that the iterative solvers are 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 (4x4 matrix) example. The objective is to write the coefficient matrix (Jacobian matrix) as a product of two matrices,

$$LU = A$$

where **L** is lower triangular (has non-zero elements only on the diagonal and below) and **U** is upper triangular (has non-zero elements only on the diagonal and above). It is further possible to require the diagonals of **L** to be equal to one. If **A** = (a_{ij}), **L** = (α_{ij}) and **U** = (β_{ij}), then for the case of a 4x4 matrix the decomposition would look like

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

For example, it can be checked by matrix multiplication that the following is an LU-decomposition of the given 4x4 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 **A** is known then the solution of the system of equations **Ax = b** can be written as

$$Ax = (LU)x = L(Ux) = b$$

The solution is obtained by solving for the vector **y** such that

$$\mathbf{L}\mathbf{y} = \mathbf{b}$$

and then solving

$$\mathbf{U}\mathbf{x} = \mathbf{y}$$

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

$$y_1 = \frac{b_1}{\alpha_{11}}$$

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

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

$$x_N = \frac{y_N}{\beta_{NN}}$$

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

Given the coefficient matrix \mathbf{A} , how are the decomposition matrices \mathbf{L} and \mathbf{U} computed? 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,



$$\sum_{k=1}^i \alpha_{ik} \beta_{kj} = a_{ij} \quad i = 1, \dots, j \quad (\text{A1})$$

$$\sum_{k=1}^j \alpha_{ik} \beta_{kj} = a_{ij} \quad i = j+1, \dots, N \quad (\text{B1})$$

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 equation (A1) by

$$\beta_{ij} = a_{ij} - \sum_{k=1}^{i-1} \alpha_{ik} \beta_{kj} \quad \text{for } i = 1, \dots, j \quad (\text{A2})$$

followed by the solution of α_{j+1j} to α_{Nj} from equation (B1) by

$$\alpha_{ij} = \frac{1}{\beta_{jj}} \left(a_{ij} - \sum_{k=1}^{j-1} \alpha_{ik} \beta_{kj} \right) \quad \text{for } i = j + 1, \dots, N. \quad (\text{B2})$$

The example will demonstrate that the α 's and β 's that occur on the right-hand side of equations (A2) and (B2) 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 roundoff errors in the arithmetic and is essential for the numerical stability of Crout's method.

Now consider the example with

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



Starting with the first column we solve for $\beta_{11} = 1$ from equation (A2) where the sum is taken to mean zero. Equation (B2) 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 (A2) compute sequentially $\beta_{12} = 1$, $\beta_{22} = 3$. Now from equation (B2) 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 Subsection.

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 $y = (4, 9, -4, 4)^T$. We then solve the system $Ux = y$. 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 $x = (1, 1, 1, 1)^T$.

4.15 Model Geometry

The mesh used in the BRAGFLO simulations attempts to incorporate radial flow phenomena at large distances from the repository and to include 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 (1992, Volume 5).

4.16 Well Models

Well behavior is described by an inflow performance relation:



$$q_l = \frac{(PI)\rho_l k_{rl}}{\mu_l} (p_l - p_{wf}),$$

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 Section 7.2.4.

The well operation is determined by the well type as specified in the input file. 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 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 Section 7.2.8.

5.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE

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 has the following capabilities and limitations, which are discussed in detail in Section 4.0:

- 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 (Subsection 4.1).
- BRAGFLO assumes that the directions of the permeability tensor are aligned with the reservoir coordinate axis; that is, $\theta = 0$ (Subsection 4.3).
- BRAGFLO evaluates brine density assuming its fluid compressibility is constant (Subsection 4.4).

- BRAGFLO uses the Redlich-Kwong-Soave equation of state to relate gas density to pressure (Subsection 4.4).
- Although viscosity could be pressure dependent for gases, BRAGFLO treats viscosity constant for both water and gas (Subsection 4.4).
- BRAGFLO assumes a no-flow Neumann type boundary condition at all exterior grid boundaries (Subsection 4.4).
- BRAGFLO uses a fully implicit formulation to solve the material balance equations (Subsection 4.5).
- BRAGFLO uses the difference approximation for the Jacobian evaluation (Subsection 4.6).
- In BRAGFLO the user can specify from input directives the iteration frequency for the Jacobian evaluation (Subsection 4.6).
- For both storage and computational considerations the linear equation solver should take advantage of the banded structure. This is true for all the BRAGFLO solvers (Subsection 4.6).
- 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 (Subsection 4.7).
- BRAGFLO assumes a water/gas system (Subsection 4.8).
- In BRAGFLO fluids are assumed to be immiscible (Subsection 4.8).
- 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).
- BRAGFLO allows for coupling to the mechanical system (rock matrix) through the introduction of rock compressibility (Subsection 4.10).
- The fracture treatment in BRAGFLO allows for pressure induced alterations to the porosity by introducing a pressure-dependent porosity (Subsection 4.10).
- The BRAGFLO fracture treatment further allows for change in the fracture material permeability (Subsection 4.10).
- Representation of the creep closure within 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).
- BRAGFLO corrects for the Klinkenberg effect (Subsection 4.12).
- BRAGFLO can model gas dissolution in brine using a Henry's law treatment (Subsection 4.17).
- Well models in BRAGFLO allow simulation of gas or brine injection or production (Subsection 4.16).

- Within BRAGFLO there are chemical reactions with the effect of consuming brine and generating gas. BRAGFLO accounts for these reactions by assuming that all 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) (Subsection 4.13).
- 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 one direct solver, which uses LU-decomposition (Subsection 4.14).
- BRAGFLO includes a successive over relaxation (SOR) solver (Subsection 4.14).
- Within BRAGFLO the LU-decomposition is done within the band structure of the Jacobian matrix. This is crucial for efficient computation (Subsection 4.14).
- 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 (Section 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 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.
3. **The BRAGFLO ASCII output (.OUT) file for the sampled vector.** This file echoes input and provides user-readable output and QA information.
4. **The BRAGFLO summary (.SUM) file for the sampled vector.** This file contains a limited amount of summary information on results at each time step.
5. **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.
6. **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 1996 WIPP PA CALCUALTIONS DO NOT 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_R001.INP  
$ DEFINE BF2_DBG$OUTPUT BF2_TEST7_R001.OUT  
$ DEFINE BF2_DBG$SUMMARY BF2_TEST7_R001.SUM  
$ DEFINE BF2_BIN$OUTPUT BF2_TEST7_R001.BIN  
$ DEFINE BF2_IN$RESTART BF2_TEST7_R001.RIN  
$ DEFINE BF2_OUT$RESTART BF2_TEST7_R001.ROT  
. .  
. .  
. .
```

If so desired, the user can modify those file names by editing the DEFINE lines using the Digital Command Language (DCL) EDIT command. This is accomplished by typing EDIT (or simply EDT) followed by the name of the .COM file, moving the cursor to the file names to be changed, changing the file names (and specifying another directory name if the file exists in another directory), and then, after all the necessary name changes have been made, typing control-Z and EXIT to save the changes to the .COM file.

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=BEATLES$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 and outputs the Files 2, 3, 4, 5, and 6, as shown in Figure 30.



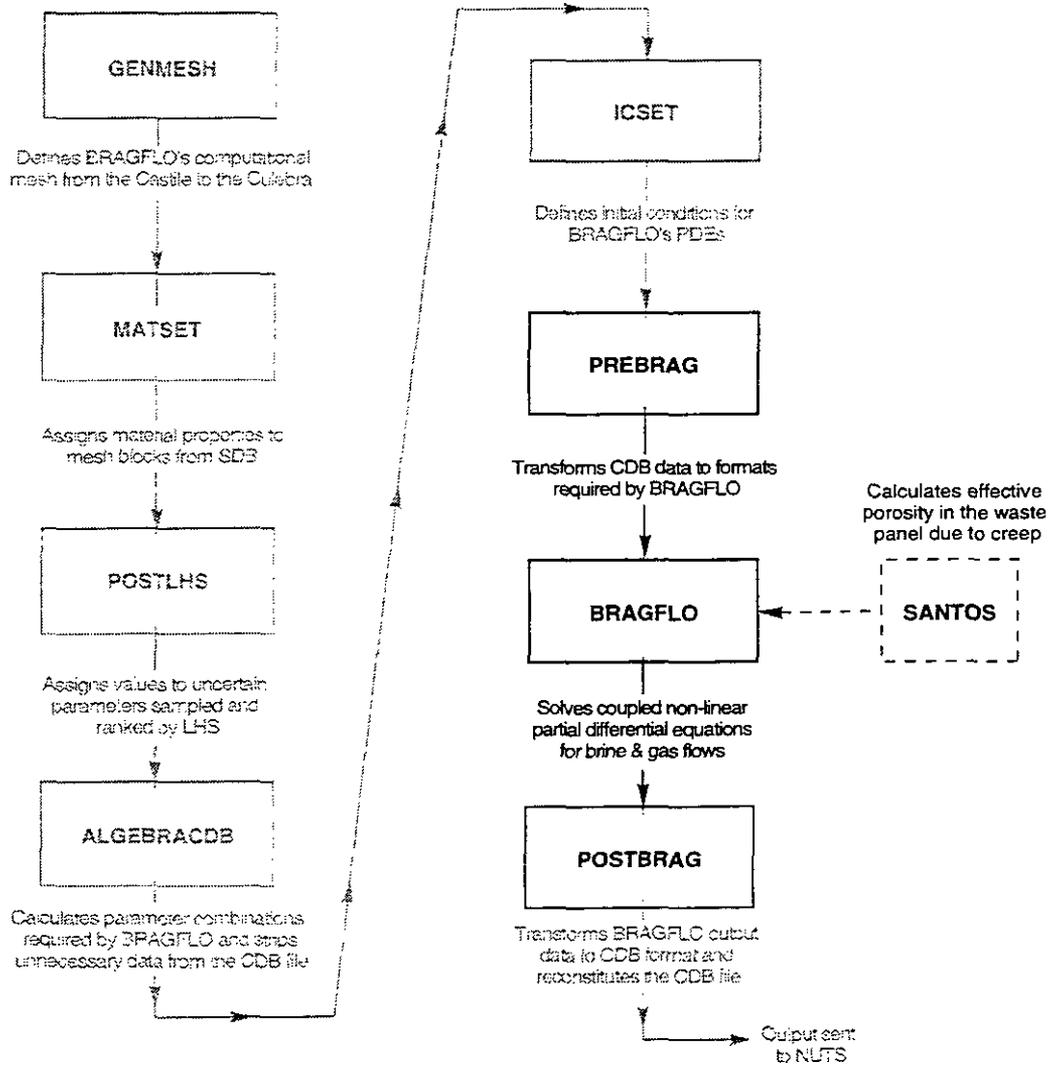
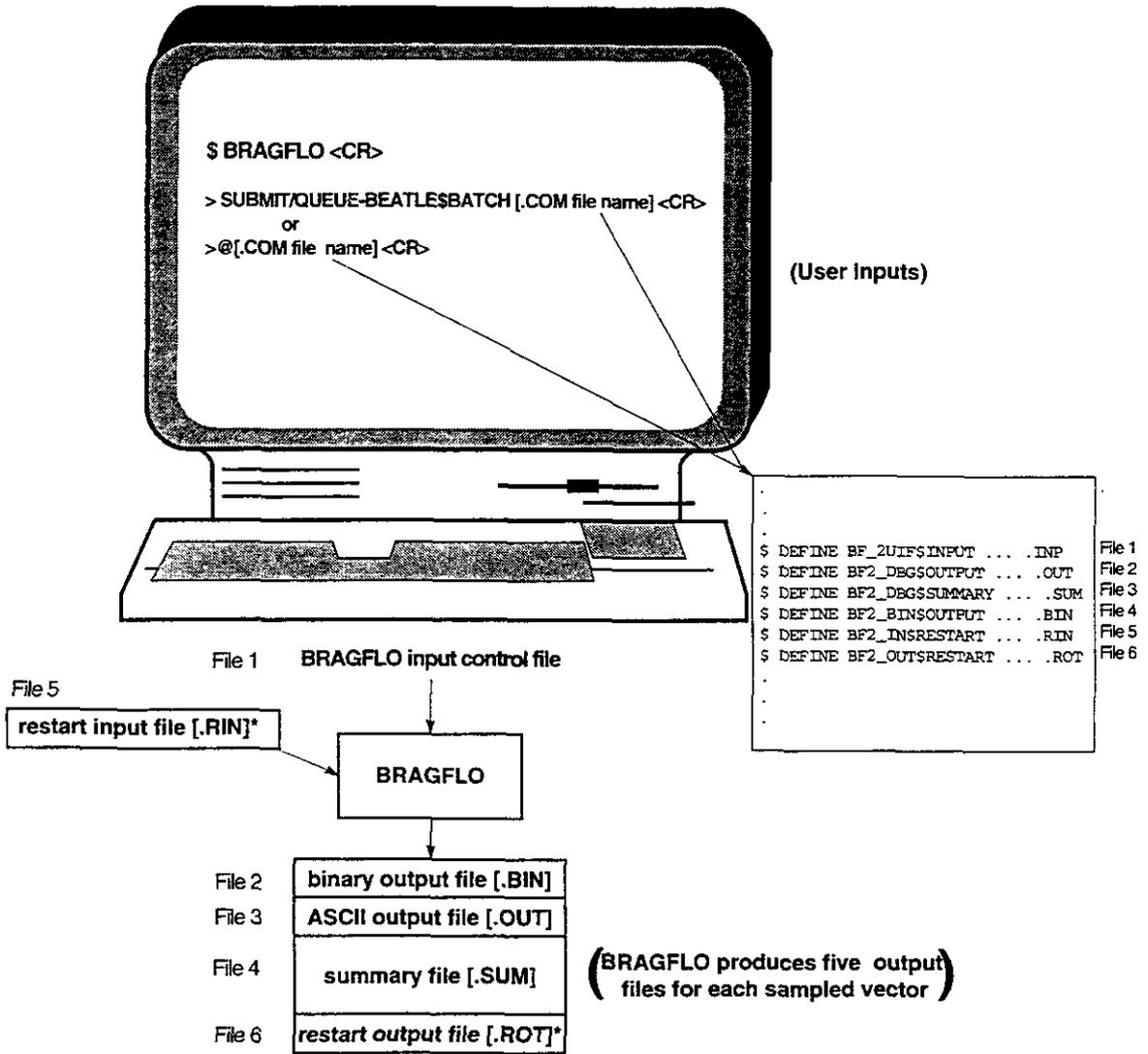


Figure 29. Sample computational flow diagram for BRAGFLO, highlighting flow to and from BRAGFLO.



*NOTE: .ROT and .RIN files not used for the 1996 WIPP PA calculation.

Figure 30. User-required file specifications for BRAGFLO.

7.0 DESCRIPTION OF INPUT FILES

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, used for the Compliance Certification Application (CCA) calculations, 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
C      1  MX          , MY          , MZ          , MG          ,
C      2  NEQ         , MGNEQ       , MDIM        , NPHASE      ,
C      3  NWTIME      , NW          , NWPERGRID   , MMAT       ,
C      4  NPINT       , NCOMP       , MGAS        , MRAD       ,
C      5  MRXYZ       , MAXPRNTASC  , MAXPRNTBIN  , MAXPRNTRST
C
C      INTEGER
C      1  MAXMATTIMES, NWTIMEP     , NDTFIXMAX   , MAXMATTIMP ,
C      2  NDTFIXMAXP , NSDATA      , NTDATA     , MKLOS     ,
C      3  MMON       , MWST        , MDRZ       , NVPR      ,
C      4  MXHIV      , MVHIV       , IBWM       , MRWXYZ    ,
C      5  MWXYZ      , MGVAR       , MSPEC      , NDIRMAX   ,
C
C      PARAMETER (MX=50, MY=40, MZ=10, MG=MX*MY*MZ, NEQ=2, MGNEQ=MG*NEQ,
C      1          MDIM=2404, NPHASE=2, NWTIME=10, NW=50, NWPERGRID=2, MMAT=80,
C      2          NPINT=10000, NCOMP=3, MGAS=6, MRAD=1, MRXYZ=MRAD*MG,
C      3          MAXPRNTASC=100, MAXPRNTBIN=100, MAXPRNTRST=100,
C      4          MAXMATTIMES=20, NWTIMEP=NWTIME+1, NDTFIXMAX=50,
C      5          MAXMATTIMP=MAXMATTIMES+1, NDTFIXMAXP=NDTFIXMAX+1,
C      6          NSDATA=13, NTDATA=214, MKLOS=4, MMON=9, MWST=2, MDRZ=1,
C      7          NVPR=95+3*MWST*(1+MRAD), MXHIV=15000, MVHIV=MG, IBWM=1,
C      8          MRWXYZ=MRAD*MWST*MG, MWXYZ=MWST*MG, MGVAR=10, MSPEC=23,
C      9          NDIRMAX=37)
```

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 1. Variables used in BF2_PARAMS.INC

Parameter	Description
MX	Maximum number of grid blocks in the x-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 y-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 z-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: $MDIM = 3 * \{NEQ * [\text{MIN}(MX * MY, MX * MZ, MY * MZ) + 1] - 1\} + 1$
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.
MMAT	Maximum number of material 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 (e. g., brine pressure or gas saturation).
IBWM	Maximum bandwidth for Jacobian used in solution of multicomponent gas transport model within BRAGFLO; value to be used is computed from the formula: $IBWM = 3 * \text{MAX}(MX * MY, MX * MZ, MY * MZ) + 1$ 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 2. 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 look-up table to obtain gas density.
NCOMP	3	Number of components in all phases. Includes gas, brine, and gas dissolved in 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.

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
12. multicomponent gas transport parameters.



INPUTS FROM ALL SECTIONS EXCEPT SECTIONS 11 AND 12 ARE ALLOWED FOR THE 1996 WIPP PA CALCULATIONS.

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 Section 7.2.2.

7.2.0 PREBRAG QA Information

Unlike previous versions of BRAGFLO, version 4.00 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. If the input file is set up manually, this section should be omitted; go directly to Section 7.2.1.

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****

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 section, 7.2.1). 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.

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 rest of the input file is the same as in BRAGFLO version 3.62ZO, beginning with Line 1.1 in Section 7.2.1.

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

```
**QA**  
PREBRAG  -- Program name  
6.00     -- PREBRAG version number  
01/19/96 -- PREBRAG revision date  
01/25/96 -- PREBRAG run date  
11:13:44 -- PREBRAG run time  
Title of the run (Line 1.1)
```

7.2.1 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 SUPPORTED FOR THE 1996 WIPP PA 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), 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 7.2.3 (Mesh Parameters). This will be discussed in more detail in Subsection 7.2.3.

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 7.2.7 (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 7.2.6). 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).
- 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 ***
```

The next line is repeated NDTFIX times, each line with these 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].

7.2.2 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:

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

ASCII Output Controls.

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

Table 3. 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	mol	lbmol	0.4535237
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	$9.8692326671601282 \times 10^{-13}$

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

Line 2.4. IPRNTASC.

IPRNTASC: ASCII output time step frequency.



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

Line 2.4: NPTMEASC.
NPTMEASC: Number of specified times.

Line 2.4a: Descriptor.

Line 2.4b: TIMESASC (NPTMEASC values).
TIMESASC: Specified output times [s or days]

Binary output controls.

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

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

Line 2.6. IPRNTBIN.
IPRNTBIN: Binary output time step frequency.

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

Line 2.6. NPTMEBIN.
NPTMEBIN: Number of output times specified.

Line 2.6a. Descriptor. Output times.

Line 2.6b. TIMESBIN (NPTMEBIN values).
TIMESBIN: Specified binary output times [s or days]

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 7.3.

NOTE: RESTART CAPABILITY IS NOT ALLOWED FOR THE 1996 WIPP PA CALCULATION.

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

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

Line 2.8. IPRNTRST.
 IPRNTRST: Restart output time step frequency.

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

Line 2.8. NPTMERST.
 NPTMERST: Number of times to specify restart output.

Line 2.8a. Descriptor. Restart output times.

Line 2.8b. TIMESRST (NPTMERST values).
 TIMESRST: Specified restart output times [s or days].

Element Variables. The next input are the ASCII and binary print control flags. These flags indicate which of at least 95 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 4. The number of element variables available to be printed out depends on the number of waste regions in the mesh (defined in Subsection 7.2.7) and the number (if any) of radionuclides being tracked in the transport calculation. There are 95 element variables that are always available, none of which is associated with radionuclide transport. Of these 95 variables, 45 (numbers 49-93) 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 $NVPR = 95 + 3 * MWST * (1 + MRAD)$, 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.

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 4, 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 postprocessing. For example, *integration of brine flow past some boundary can be done in postprocessing 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 hard-wired to a particular mesh. Without history variables, postprocessing can only be done using the element variables, which are usually output at multistep intervals. Then, variables that change rapidly over a short period of time cannot be integrated accurately.

Line 2.13. Descriptor. History variables.

Line 2.14. NHIV.

NHIV: Total number of element variables (from the list in Table 1) 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.

LH: Element variable number from Table 1.

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

Table 4. Element variables available for printout in BRAGFLO. Variables 1 - 95 are, by default, available in any run. Variables 96 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 = 95 + 3 * MWST * (1 + MRAD) = 107 element variables.

No.	CAMCON Element Variable Name	Description	SI Units
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, x-direction	m ²
12	PERMBRY	Permeability to brine, y-direction	m ²
13	PERMBRZ	Permeability to brine, z-direction	m ²
14	PERMGASX	Permeability to gas, x-direction	m ²
15	PERMGASY	Permeability to gas, y-direction	m ²
16	PERMGASZ	Permeability to gas, z-direction	m ²
17	SATBRINE	Brine saturation	fraction void volume
18	SATGAS	Gas saturation	fraction void volume
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	fr Orig. Brine In Place
24	CWELLGAS	Cumulative well gas flow	fr Orig. Gas In Place
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. interblock brine flow, x-direction	m ³ /s (@ ref. conds)
32	FLOWBRY	Time-avg. interblock brine flow, y-direction	m ³ /s (@ ref. conds)

No.	CAMCON Element Variable Name	Description	SI Units
33	FLOWBRZ	Time-avg. interblock brine flow, z-direction	m ³ /s (@ ref. conds)
34	FLOWGASX	Time-avg. interblock gas flow, x-direction	m ³ /s (@ ref. conds)
35	FLOWGASY	Time-avg. interblock gas flow, y-direction	m ³ /s (@ ref. conds)
36	FLOWGASZ	Time-avg. interblock 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	mol/s
40	CORRATH	Humid corrosion rate-simple model	mol/s
41	BIORATI	Inundated biodegradation rate-simple model	mol/s
42	BIORATH	Humid biodegradation rate-simple model	mol/s
43	H2RATE	H ₂ generation rate-simple model	kg/(sm ³)
44	BRINRATE	Brine consumption rate-simple model	kg/(sm ³)
45	FERATE	Fe consumption rate-simple model	kg/(sm ³)
46	CELLRATE	Biodegrad consumption rate-simple model	kg/(sm ³)
47	FECONC	Fe concentration-simple model	kg/m ³
48	CELLCONC	Biodegradables concentration-simple model	kg/m ³
49	H2_R	H ₂ generation rate-reaction path model	kg/(sm ³)
50	CO2_R	CO ₂ generation rate-reaction path model	kg/(sm ³)
51	CH4_R	CH ₄ generation rate-reaction path model	kg/(sm ³)
52	N2_R	N ₂ generation rate-reaction path model	kg/(sm ³)
53	H2S_R	H ₂ S generation rate-reaction path model	kg/(sm ³)
54	O2_R	O ₂ generation rate-reaction path model	kg/(sm ³)
55	H2O_R	H ₂ O generation rate-reaction path model	kg/(sm ³)
56	H2SO4_R	H ₂ SO ₄ generation rate-reaction path model	kg/(sm ³)
57	HNO3_R	HNO ₃ generation rate-reaction path model	kg/(sm ³)
58	CH2O_R	Biodegrad consumption rate-reaction path model	kg/(sm ³)
59	FE_R	Fe consumption rate-reaction path model	kg/(sm ³)
60	FES2F_R	FeS ₂ generation rate-reaction path model	kg/(sm ³)
61	FES2O_R	FeS ₂ generation rate-reaction path model	kg/(sm ³)
62	FECO3F_R	FeCO ₃ generation rate-reaction path model	kg/(sm ³)
63	FECO3O_R	FeCO ₃ generation rate-reaction path model	kg/(sm ³)
64	FEOH2_R	Fe(OH) ₂ generation rate-reaction path model	kg/(sm ³)
65	FEOOH_R	FeO(OH) generation rate-reaction path model	kg/(sm ³)

No.	CAMCON Element Variable Name	Description	SI Units
66	FE3O4_R	Fe ₃ O ₄ generation rate–reaction path model	kg/(sm ³)
67	FES_R	FeS generation rate–reaction path model	kg/(sm ³)
68	CAO_R	CaO generation rate–reaction path model	kg/(sm ³)
69	CAOH2_R	Ca(OH) ₂ generation rate–reaction path model	kg/(sm ³)
70	CACO3_R	CaCO ₃ generation rate–reaction path model	kg/(sm ³)
71	H2_RAD_R	H ₂ generation rate–radiolysis	kg/(sm ³)
72	H2_C	H ₂ concentration–reaction path model	kg/(sm ³)
73	CO2_C	CO ₂ concentration–reaction path model	kg/m ³
74	CH4_C	CH ₄ concentration–reaction path model	kg/m ³
75	N2_C	N ₂ concentration–reaction path model	kg/m ³
76	H2S_C	H ₂ S concentration–reaction path model	kg/m ³
77	O2_C	O ₂ concentration–reaction path model	kg/m ³
78	H2O_C	H ₂ O concentration–reaction path model	kg/m ³
79	H2SO4_C	H ₂ SO ₄ concentration–reaction path model	kg/m ³
80	HNO3_C	HNO ₃ concentration–reaction path model	kg/m ³
81	CH2O_C	Biodegradables concentration–reaction path model	kg/m ³
82	FE_C	Fe concentration–reaction path model	kg/m ³
83	FES2F_C	FeS ₂ concentration–reaction path model	kg/m ³
84	FES2O_C	FeS ₂ concentration–reaction path model	kg/m ³
85	FECO3F_C	FeCO ₃ concentration–reaction path model	kg/m ³
86	FECO3O_C	FeCO ₃ concentration–reaction path model	kg/m ³
87	FEOH2_C	Fe(OH) ₂ concentration–reaction path model	kg/m ³
88	FEOOH_C	FeO(OH) concentration–reaction path model	kg/m ³
89	FE3O4_C	Fe ₃ O ₄ concentration–reaction path model	kg/m ³
90	FES_C	FeS concentration–reaction path model	kg/m ³
91	CAO_C	CaO concentration–reaction path model	kg/m ³
92	CAOH2_C	Ca(OH) ₂ concentration–reaction path model	kg/m ³
93	CACO3_C	CaCO ₃ concentration–reaction path model	kg/m ³
94	H2_RAD_C	H ₂ concentration–radiolysis	kg/m ³
95	H2OFLOWI	Water inflow rate	kg/s
96	BM1TOT	Total isotope mass from Waste Region 1	kg
97	BC1TOT	Total isotope conc. from Waste Region 1	kg/m ³
98	SM1TOT	Total solid isotope mass from Waste Region 1	kg

No.	CAMCON Element Variable Name	Description	SI Units
99	BM1PU240	Mass of isotope 1 (Pu240) from Waste Region 1	kg
100	BM1U236	Mass of isotope 2 (U236) from Waste Region 1	kg
101	BM1TH232	Mass of isotope 3 (Th232) from Waste Region 1	kg
102	BC1PU240	Conc. of isotope 1 from Waste Region 1	kg/m ³
103	BC1U236	Conc. of isotope 2 from Waste Region 1	kg/m ³
104	BC1TH232	Conc. of isotope 3 from Waste Region 1	kg/m ³
105	SM1PU240	Solid mass of isotope 1 from Waste Region 1	kg
106	SM1U236	Solid mass of isotope 2 from Waste Region 1	kg
107	SM1TH232	Solid mass of isotope 3 from Waste Region 1	kg

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

IJHIV: 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 7.2.15). In addition, the summary 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.

In the current version of BRAGFLO, the following nine variables are printed at the monitor grid blocks: PO (brine pressure, Pa), PG (gas pressure, Pa), SO (brine saturation), PHI (porosity), PERMGX (permeability to gas in the x-direction, m²), CONCFE (iron concentration, kg/m³), CONCBIO (cellulosics concentration, kg/m³), QR(1) [H₂ generation rate, kg/(s m³)], QOBLOCKI (interblock brine flow in x-direction, m³/s at reference conditions), QOBLOCKJ (interblock brine flow in y-direction, m³/s at reference conditions), QGBLOCKI (interblock gas flow in x-direction, m³/s at reference conditions), QGBLOCKJ (interblock gas flow in y-direction, m³/s at reference conditions).

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 statement>
*** 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.

7.2.3 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) are to be read.

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

IDZFLAG: Specifies how grid block width Δz (DZGRID) are 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.

IDDEPTHFLAG = 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.
= 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 ***

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 = 0:

Line 3.4. DXCONST.

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

If IDXFLAG = 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 = 0:

Line 3.6. DYCONST.

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

If IDYFLAG = 1:

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

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

If IDYFLAG = 2:

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

DYGRID(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 = 0:

Line 3.8. DZCONST.

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

If IDZFLAG = 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 = 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 = 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 = 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 = 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 = 1:

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

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

If IDEPTHFLAG = 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 = 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 = 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 = 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 = 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 = 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].

If IDEPTHFLAG < 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 = -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 place holder values (three integers and four real numbers) must be input.

If IDEPTHFLAG = -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 place holder values (three integers and four real numbers) must be input.

If IDEPTHFLAG < -2:

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.

7.2.4 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) are 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. These problems can be eliminated by specifying Dirichlet bound-

ary conditions. 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.

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 have 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 $\text{bbl}\cdot\text{cP}/(\text{day}\cdot\text{psi})$]. 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 km x 60 km x 100 m, a productivity index of $1.0 \times 10^{-6} \text{ m}^3$ [$3.7 \times 10^{12} \text{ bbl}\cdot\text{cP}/(\text{day}\cdot\text{psi})$] 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.

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.

7.2.5 Initial Conditions

Initial conditions must be input for brine pressure, brine saturation, iron concentration, and cellulose 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. Cellulose concentration initial conditions.

Line 5.8. (((**CONCBIO**(I,J,K), I=1, NX), J=1, NY), K=1, NZ).
CONCBIO: Initial cellulose 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 cellulose), 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 $START \geq TIMEICRESET$ (described in Subsection 7.2.7; generally, $TIMEICRESET = 0.$), 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 $START < TIMEICRESET$, 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, $CONCFE$ and $CONCBIO$, are not used until after $TIMEICRESET$; furthermore, reactions that affect the values of $CONCFE$ and $CONCBIO$ 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 $CONCFE$ and $CONCBIO$ 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 $TIMEICRESET$.

7.2.6 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: $1.0 + DEPLIMIT(1) > S_g > -DEPLIMIT(1)$. 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: $DEPLIMIT(1) = 0.2$.

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: $PO > DEPLIMIT(2)$. If $PO \leq DEPLIMIT(2)$, 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; interstep 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: $1.0 + SATLIMIT > S_g > -SATLIMIT$ provided that $DEPLIMIT(1) > SATLIMIT$. Nonconvergence 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 $DEPLIMIT(1) > SATLIMIT$. 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 variables changes for normal convergence.



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: 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: 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 simply 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 for use in PA 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: 2.0.

EPSLOOSE(2): Same meaning as EPSNORM(2); used after IJACSWITCH time step reductions have occurred. Recommended value: 0.01.

Line 6.13. Descriptor. Normal right-hand-side function (or residual) criteria. 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, roundoff errors, discontinuous functional dependencies, property functions with discontinuous derivatives, and nonlinearities 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: 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: 1.0×10^{-2} .

Line 6.15. Descriptor. Loosened right-hand-side function criteria. *This feature has not been tested for use in PA 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: 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: 1.0×10^{-1} .

Line 6.17. Descriptor. Multicomponent 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 [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 [mol/m^3].

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

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 4.00 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.

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.

LSOR: Point successive overrelaxation (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.

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 nonconvergence 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 nonconvergence 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 nonconvergence 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 impracticably 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 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 roundoff 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 roundoff 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_a and P_o . P_a 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_a , which is directly proportional to the mass or mole fraction of gas dissolved in brine:

$$P_a = x_g H,$$

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 = 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 = 1), because this may cause the solution to oscillate and fail to converge. Recommended value: same as ITMAX, 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 7.2.8); 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.* Recommended value: same as ITMAX, 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.

DELTFACTOR: Time step reduction factor when nonconvergence 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 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, strictly 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; 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*; 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.

7.2.7 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 MAXMAT-

TIMES, 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.

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 generally applications. The material 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. In addition, 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. 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, 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 7.2.5. Then, at some later time (TIMEICRESET), the conditions in the Waste can be reset to the initial conditions specified in Subsection 7.2.5.

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 submodel only for this material type (provided that model is turned on; input controlling this submodel 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_WASTE(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 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 (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 7.2.5. This differs from DRZ material in that both saturation and pressure are reset at time TIMEICRESET, and they are reset to the Subsection 7.2.5 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 7.2.5 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 easily provided in the original conditions in Subsection 7.2.5.

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 $\text{NMATRESET} \leq 0$, the next two lines (7.19 and 7.20) are omitted. If $\text{NMATRESET} > \text{NMAT}$, the run will abort.

Line 7.19. Descriptor. "Reset" materials.

Line 7.20. (MATRESET(I), I=1, NMATRESET).

MATRESET: Material type index numbers for materials in which the brine pressure, PO, and brine saturation, SO, will be reset to the original (Subsection 7.2.5) 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 postprocessing 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 reports, 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.

ICWASTE: Flag to indicate that waste initial conditions will differ from the initial conditions specified in Subsection 7.2.5. 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.

If TIMEICRESET = START, the ICWASTE must be 0. Otherwise, BRAGFLO will abort with the message:

```
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].

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 7.31. Descriptor. Relative permeability and capillary pressure model parameters.

The next line is repeated NMAT times. 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.

Line 7.32. 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 7.33. Descriptor. More relative permeability and capillary pressure model parameters.

Line 7.34. 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 $SBMIN(I) \geq SBR(I)$. If $SBMIN(I) < SBR(I)$, BRAGFLO will abort, even if $KPC(I) \neq 3$. Recommended value: $1.05 \times SBR(I)$.

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 $POMIN(I) = 1.01325 \times 10^5$ 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 $PCMAX(I) = 1.0 \times 10^8$ 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.

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: $P_{ct} = a k^n$, 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: $P_{ct} = a k^n$, 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 7.35. Descriptor. Intrinsic properties.

The next line is repeated NMAT times.

Line 7.36. 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].

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.

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];
 ϕ_o = intact porosity [m^3 void/ m^3 rock];
 n = exponent [dimensionless].

Line 7.37. Descriptor. Fracture model control.

Line 7.38. 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 7.39 -7.42 are input *only* if K FRACTURE = .TRUE.

Line 7.39. Descriptor. Number of materials in which the fracture model can be applied.

Line 7.40. NFRAC.

NFRAC: Number of materials in which the fracture model can be applied.

The following two lines are repeated NFRAC times.

Line 7.41. Descriptor. Fracture model parameters.

Line 7.42. I, FRPI(I), FRPF(I), FRPHIMAX(I), FRPRMEXP(I), IFRX(I), IFRY(I), IFRZ(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.

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.

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]

$$= BKLINK \cdot (k_w)^{EXPKLINK}$$

$BKLINK$ = linear parameter in Klinkenberg equation [Pa],

$EXPKLINK$ = exponent in Klinkenberg equation [dimensionless].

It is assumed in BRAGFLO that input values of intrinsic permeability (Line 7.36) 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; K FRACTURE = .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.

Line 7.43. Descriptor. Klinkenberg effect control parameter.

Line 7.44. 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 7.45. Descriptor. Klinkenberg parameters.

Line 7.46. `BKLINK`, `EXPKLINK`.

`BKLINK`: Linear parameter in Klinkenberg equation [Pa]. Recommended value:
 9.8×10^{-1} Pa.

`EXPKLINK`: Exponent in Klinkenberg equation [dimensionless]. Recommended
value: -0.33.

7.2.8 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 (H_2), carbon dioxide (CO_2), methane (CH_4), nitrogen (N_2), oxygen (O_2), and hydrogen sulfide (H_2S). 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.

Line 8.1. Descriptor. Reference conditions.

Line 8.2. `TREF`, `PREF`.

`TREF`: Reference temperature for standard densities [K or °R].

`PREF`: Reference pressure for standard densities [Pa or psi].

Line 8.3. Descriptor. Brine property parameters.

Line 8.4. `SALT`, `DENOSC`, `KGSAT`, `IDGAS`, `BRCOMP`.

`SALT`: Brine salinity [wt % solute]. Lambert (1983) reports two values of solute concentrations in groundwaters from the Salado Formation: 355,100 mg/L and 372,000 mg/L; using the average value of 363,550 mg/L, assuming the reported values are total dissolved solids, and using brine density at 27 °C (300.15 K) of 1230 kg/m^3 , the salinity of Salado brine is 29.6 wt %.

`DENOSC`: Density of brine at reference conditions [kg/m^3 or lb/ft^3]. The density of WIPP brine at 101.325 kPa and 27 °C (300.15 K) averages 1230 kg/m^3 .

`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 $2.5 \times 10^{-10} \text{ Pa}^{-1}$. 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/m^3].

If IDGAS = 0, no additional gas dissolution parameters are read in; skip to Line 8.5.

If IDGAS = 1, input Lines 8.4a, 8.4b, 8.4c, and 8.4d:

Line 8.4a. 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 8.4b. 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 8.4c. Descriptor. Slopes of parameters at pressures greater than the bubble pressure.

Line 8.4d. BSLOPE, RSLOPE, VSLOPE.

BSLOPE: Slope of the brine formation volume factor versus pressure curve for undersaturated brine (pressure above initial brine bubble point pres-

sure): 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): $d(R_{so}) / dP$ [Pa^{-1} or $\text{ft}^3/(\text{bbl}\cdot\text{psi})$]. 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 IDGAS = 2, read Lines 8.4a and 8.4b.

Line 8.4a. Descriptor. Henry's law constant.

Line 8.4b. HENRYC.

HENRYC: Henry's law constant [Pa/mol fraction gas dissolved in brine]. 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 IDGAS = 2, a value for LVARSWTCH = T should be used; see Line 6.22.

Line 8.5. 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 8.6. VISO, VISG.

VISO: Brine viscosity [Pa*s or cP]. The viscosity of WIPP brine at 27 °C (300.15 K) and 101.325 kPa is 1.8×10^{-3} Pa*s.

VISG: Gas viscosity [Pa*s or cP]. The viscosity of hydrogen at 27 °C (300.15 K) and 101.325 kPa is 8.92×10^{-6} Pa*s.

Line 8.11. Descriptor. Gas density flag.



Line 8.12. 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: H_2 , CO_2 , CH_4 , N_2 , O_2 , and H_2S . 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 multicomponent 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 equation of state (INTERPDENG = 0) must be solved each time a new density is needed.

Line 8.13. Descriptor. Gas composition.

Line 8.14. (YGAS(I), I=1, MGAS), NGAS, N1GAS.

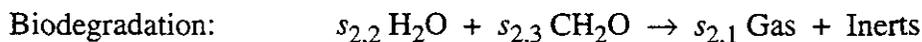
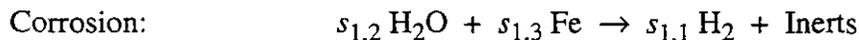
YGAS: Initial mole fraction of each of the MGAS gases currently available in BRAGFLO (MGAS = 6; set in the PARAMETER statement). If the gas transport option is used, this composition can change during the run. If gas transport is not used, this initial gas composition will remain fixed for all time.

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 = O₂, 6 = H₂S. 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.

7.2.9 Chemical Reaction Parameters

These parameters govern the chemical reactions that are modeled in BRAGFLO. Two reactions are modeled: corrosion of iron and microbial degradation of cellulose. These reactions take place only in the Waste. Cellulose is approximated by the pseudo-molecule CH₂O, having a molecular weight of 30.02628 x 10⁻³ kg/mol. The reactions are written as:



Both reactions are assumed to be zeroth order in kinetics with respect to the solid reactants. In other words, the rate of reaction is independent of the iron or cellulose concentration. The gas produced in the biodegradation reaction 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 CH₂O consumption and no gas generation.

= 1: Fe and CH₂O consumption with gas generation.

= 2: Reaction path gas generation model. (Not yet available.)

If IGASVAR = 0, no more chemical reaction parameters are input; go to Section 10.

Line 9.3. Descriptor. Reaction rate constants for brine-inundated conditions.

Line 9.4. RK(1), RK(2).

RK(1): Corrosion reaction rate constant under brine-inundated conditions [mol Fe/(s•m³) or lbmol Fe/(day•ft³)].

RK(2): Biodegradation reaction rate constant under brine-inundated conditions [mol CH₂O/(s•m³) or lbmol CH₂O/(day•ft³)].

Line 9.5. Descriptor. Humid rate factors.

Line 9.6. HF(1), HF(2).

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. Stoichiometry for corrosion.

BRAGFLO currently assumes that the two gas generation reactions are written with $s_{1,3} = s_{2,3} = 1.0$. Both of these stoichiometric coefficients must be input with a value of 1.0; if a value other than 1.0 is input, the results will be wrong.

Line 9.8. S(1,1), S(1,2), S(1,3).

S(1,1): Stoichiometric coefficient $s_{1,1}$ for the corrosion reaction [mol H₂/mol Fe].

S(1,2): Stoichiometric coefficient $s_{1,2}$ for the corrosion reaction [mol H₂O/mol Fe].

S(1,3): Stoichiometric coefficient $s_{1,3}$ for the corrosion reaction [mol Fe/mol Fe].

Required input value: 1.0 mol Fe/mol Fe.

Line 9.9. Descriptor. Stoichiometry for biodegradation.

Line 9.10. S(2,1), S(2,2), S(2,3).

S(2,1): Stoichiometric coefficient $s_{2,1}$ for the biodegradation reaction [mol H₂/mol CH₂O].

S(2,2): Stoichiometric coefficient $s_{2,2}$ for the biodegradation reaction [mol H₂O/mol CH₂O].

S(2,3): Stoichiometric coefficient $s_{2,3}$ for the biodegradation reaction [mol CH₂O/mol CH₂O]. Required input value: 1.0 mol CH₂O/mol CH₂O.

Line 9.11. Descriptor. Additional reaction parameters.

Line 9.12. SATWICK, LARXN, 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 the actual brine saturation, S_b , to calculate reaction rates, an effective brine saturation, $S_{b,eff}$ is used, where

$$S_{b,eff} = S_b + S_w(1 - e^{\alpha S_b})$$

The factor α is ALPHARXN, and S_w is SATWICK. This function smoothes $S_{b,eff}$; it was intended originally for $S_{b,eff}$ to be $S_b + S_w$ but this function is discontinuous at $S_b = 0$, which can cause numerical difficulties that may lead to incorrect results.

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.

ALPHARXN: Term used in smoothing functions to eliminate a discontinuity at brine saturation, $S_b = 0$. Always used in expression to obtain $S_{b,eff}$ when wicking is modeled (i. e., when SATWICK > 0.). When LARXN = T, ALPHARXN (or α) is used in the smoothing function for both humid corrosion and biodegradation rates:

$$r_{h,eff} = r_h(1 - e^{\alpha S_b})$$

where:

r_h = humid corrosion or biodegradation rate
 = HF(1) x RK(1), or HF(2) x RK(2);
 $r_{h,eff}$ = effective (smoothed) humid corrosion or biodegradation rate.

If LARXN = F, then ALPHARXN is not used for the humid corrosion and biodegradation rates, and $r_{h,eff} = r_h$. The full corrosion or biodegradation rate is given by [where r_i is the inundated rate, RK(1) or RK(2)]:

$$r = S_b r_i + (1 - S_b) r_{h,eff}, \quad S_b > 0$$

$$= 0, \quad S_b = 0$$



so, unless $r_{h,eff} = 0$, r will be discontinuous at $S_b = 0$. 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.

7.2.10 Creep Closure Parameters

These parameters activate the creep closure submodel. 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 nonbackfilled 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 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 CLOSURE = .FALSE., no more closure data are input; go to Subsection 7.2.11.

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.

= 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), CLOSPERFACT(I), CLOSPERMEXP(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 7.36. 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 circum-

stances. 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.

CLOSPERMFACT(I): Constant factor, a , in expression relating permeability, k , to porosity, ϕ , in each region undergoing dynamic creep closure [m^2]:

$$k = a\phi^\eta$$

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 7.36). If KLOSAVE = 1, all grid blocks using the same closure surface will have the same porosity and, consequently, the same permeability. Recommended value: $1.0 \times 10^{-11} m^2$.

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.

Line 10.7. Descriptor. Creep closure material control parameter.

Line 10.8. 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 7.2.11.

Line 10.9. Descriptor. Creep closure parameters associating a material number with a creep closure model number.

The following line is repeated NMATCLOS times:

Line 10.10. 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)



7.2.11 Radionuclide Transport and Decay Parameters

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.

Because of stability limitations and potentially extreme run times associated with the current implementation of transport and radionuclide decay, this submodel of BRAGFLO is of limited use and is being phased out. It is being 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 7.2.12.

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.

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 [mol O₂/mol H₂]:
 $H_2O \rightarrow H_2 + (SRADO2) O_2$.

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:

$$M_{w,O_2} \cdot SRADO2 = 31.9988 \times 10^{-3} SRADO2 \text{ [kg O}_2 \text{ / mol H}_2 \text{] ,}$$

where:

M_{w,O_2} = molecular weight of O₂ [kg O₂ / mol O₂],

M_{w,H_2} = molecular weight of H₂ [kg H₂ / mol H₂].

When this mass is treated as an equal mass of H₂, it is equivalent to:



$$\begin{aligned} \frac{M_{w,O_2} \cdot SRADO2}{M_{w,H_2}} &= \frac{31.9988 \times 10^{-3} SRADO2 \left[\frac{\text{kg H}_2 (= \text{kg O}_2)}{\text{mol H}_2} \right]}{2.01588 \times 10^{-3} \left[\frac{\text{kg H}_2}{\text{mol H}_2} \right]} \\ &= 15.8734 \cdot SRADO2 \text{ [mol H}_2 \text{ / mol H}_2 \text{]} \\ &= 7.93668 \text{ [mol H}_2 \text{ / mol H}_2 \text{]} \end{aligned}$$

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., $H_2O \rightarrow H_2 + 1/2 H_2$), rather than

$M_{w,O_2} \cdot SRADO2$ kg of H_2 . Then the value $SRADO2$ should have in order to produce 0.5 mol H_2 can be calculated from:

$$\frac{1}{2}[\text{mol } H_2 / \text{mol } H_2] = \frac{M_{w,O_2} \cdot SRADO2}{M_{w,H_2}},$$

or,

$$\begin{aligned} SRADO2 &= \frac{\frac{1}{2} M_{w,H_2}}{M_{w,O_2}} \\ &= \frac{\left(\frac{1}{2}\right) 2.01588 \times 10^{-3}}{31.9988 \times 10^{-3}} \\ &= 0.0314993. \end{aligned}$$

GH2AVG: Average "G" value for H_2 [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].

Line 11.19. Descriptor. Atomic weights.

Line 11.20. (AWT(I),I=1,NRAD).
AWT: Atomic weight of isotope IDION [kg/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 [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 gridblocks 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 interblock 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 increased, but should remain below 1.0. Increasing either of these will increase the computational effort.

7.2.12 Multicomponent Gas Transport Parameters

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 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 input.



7.3 Restart Capability

NOTE: THE RESTART CAPABILITY IS NOT ALLOWED FOR THE 1996 WIPP CALCULATIONS.

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 something, 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 postprocessing 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 instances, 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. Postprocessing. The binary file from the restart run will have the same structure as the initial run, but start from the restart time. Before postprocessing 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.

8.0 ERROR MESSAGES

BRAGFLO outputs a number of error messages and aborts execution when it detects invalid input parameters. Explanations of these error messages can be found in Section 7.0.

9.0 DESCRIPTION OF OUTPUT FILES

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 postprocessing 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 postprocessing.

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 postprocessing.

PROGRAM BINREAD

```
C
C   Translates BRAGFLO binary file into ASCII file.
C   J. Schreiber, SAIC, 03/08/96
C
C   PARAMETER (MX=50,MY=40,MZ=10,NVPR=107,MXHIV=15000,
1    MVHIV=MX*MY*MZ,MGVAR=10)
C
C   CHARACTER*8   RTIME(2),PNAME(2),VRSION(2),UNITS,REVDATE(2)
C   CHARACTER*8   NAMVAREL(NVPR),NAMVARHI(MXHIV),NAMVARGL(MGVAR)
C   CHARACTER*50  LABEL(L,NVPR),LABELHI(MXHIV),LABELGL(MGVAR)
C   CHARACTER*20  LABUNTEL(NVPR),LABUNTHI(MXHIV),LABUNTGL(MGVAR)
C   CHARACTER*9   DATE(2)
C   CHARACTER*32  CPUNAME
C   CHARACTER*1   FILTYP
C   CHARACTER*80  FILNAM(6),BRAGNAM
C   CHARACTER*132 TITLE
C   DIMENSION IIVHIV(MVHIV,NVPR),JJHIV(MVHIV,NVPR),KKHIV(MVHIV,NVPR)
C   DIMENSION UNTCNVEL(NVPR),UNTCNVHI(MXHIV),UNTCNVGL(MGVAR)
C   DIMENSION DXGRID(MX,MY,MZ),DYGRID(MX,MY,MZ),DZGRID(MX,MY,MZ)
C   DIMENSION GRIDVOL(MX,MY,MZ),LHI(NVPR),LE(NVPR),LH(MXHIV),LG(MGVAR)
C   DIMENSION HVAR(MXHIV),YY(MX,MY,MZ),NGBHIV(NVPR)
C   REAL IBBALMX,JBBALMX,KBBALMX,IGBALMX,JGBALMX,KGBALMX
C
C
C   WRITE (*,*) 'Enter name of BRAGFLO binary file.'
C   READ (*,'(A)') BRAGNAM
C
C   OPEN (8,FILE=BRAGNAM,STATUS='OLD',FORM='UNFORMATTED')
C   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 vbIs printed
C at each time step.
C NHIV = No. of element vbIs that are printed as history vbIs.
C NGVAR = Number of global variables.
C

```
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 4 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 LABLEL = 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

```
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),LABLEL(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   Mesh dimensions and grid block volumes.
```

```
C
C   READ (8) ((DXGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
C   READ (8) ((DYGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
C   READ (8) ((DZGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
C   READ (8) ((GRIDVOL(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
```

```
C
C   *** End of header section (READ) ***
```

```
C
C
C   IF (PNAME(1)(1:7) .EQ. 'PREBRAG') THEN
C     WRITE (9,*) '** PREBRAG Program Name **'
C     WRITE (9,*) PNAME(1)
C     WRITE (9,*) '** PREBRAG Version Number **'
C     WRITE (9,*) VRSION(1)
C     WRITE (9,*) '** PREBRAG Revision Date **'
C     WRITE (9,*) REVDATE(1)
C     WRITE (9,*) '** PREBRAG Run Date **'
C     WRITE (9,*) DATE(1)
C     WRITE (9,*) '** PREBRAG Run Time **'
C     WRITE (9,*) RTIME(1)
C   END IF
```

```
C
C   WRITE (9,*) '** BRAGFLO Run Date **'
C   WRITE (9,*) DATE(2)
C   WRITE (9,*) '** BRAGFLO Run Time **'
C   WRITE (9,*) RTIME(2)
C   WRITE (9,*) '** BRAGFLO Program Name **'
C   WRITE (9,*) PNAME(2)
C   WRITE (9,*) '** BRAGFLO Version Number **'
C   WRITE (9,*) VRSION(2)
C   WRITE (9,*) '** BRAGFLO Revision Date **'
C   WRITE (9,*) REVDATE(2)
```

```
C
C   WRITE (9,*) '** Computer Name **'
C   WRITE (9,*) CPUNAME
C   WRITE (9,*) '** Output File Type **'
C   WRITE (9,*) FILTYP
C   WRITE (9,*) '** Number of Files Used **'
C   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        LABELEL(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  
C  
C  
*** End of header section (WRITE) ***
```



```
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 vbls and global and element vbls output
C                       will follow at this time step.
C
C     NPO = 0
110 READ (8,END=130) TIME,TIMED,TIMEYR,DELT,DELTD,DELTyr,AVGITER,
1   CPUS,CPUHR,RNSTEP,RITERTOT,KBIN
   IF (MHIV .GT. 0) READ (8,END=130) (HVAR(I),I=1,MHIV)
C
C   WRITE (9,*)
C   WRITE (9,*)
C   WRITE (9,*) '*** TIME (s,d,y), DELT (s,d,y), IterAvg, CPU (s,hr), '
1  //' Step No., IterTot, KBIN'
C   WRITE (9,*) TIME,TIMED,TIMEYR,DELT,DELTD,DELTyr,AVGITER,
1  CPUS,CPUHR,RNSTEP,RITERTOT,KBIN
C   WRITE (9,*)
C   WRITE (9,*) '*** History Vbls at Time Step',RNSTEP
C   IF (MHIV .LE. 0) THEN
C     WRITE (9,*) ' (no element-variable-based history variables)'
C   ELSE
C     WRITE (9,*) (HVAR(I),I=1,MHIV)
C   END IF
C
C   (History vbls only, if KBIN=0)
C
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
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
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 Appendix B.

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, PHI,	PERMGX, CONCFE, CONCBIO, QR(1),						
6		QOBLOCKI, QOBLOCKJ, QGBLOCKI, QGBLOCKJ							
7	Monitor Block # 1:	(11, 10, 1)							
8		6.8534030052E+06	6.8534030052E+06	9.9993392867E-01	3.7000000000E-01				
9		3.1650984593E-12	1.3691991909E+02	8.0880900000E+01	0.0000000000E+00				
10		1.8074126802E-07	2.3477482289E-09	0.0000000000E+00	2.4378208877E-14				
11	Monitor Block # 2:	(17, 10, 1)							
12		6.7853807274E+06	6.7919359916E+06	2.0800797783E-03	1.3559451410E-01				
13		5.5888660300E-12	1.3614295550E+02	8.0880900000E+01	7.1966507423E-12				
14		0.0000000000E+00	0.0000000000E+00	1.3059617970E-04	-6.8230599392E-05				
15	Monitor Block # 3:	(25, 12, 1)							
16		7.3286118606E+06	7.3323394444E+06	1.0000000000E+00	1.7791276293E-02				
17		1.8197020000E-19	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00				
18		-3.3526725094E-09	-1.5699372612E-09	0.0000000000E+00	0.0000000000E+00				

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

$$EPSMAX(1) = \max(\Delta S_g \times 10^{\epsilon_1}),$$

$$EPSMAX(2) = \max\left(\frac{\Delta P_b}{P_b \epsilon_2}\right),$$



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.

$$FTOLMAX(1) = \begin{cases} \max\left(\frac{F_1/T_{3g}}{f_1}\right), & T_{3g} \geq T_{3o} \text{ and } F_1 > f_1, \\ \max\left(\frac{F_1}{f_1}\right), & T_{3g} \geq T_{3o} \text{ and } F_1 \leq f_1, \\ 0., & T_{3g} < T_{3o}, \end{cases}$$

$$FTOLMAX(2) = \begin{cases} \max\left(\frac{F_2/T_{3b}}{f_2}\right), & T_{3b} \geq T_{3o} \text{ and } F_2 > f_2, \\ \max\left(\frac{F_2}{f_2}\right), & T_{3b} \geq T_{3o} \text{ and } F_2 \leq f_2, \\ 0., & T_{3b} < T_{3o}, \end{cases}$$

F_1 = discretized gas mass balance equation (see p. 38),
 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 roundoff.

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]:

$\epsilon_1 = EPSNORM(1)$ = required number of digits of accuracy to the right of the decimal in the change in gas saturation from the last time step.
 $\epsilon_2 = EPSNORM(2)$ = 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] 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 $\text{ICONVTEST} = 0$.

When convergence is *not* obtained within ITMAX [Line 6.22] 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),
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].

GASBALMAX and BRNBALMAX are computed as follows:

$$\text{GASBALMAX} = \max(F_1),$$

$$\text{BRNBALMAX} = \max(F_2).$$

These mass balance measures are closely related to FTOLMAX (1) and FTOLMAX (2), respectively, the latter being normalized by $T_{3g}f_1$ or $T_{3b}f_2$ in the denominator.

Lines 5 and 6 indicate which arrays are being monitored (see discussion of Monitor Blocks, Lines 2.17 - 2.22, in Section 7.2.2). In this example, three grid blocks are being monitored; the grid block locations are indicated on lines 7, 11, and 15. For each monitored grid block, the 12 array values being monitored are listed on the three lines that follow the grid block location.

9.4 Restart Output (.ROT) File



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.

10.0 REFERENCES

- Aziz, K. and Settari, A., 1979, *Petroleum Reservoir Simulation*, Applied Science Publishers, Essex, England.
- Brooks, R.H. and Corey, A.T., 1964, "Hydraulic Properties of Porous Media," Hydrology Paper No. 3. Fort Collins, CO: Colorado State University.
- Butcher, B.M., S.W. Webb, and J.W. Berglund. 1995. *System Prioritization Method—Iteration 2. Baseline Position Paper: Disposal Room and Cuttings Models, Volume 2, Appendix F*. March 28, 1995. Albuquerque, NM: Sandia National Laboratories.
- Corey, A.T., 1990, *Mechanics of Immiscible Fluids in Porous Media*, Water Resources Publications, Littleton, CO, pg. 98.
- Darcy, H. 1856. *Les fontaines publiques de la ville de Dijon*. Dalmont, Paris.
- Key, S., Fewell, M., Vaughn, P., Lord, M. and Labreche, D., 1994. *Background and Basis for the Fluid Flow Model Incorporated in BRAGFLO for Representing Pore Pressure-Induced Alterations in Permeability and Porosity in the Anhydrite Interbeds Above and Below the WIPP Repository Horizon*, SAND94-0381. Albuquerque, NM: Sandia National Laboratories.
- Klinkenberg, L.J., 1941, "The Permeability of Porous Media to Liquids and Gases," *Drilling and Production Prac.*, API, pp. 200-213.
- Lambert, S. J. 1983. *Dissolution of Evaporites in and Around the Delaware Basin, Southeastern New Mexico and West Texas*. SAND82-0461. Albuquerque, NM: Sandia National Laboratories.
- Maron, M.J. 1982. *Numerical Analysis: A Practical Approach*. Macmillan Publishing Co., Inc.: New York, New York.
- Peaceman, D.W., 1977, *Fundamentals of Numerical Reservoir Simulation*, Elsevier Scientific Publishing Co., Amsterdam.
- Stone, C.M. 1995, "Transfer of Porosity and Gas Curves From SANTOS for the Final Porosity Surface," Memorandum to B.M. Butcher, Sandia National Laboratories, Albuquerque, NM. December 19, 1995.
- Thomas, G.W., 1982, *Principals of Hydrocarbon Reservoir Simulation*, IHRDC, Publishers, Boston.

Van Genuchten, R., 1978, *Calculating the Unsaturated Hydraulic Conductivity with a New Closed-Form Analytical Model*, Research Report 78-WR-08. Princeton, NJ: Princeton University, Department of Civil Engineering.

Walas, S.M. 1985. *Phase Equilibria in Chemical Engineering*. Butterworth Publishers, Boston, MA, pp. 43-54.

WIPP PA (Performance Assessment) Department, 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992-Volume 3: Model Parameters*. SAND92-0700/3, Albuquerque, NM: Sandia National Laboratories.

WIPP PA (Performance Assessment) Department, 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992-Volume 5: Uncertainty and Sensitivity Analyses of Gas and Brine Migration for Undisturbed Performance*. SAND92-0700/5, Albuquerque, NM: Sandia National Laboratories.

