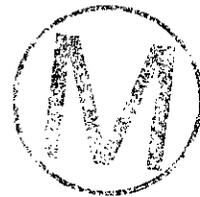

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Application
for the
Waste Isolation Pilot Plant**

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WIPP PA
User's Manual

for

GRASP-INV (Version 2.01)



Document Version 1.00

WPO # 30636

January 31, 1996

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GLOSSARY

Categorical indicator variograms - A variogram that describes the increase in probability versus distance that a categorical variable (or indicator) will change to another categorical variable.

Conditionally simulated transmissivity field - A transmissivity field that has been produced using a geostatistical algorithm to reflect the "natural" variability in the permeability field, yet which honors the observed transmissivity data at the measurement locations.

Covariance function - A mathematical expression of the reduction in correlation between two variables (e.g., permeability) versus distance.

Ensemble of simulated transmissivity fields - A set of realizations of simulated transmissivity fields that could be either conditioned to observed data (i.e., honor the observed measurements) or unconditioned in the absence of observed data (e.g., a random transmissivity field).

Geostatistical simulation grid - A finely spaced grid upon which the geostatistical calculations are performed. Can be much finer than the finite difference grid used for groundwater flow calculations.

Indicator(s) - Also referred to as categories. Usually used to describe a set or sets of data whose covariance properties are independent from one another. For example, the covariance of permeability data from a sand could be considered independent from the covariance of the permeability data from a clay. Thus, two indicators could be used to represent the sand and clay units separately for the geostatistical simulation.

Indicator simulation - A geostatistical calculation in which the occurrence of an indicator is simulated by employing indicator variograms and the relative frequency of the indicator's occurrence. Also referred to as a simulated categorical field.

Kriged estimate - A geostatistical calculation that produces the best linear unbiased estimate of a variable's value given the variogram of the variable, the observed data locations, and the number of neighboring data points to use in the calculation.

Model calibration - The process of reducing the difference between observed freshwater head or pressure data and calculated heads or pressures of a model (e.g., groundwater flow model) through the modification of model parameters such as transmissivity, storativity, or the assigned boundary conditions.

Sequential gaussian simulation - A technique used to generate a conditional or unconditional random field for a variable with a Gaussian statistical distribution. The field is produced by choosing a point in the simulation grid and then determining the kriged estimate and kriged standard error for the simulation variable at this point by using the observed data and a selected



number of previously simulated values. This process is used to obtain the variable's local Gaussian distribution at this particular point in space. This distribution is then sampled and the sample value is assigned to this point. The process continues until each point in the simulation grid has been simulated.

Variogram model - A mathematical expression of the increase in variation (or variance) between two variables (e.g., permeability) versus distance. It may be obtained by subtracting the covariance function from 1.0.



1.0 INTRODUCTION

This document serves as a User's Manual for GRASP-INV (Version 2.01) to be used in the 1996 Waste Isolation Pilot Plant (WIPP) Performance Assessment (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.

1.1 Problem Definition

The objective of the study of the Culebra Dolomite aquifer at the WIPP site is to assess a scenario where radionuclides would escape from the repository through an unplugged well sometime in the future and invade the Culebra Dolomite aquifer, which is the most significant aquifer lying above the Salado salts beds that would host the wastes. The radionuclides would then migrate into this aquifer and eventually reach the WIPP site boundaries, (referred to as the land withdrawal boundaries), a 4 mile square surrounding the potential disposal site. Due to federal regulations, two important quantities will play a role in the assessment of the site:

- what is the travel time in the Culebra from any given release point to these boundaries?
- what will be the concentration of radionuclides in the Culebra at these boundaries, regardless of boundary section?

The performance assessment methodology employed at the WIPP site is probabilistic; therefore, the modelers of the Culebra aquifer are not being asked to give a single "optimal" estimate of the aquifer properties, which would result in the prediction of a single travel time or concentration, but rather to provide a range of possible "realizations" of these properties. These realizations should all be consistent with the available information on the site and, should also be equally likely; thus they would provide a means of displaying the uncertainty with regard to knowledge about the aquifer. In the probabilistic performance assessment, each realization is implied as an alternative description of the aquifer among an ensemble of other parameters describing the release scenario (about sixty different classes of parameters in the analysis WIPP PA, 1992, analysis).

In this document, we will concentrate on the determination of one set of parameters, the transmissivity field in the Culebra, based on the available hydrogeologic information, which consists of

- local transmissivity measurements (slug tests and short-term pumping tests),
- quasi-steady-state head measurements, and
- transient responses of the aquifer during several long term pumping tests.



1.2 Software Identifier

Code Name: GRASP-INV

WIPP Prefix: GRI

Version Number: 2.01

Platform: FORTRAN 77 for Open VMS AXP, ver. 6.1, on DEC Alpha

1.3 Points of Contact

1.3.1 Code Sponsor

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1.3.2 Code Consultant

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INTERA, Inc.
6850 Austin Center Blvd., Suite 300
Austin, TX 78731
(512) 346-2000



2.0 FUNCTIONAL REQUIREMENTS

The overall functionality of the GRASP-INV code may be summarized as follows; given (1) a discretized domain (i.e., numerical model grid), (2) a set of boundary conditions for that domain, (3) a set of observed transmissivity or permeability data, (4) a set of steady-state or observed fresh-water heads, (5) a set of characteristic parameters of the water and geologic media (e.g., water compressibility, water temperature, water density, water viscosity, rock porosity, rock compressibility, rock density) and (6) an estimate of the covariance function for the transmissivity or permeability data, determine the transmissivity field across the model domain that reproduces the observed transmissivity and freshwater head data.

GRASP-INV first generates an initial guess of the transmissivity field given the observed transmissivity data and the covariance function(s) describing the correlation among the transmissivity data. If the transmissivity data come from distinctly different statistical populations (e.g., from a fractured zone and a non-fractured zone), the transmissivity data may be subdivided into separate geostatistical populations, referred to as indicators or categories, prior to developing the initial guess of the transmissivity field. In this situation, GRASP-INV uses the indicator simulation approach to determine the category for each of the model grid blocks (see Section 4.1.6.1). A second pass is then made to "fill in" the spatial properties for each of the categories independently. GRASP-INV utilizes a technique called sequential gaussian simulation to "fill in" a category's spatial properties (see Section 4.1.6.2) by assuming the properties may be statistically represented by a Gaussian distribution. Once this second pass is complete, the initial transmissivity field is obtained and GRASP-INV begins to calibrate the field to the observed freshwater head data (see Sections 4.2 through 4.5)

In terms of specific functional requirements, GRASP-INV must be capable of the following:

R.1 - Given observed transmissivity data, determine the kriged estimate of transmissivity at an estimate location using an exponential or spherical variogram model (see Section 4.1).

R.2 - Given an exponential or spherical variogram model, use sequential simulation to produce an ensemble of simulated transmissivity fields which reproduce the input variogram (see Section 4.1).

R.3 - Given categorical indicator variograms and relative frequency of occurrence, produce an ensemble of simulated categorical fields which reproduce the input categorical variograms for two dimensional fields (see Section 4.1).

R.4 - Given categorical indicator variograms, relative frequencies of categorical occurrence, transmissivity (continuous variable) variograms for each category, produce an ensemble of simulated transmissivity fields which reproduce the categorical variograms as well as the transmissivity variograms within each of the categories for two dimensional and three dimensional fields (see Section 4.1).



R.5 - Given a set of transmissivity values for each category over a regularly or irregularly spaced geostatistical simulation grid, determine the transmissivity values for an irregularly spaced finite difference grid which is superimposed upon the regularly spaced geostatistical simulation grid. Assign the grid block a category by determining the highest number of points for each category which lie within the grid block and selecting this category for the grid block. Assign either (1) the geometrical average of the transmissivity values of the simulation points (if they are read as an external file) within the grid block as the isotropic transmissivity value or (2) the electrical analog equivalent transmissivity value of the simulation points falling within the grid block if the geostatistical simulation grid is generated within the GRASP-INV code (see Section 4.1.7).

R.6 - Given a set of grid block transmissivity values, demonstrate that the steady-state pressures and the transient pressures are calculated properly for multi-dimensions (see Section 4.2).

R.7 - Calculate the sensitivity of a performance measure to various system parameters in one or two dimensional flow fields using the adjoint technique. The performance measures are pressure at a selected location within the model domain (and if applicable at a selected time), and weighted least squares objective function of calculated and observed pressure. The sensitivity parameter is grid block permeability (see Section 4.3).

R.8 - Given categorical indicator variograms, relative frequencies of categorical occurrence, transmissivity (continuous variable) variograms for each category, observed transmissivity and head data, produce a conditionally simulated transmissivity field which reproduces the categorical variograms as well as the transmissivity variograms within each of the categories for two dimensional fields. Calibrate this transmissivity field to the observed head data using a weighted least-squares objective function of computed and observed pressures. Reduce the objective function to a specified minimum value by adding pilot points in the regions of highest sensitivity and subsequently optimizing the transmissivity assigned to the pilot points (see Section 4.4).



3.0 REQUIRED USER TRAINING and/or BACKGROUND

To use GRASP-INV, users should have basic knowledge of (1) Open VMS, (2) Digital Command Language, and (3) access to the WIPP PA cluster of DEC Alpha VAX microcomputers or their equivalent.

In addition, users should have an educational background or professional experience related to stochastic hydrogeology to properly interpret the results of the GRASP-INV code.





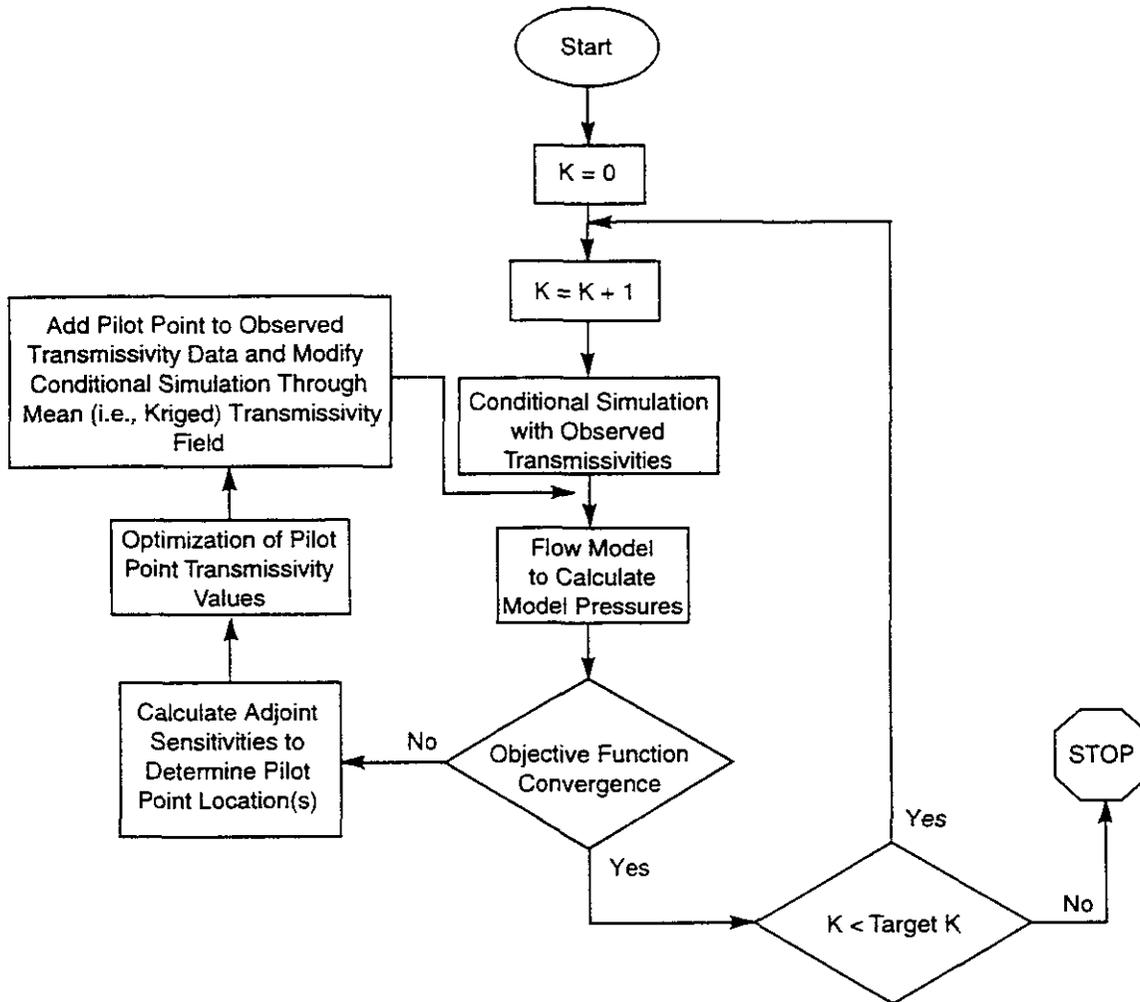
4.0 DESCRIPTION OF THE MODELS AND METHODS

GRASP-INV solves the inverse problem for Darcy's Law of groundwater flow. That is, given information concerning the physical characteristics of an aquifer and its groundwater heads spatially and/or temporally, GRASP-INV determines a spatially varying transmissivity field that will reproduce the observed heads (within the head uncertainty bounds). GRASP-INV was designed to meet the needs of the WIPP PA program by solving the inverse problem to determine the Culebra transmissivity field using the measured heads within the Culebra Dolomite. However, because the Total System PA calculations employ Monte Carlo simulation, numerous calibrated Culebra transmissivity fields are required. Therefore, GRASP-INV calibrates numerous transmissivity fields (T-fields), each of which has different spatial characteristics.

The general process used in the GRASP-INV code is illustrated by the flow chart in Figure 1. The initial transmissivity field is generated through a geostatistical simulation routine called CONSIM II. This simulation is usually performed on a grid much finer than the flow model finite difference grid. Once a field is generated, the flow model grid is superimposed upon the geostatistical simulation grid and average transmissivity values are calculated for each flow model grid block by analyzing the simulation grid point values falling within each grid block. The grid-block transmissivity values are then sent to the flow model, SWIFT II. SWIFT II calculates groundwater pressures and velocities across the flow model domain and sends this information to GRASP II, a sensitivity analysis routine.

GRASP II first determines the objective function, which in the case of the Culebra flow model is the weighted least squares error between computed and measured steady-state and/or transient pressures. GRASP II then calculates adjoint sensitivities of the objective function to the addition a pilot point. Having determined the most sensitive location for the addition of a pilot point into the model transmissivity field, the transmissivity value assigned to the pilot point is optimized by the PAREST routine to reduce the objective function. Constraints are assigned to the optimization process to ensure realistic transmissivity values at the pilot point locations. Once a pilot point's x,y,z location is selected and the transmissivity assigned, the transmissivity field is modified by determining the influence of the pilot point upon the surrounding grid block transmissivity values (Figure 2). The modified transmissivity field is then sent back to SWIFT II and the process repeats until the objective function is reduced to a specified minimum or until a selected maximum number of pilot points has been added.

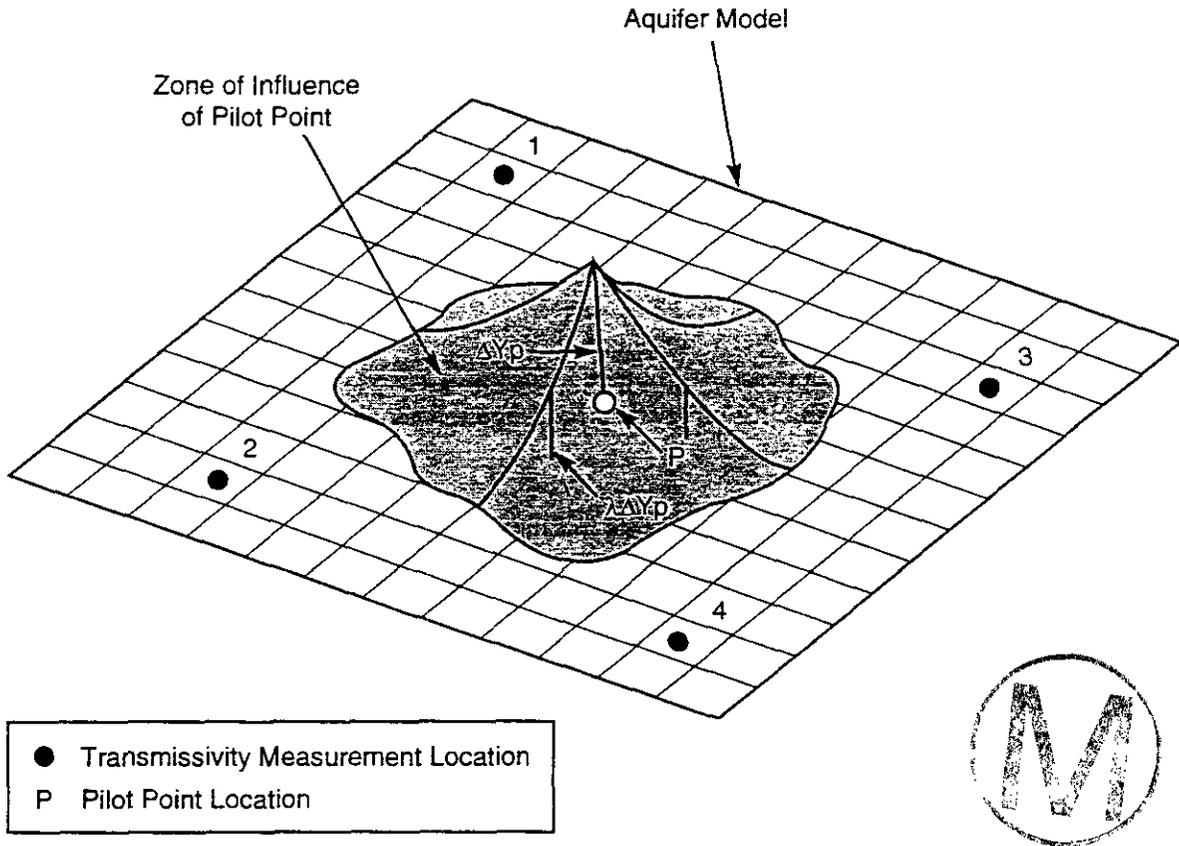
One may ask "Why use pilot points to calibrate the model?" Another approach to solving the inverse problem consists of dividing the model domain into a few zones; in each of these zones, the transmissivity is treated as constant. The transmissivities in the different zones constitute the parameters to be adjusted in the optimization process. Clearly, the delineation of zones is a subjective process that affects the results of the calibration. Several alternative zonation patterns may have to be considered for calibration; also, uniform transmissivities are assigned to each zone. This approach was found to be inadequate for addressing the issues of spatial variability,



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Figure 1. Flow Chart of GRASP-INV



● Transmissivity Measurement Location
 P Pilot Point Location

Pilot Point - Schematic

		X	Y	T	y (log ₁₀ T)	σ _y
Measured Transmissivity	1	150	1050	10 ^{-3.1}	-3.1	0.5
	2					
	⋮					
	4					
Pilot Points added in Calibration	P ₁	650	620	10 ^{-4.81}	-4.81	0.84
	P ₂					
	⋮					
	P _n					

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Figure 2. Spatial Influence of a Pilot Point Upon Model Grid-Block Transmissivities

as indicated by the study described in Niou and Pietz (1987). These authors attempted to match the hydraulic response to the H-3 Multipad pumping test using a zonation approach. Their study produced a set of transmissivity zones within which the transmissivities were constant.

To avoid the above difficulties of the zonation approach, an approach using pilot points (deMarsily et al., 1984; LaVenue and Pickens, 1992) as parameters is adopted. Conceptually, a pilot point may be viewed as a simple mechanism to effect realistic modifications of transmissivity in the region of the model surrounding the pilot-point location. The definition of the T field using the pilot point method, as presented by deMarsily et al. (1984), Certes and deMarsily (1991), LaVenue and Pickens (1992), Gomez-Hernandez (1992) was compared with other methods by Keidser and Rosbjerg (1991). Keidser and Rosbjerg concluded their comparison of the pilot point approach with other techniques based on zoning by stating that "it [pilot point] is the best at reproducing large local heterogeneities due to the influence of the pilot points on the kriged T fields."

The question arises whether the generated fields are indeed equally plausible (i.e., each field has the same probability of representing the real field). It is well known that unconditional simulations, such as those generated by the Sequential Simulation method, are in principle independent and equally likely if the random number generator used to produce them is adequate. Conditioning these simulations on measured T data maintains this equal-likeliness. Is it still the same after a second conditioning by the head measurements through an inverse? To ensure this, we will first prescribe a constant number of pilot points for each simulation, so that the calibration has the same degree of freedom and plausibility. If the calibration criterion reached through optimization (a L_2 norm based on the difference between observed and calculated heads) was identical for all simulations, one would be justified in claiming that the equal-likeliness of the simulations would be preserved. This will not be exactly the case in practice: each conditionally simulated and calibrated field will reach a slightly different minimal norm. One might then think that those fields with a lesser norm could be slightly more likely than the ones with a larger norm. In practice, we will neglect this difference, since the difference in norm will be very small.

The drawback of the proposed methodology is that it is computationally intensive, as each simulated field requires the solution of a new inverse problem. It also assumes that the distribution of the T field is lognormal, which, in the case of the Culebra Dolomite, is reasonably verified by the data.

GRASP-INV is composed of four main routines as discussed above: CONSIM II, SWIFT II, GRASP II, and PAREST. The following sections will present the theory used in these routines in an attempt to give the reader the ability to construct the appropriate data sets for GRASP-INV.

4.1 CONSIM II

CONSIM II is a computer program for the geostatistical simulation of heterogeneous geologic media and related spatial random variables. It creates one-, two- or three-dimensional simulated



fields of spatially correlated random variables that may be conditioned to measured values. CONSIM II also produces estimated fields based on the measured values via kriging. The program is written in FORTRAN-77, and is developed from GSLIB, the well-known library of geostatistical programs published by Deutsch and Journel (1992). Both the FORTRAN code and the text in this section have borrowed extensively from GSLIB and the associated text by Deutsch and Journel (1992).

CONSIM II uses a two-step approach to simulating geologic media. The first step is to simulate lithology or structure within a formation as discrete categories using Indicator Categorical Simulation (iCs). The second step simulates a continuous variable for the property of interest of each category, e.g., permeability for each rock type. The continuous variable is simulated parametrically by Sequential Gaussian Simulation (sGs). If observed values of the variable of interest are available, the simulations will reproduce the observations at their locations while providing alternative, equally plausible realizations for the unmeasured regions of the field.

CONSIM II may be used to simulate a variety of geologic media; examples include

- The permeabilities of both sand and shale layers within a single formation.
- The transmissivities of both fractured and massive units within a limestone aquifer.
- Facies changes and the associated material properties for an alluvial or aeolian deposit.

4.1.1 CONSIM II: Normal Scores Transform

Gaussian based simulation programs such as CONSIM II work with normal scores of the original data. The conditioning data used in the simulations are first transformed to their normal scores, calculations are then performed in the normal space, then the results (i.e., kriging results or simulation results) are back transformed. This section provides details of the normal scores transformation step. CONSIM II will also accept data that have already been transformed.

Consider the original data $T_i, i = 1, \dots, n$, each with a specified probability

$$p_i, i = 1, \dots, n, \text{ (with } \sum_{i=1}^n p_i = 1.0 \text{)} \quad (1)$$

to account for clustering. If clustering is not considered important then all the p_i 's can be set equal to $1/n$. Tied T -data values are randomly ordered. When there is a large proportion of T -data in a tie, these tied values should be ranked (despiked) prior to using CONSIM II.

Because of the limited sample size available in most applications, one should consider a non-zero probability for values less than the data minimum or greater than the data maximum. Thus some assumptions must be made about the (unsampled) tails of the attribute distribution.



One common solution is to standardize all previous probabilities p_j to a sum slightly less than one, e.g., to $n/n+1$ if there are n data. This solution is sensitive to the number of data (sample size), and it does not offer any flexibility in modeling the distribution tails.

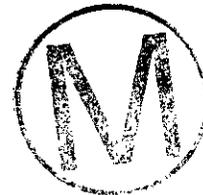
To avoid the problem of sensitivity to sample size, the cumulative probability associated with each data value is reset to the average between its cumulative probability and that of the next lowest datum. This allows finite probabilities to be lower than the data minimum and greater than the data maximum.

For notation, let c_i be the cumulative probability associated with the i th largest data value, T_i , that is

$$c_i = \sum_{j=1}^i p_j \quad (2)$$

The normal score transform y_i associated with T_i is then calculated as:

$$y_i = G^{-1}\left(\frac{c_i + c_{i-1}}{2}\right) \quad (3)$$



with $G(y)$ being the standard normal cumulative distribution function (CDF), $y_c = G^{-1}(c)$ being the corresponding standard normal c -quantile, and $c_0 = 0.0$. GSLIB utilizes the numerical approximation to $G^{-1}(\cdot)$ proposed by Kennedy and Gentle (1980).

The normal scores transformation is automatically performed in the sequential Gaussian simulation (sGs) algorithm and the transformed data are saved to a file for later use in the back transformation of the results into the real space. The back transformation T_i of the standard normal deviate y_i is given by

$$T_i = F^{-1}(G(y_i)) \quad (4)$$

where $F(T)$ is the (declustered) CDF of the original data.

Almost always, the value $G(y_i)$ will not correspond exactly to an original sample CDF value F ; therefore, some interpolation between the original sample T -values or extrapolation beyond the smallest and largest T -value will be required. Linear interpolation is always performed between two known values. A variety of options is available on how the tails of the distribution will be treated; these options are discussed in the next section.

The normal score back transform aims at exactly reproducing the sample CDF $F(T)$, except for the within class interpolation and the two extreme class extrapolations. Hence details of the sample CDF that are deemed not representative of the population should be smoothed out prior to using CONSIM II.

4.1.2 CONSIM II: CDF Interpolation Models

Both the normal scores transform algorithm and the indicator conditional cumulative distribution function (CCDF) transform result in discrete CDF's (e.g., Figure 3). Because estimated or simulated values may not correspond to the cutoff values, these methods will require interpolating between cutoffs and at the tail values.

The within-class CDF interpolation models considered in CONSIM II are:

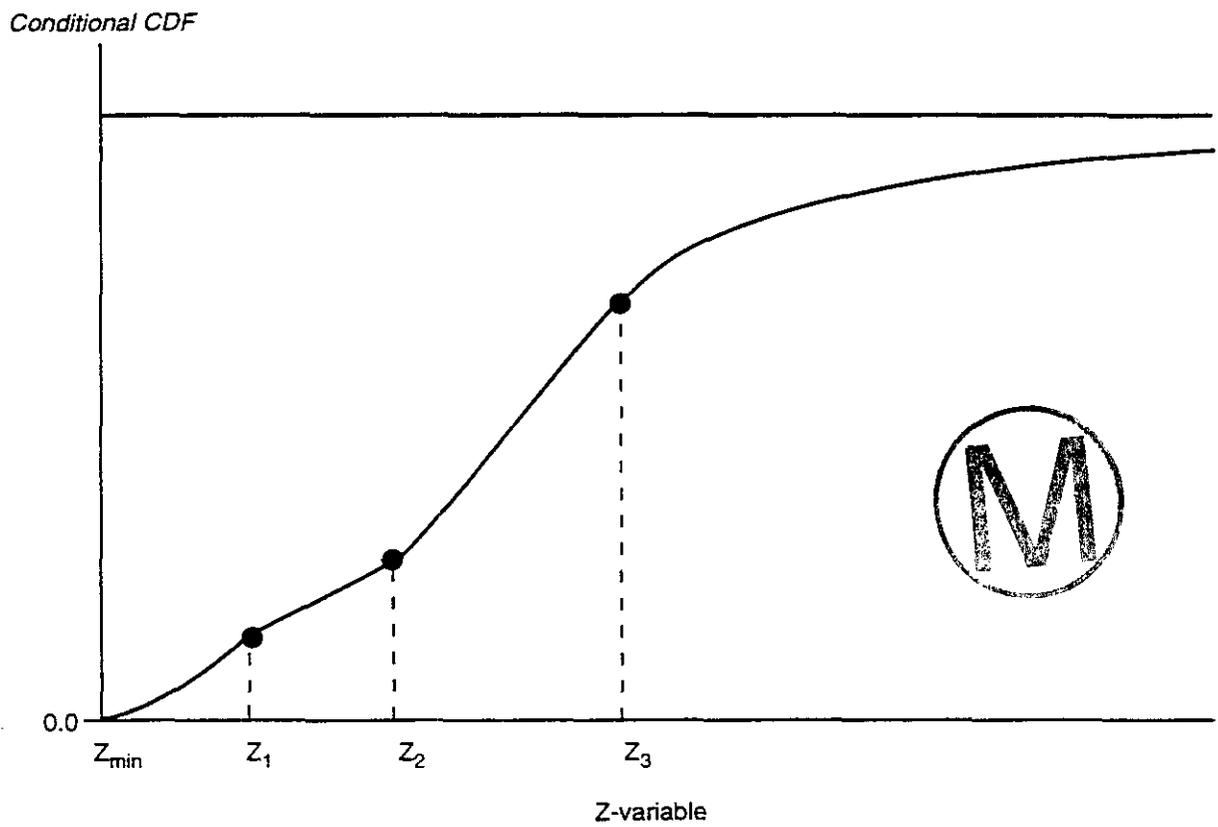
Power model: For a finite class interval $(T_{k-1}, T_k]$ and a parameter (the power) $w > 0$, this CDF model is written:

$$F_{T_{k-1}, T_k}^w(T) = \begin{cases} 0, & \forall T \leq T_{k-1} \\ \left[\frac{T - T_{k-1}}{T_k - T_{k-1}} \right]^w, & \forall T \in (T_{k-1}, T_k) \\ 1, & \forall T \geq T_k \end{cases} \quad \text{M} \quad (5)$$

In practice, this CDF model is scaled between the calculated CDF values at T_{k-1} and T_k rather than between 0 and 1. Distributions with $w < 1$ are positively skewed, $w = 1$ corresponds to the linear CDF model (uniform distribution), and distributions with $w > 1$ are negatively skewed; see Figure 4.

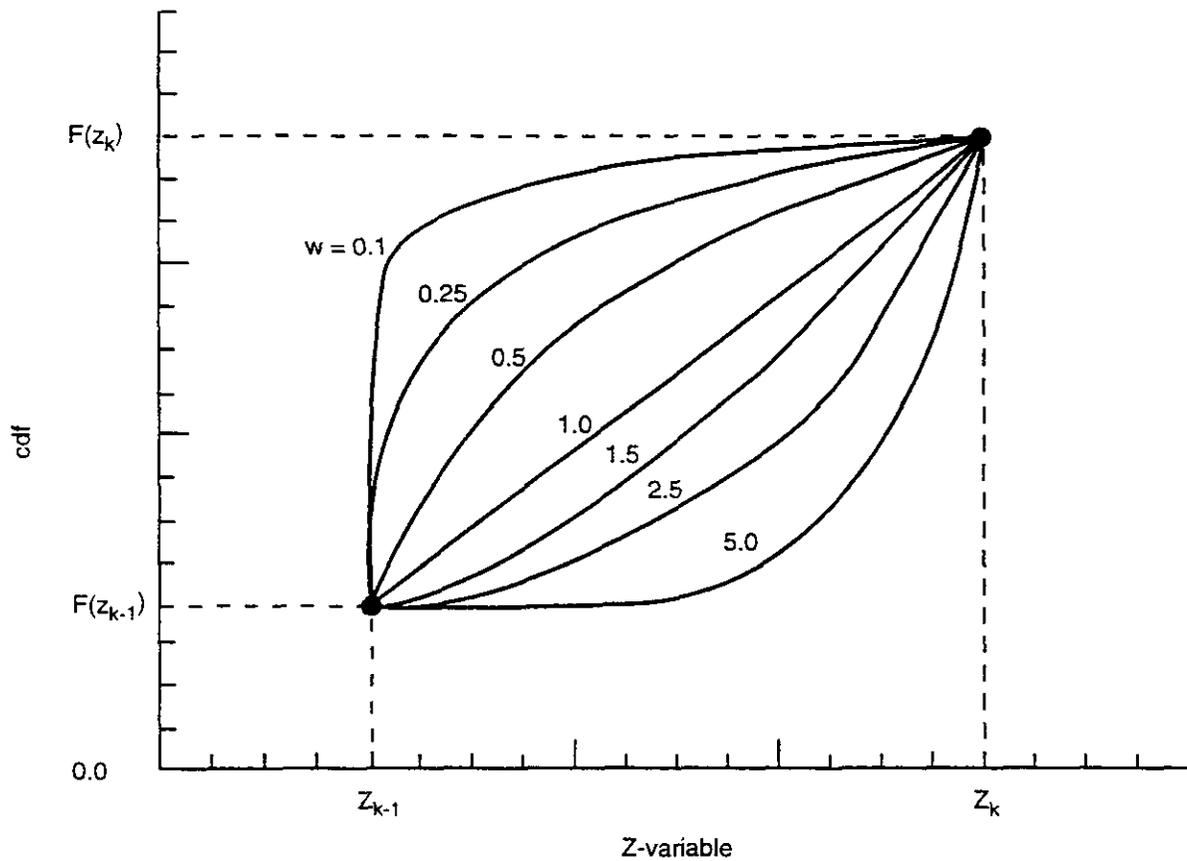
Linear interpolation between tabulated bound values: This option considers a fixed number of sub-classes with given bound values within each class (T_{k-1}, T_k) . For example, the three bound values a_{k1}, a_{k2}, a_{k3} can be tabulated defining four sub-classes $(T_{k-1}, a_{k1}), (a_{k1}, a_{k2}), (a_{k2}, a_{k3}), (a_{k3}, T_k)$ that share the probability p_k calculated for class (T_{k-1}, T_k) ; p_k is shared equally unless specified otherwise. Then, linear CDF interpolation is performed separately within each sub-class.

This option allows the user to add detail to the distribution within the classes defined by the cutoff T_k . That detail, i.e., the sub-class bound values, can be attributed to some or all of the



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Figure 3. Discrete CDF



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Figure 4. Power Model Fit Between CDF Points



original data values falling within each class (T_{k-1}, T_k) of the marginal (sample) distribution. Thus, some of the resolution lost through discretization by the T_k values can be recovered. More generally, the sub-class bound values a_k can be taken from any parametric model, e.g., beta or gamma distribution.

Hyperbolic model: This last option is to be used only for the upper tail of a positively skewed distribution. Decisions regarding the upper tail of CCDF's are often the most consequential; therefore, a great deal of flexibility is needed, including the possibility of a very long tail.

The hyperbolic CDF upper tail model (Figure 5) for a strictly positive variable is a two parameter distribution:

$$F_{w,\lambda}(T) = 1 - \frac{\lambda}{T^w}, w \geq 1, T^w > \lambda > 0 \quad (6)$$

The scaling parameter λ allows identification of any pre-calculated quantile value, for example, the p -quantile T_p such that $F_{w,\lambda}(T_p) = p$, then:

$$\lambda = T_p^w (1-p). \quad (7)$$

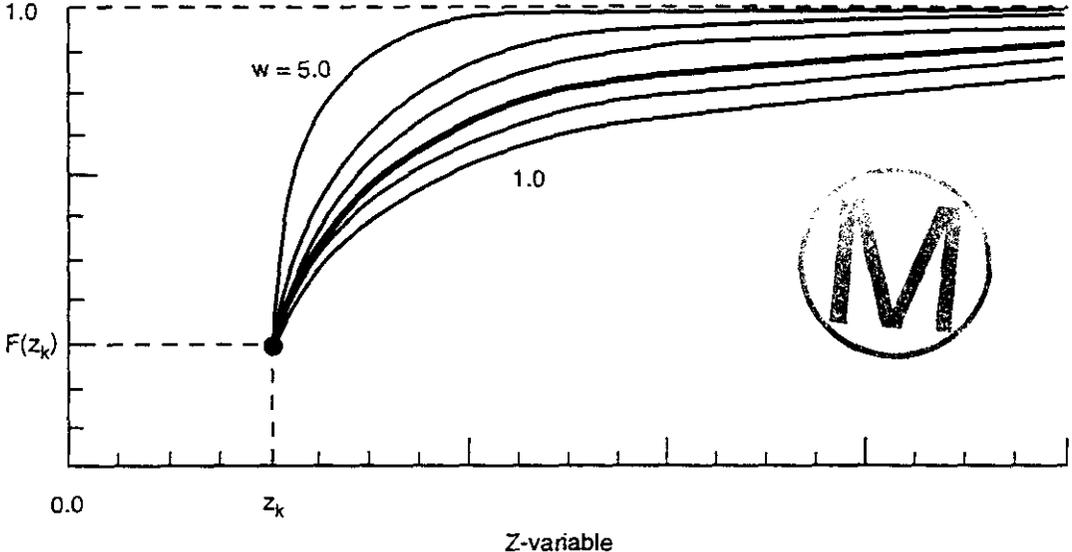
The parameter $w > 1$ controls how fast the CDF reaches its upper limit value 1; the smaller w , the longer the tail of the distribution.

The mean T -value above the p -quantile value T_p is:

$$m_p = \frac{w}{w-1} T_p > T_p. \quad (8)$$

Hence the smaller w , the larger the mean above T_p . At its minimum value, $w = 1$ identifies the Pareto distribution which has an infinite mean $m_p, \forall p$, corresponding to a very long tail. $w = 1.5$ is suggested.





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Figure 5. Hyperbolic Model for Fitting Tails

CONSIM II allows different sets of options depending on whether interpolation is needed within the middle classes or extrapolation for the lower and upper tails. The available options are:

Lower Tail: Below the first calculated CDF value:

1. Linear model or uniform distribution
2. Power model
3. Tabulated bound values

Middle: Between any two calculated CDF values:

1. Linear model (uniform distribution)
2. Power model
3. Tabulated bound values

Upper Tail: Above the last calculated CDF value:

1. Linear model (uniform distribution)
2. Power model
3. Tabulated bound values
4. Hyperbolic model



The user is asked for a specific model for each of these regions (the integer number identifying each model in the list above is used).

4.1.3 **CONSIM II: Variogram Model Specification**

This section describes the conventions for describing a variogram model and can be scanned quickly the first time through. Most of the kriging and simulation subroutines call for covariance or pseudo-covariance values; however, a semivariogram model rather than a covariance model must be specified for the normal scores data. This apparent inconsistency allows for the traditional practice of modeling variograms and also permits the straightforward incorporation of the power model, which has no covariance counterpart.

4.1.3.1 Model Types

An acceptable semivariogram model for CONSIM II consists of an isotropic nugget effect and any positive linear combination of up to four of the standard semivariogram models. The standard models are:

1. **Spherical** model defined by an actual range a and positive variance contribution or sill value c .

$$\gamma(h) = c \cdot \text{Sph}\left(\frac{h}{a}\right) = \begin{cases} c \cdot \left[1.5\frac{h}{a} - 0.5\left(\frac{h}{a}\right)^3\right], & \text{if } h \leq a \\ c & \text{if } h \geq a \end{cases} \quad (9)$$

2. **Exponential** model defined by a parameter a (effective range $3a$) and positive variance contribution value c .

$$\gamma(h) = c \cdot \text{Exp}\left(\frac{h}{a}\right) = c \cdot \left[1 - \exp\left(-\frac{h}{a}\right)\right] \quad (10)$$

3. **Gaussian** model defined by a parameter a (effective range $a\sqrt{3}$) and positive variance contribution value c .

$$\gamma(h) = c \cdot \left[1 - \exp\left(-\frac{h^2}{a^2}\right)\right] \quad (11)$$



4. **Power** model defined by a power $0 < a < 2$ and positive slope c .

$$\gamma(h) = c \cdot h^a \quad (12)$$

The type of variogram structure is specified by an integer code, which is the order in the above list, i.e., $it = 1$: spherical model, $it = 2$: exponential model, $it = 3$: Gaussian model, and $it = 4$: power model. The a and c parameter values, which correspond to the description in the above list, are also needed.

For the first three semivariograms parameter a has units length (L) and parameter c is dimensionless. For the power model, a is dimensionless and c has inverse length units (L^{-a}). Length units must be consistent with the length unit used for the geostatistical simulation grid (and thus the same as for the coordinates of the conditioning data).

4.1.3.2 Variogram Anisotropy

Each nested structure requires an additional two or five parameters that define its own geometric anisotropy in 2-D or 3-D. Figure 6 illustrates the angle and anisotropy factor required in 2-D:

- The rotation angle *ang* corresponds to an azimuth angle measured in degrees clockwise from the positive Y or north direction. The range parameter *a* is applied directly to this principal direction. The distances along the minor direction, that is, at 90 degrees from the principal direction, are obtained by multiplying *a* by the second parameter *anis*.

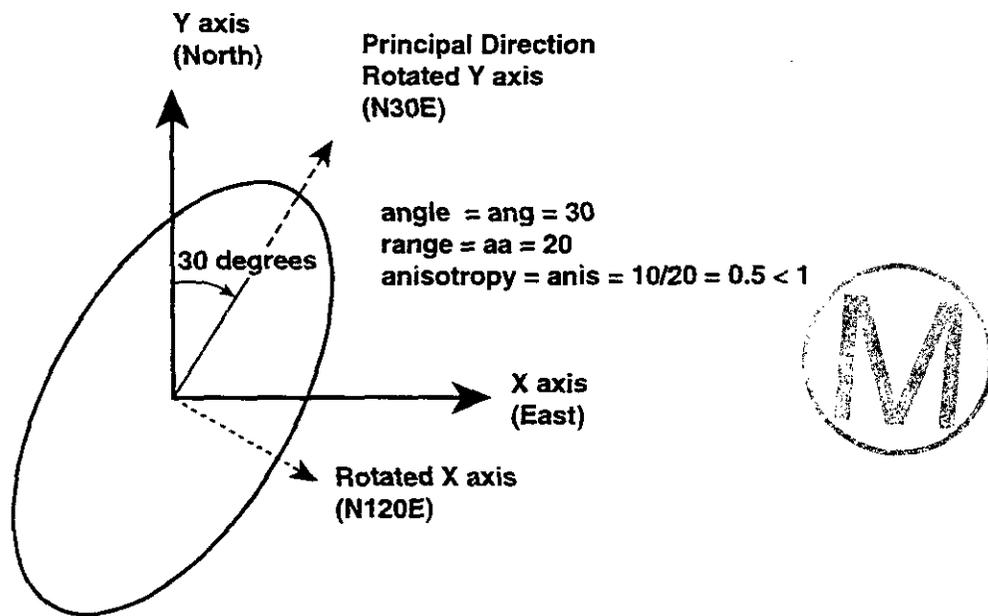
The anisotropy factor *anis* is the range in the minor direction divided by the range in the principal direction. Hence, it is normally less than one. There is no requirement, however, that the *anis* parameter be less than one; for example, it may be set very large to model a zonal anisotropy (discussed below). Note that a very large anisotropy factor will add the variogram structure in the principal direction and add nothing in any other direction, a feature known as "zonal anisotropy."

With CONSIM II the actual distance is corrected so that it accounts for the specified anisotropy. That is, the distance component in the rotated X axis (see Figure 6) is divided by *anis*. In other words, the anisotropy parameters do not apply to the *a* parameter of the variogram. Consequently, the anisotropy of the power model is handled in an intuitively correct manner; an anisotropic distance is calculated and the power *a* is left unchanged.

Figure 7 illustrates the angles and anisotropy factors required in 3-D. It is quite straightforward to visualize a phenomenon that is dipping with respect to the horizontal at a dip azimuth that is not aligned with a coordinate axis. The third angle is required to account for the geological concept of a plunge or rake. One example that requires a third angle is modeling the geometric anisotropy within the limbs of a plunging syncline.

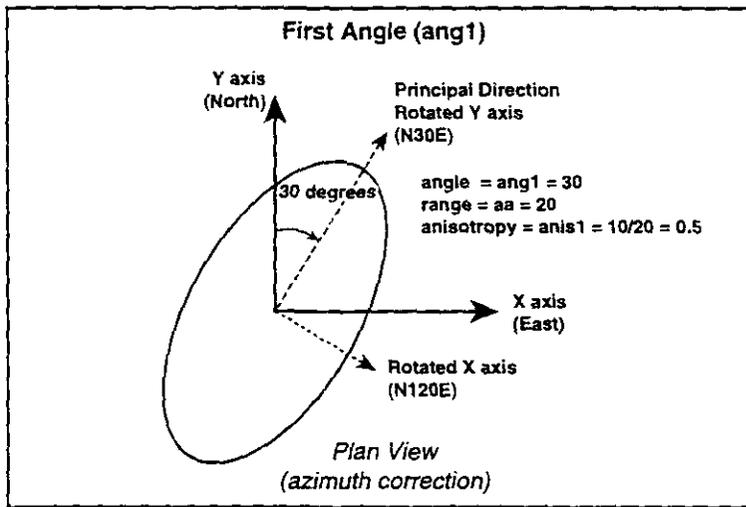
The easiest way to describe the three angles and two anisotropy factors is to imagine the rotations and squeezing that would be required to transform a sphere into an ellipsoid. The outer shell of the ellipsoid consists of points at the same structural distance, e.g., if the ellipsoid is one half as large in one direction then the attribute is one half as continuous. We will refer to the original y axis as the principal direction and consider the rotations such that it ends up being the actual principal structural direction (direction of maximum continuity):



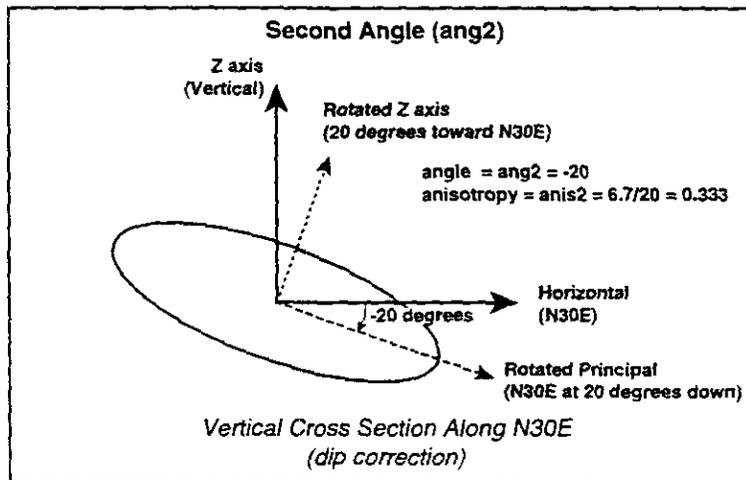


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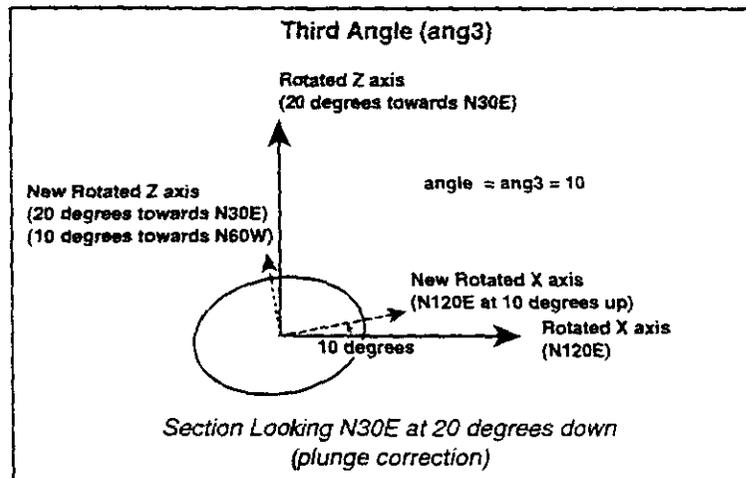
Figure 6. Angle and Axis Rotation Used in 2-D Variogram Analysis



First Step



Second Step



Third Step



Figure 7. Angle and Axis Rotation Used in 3-D Variogram Analysis

- the first rotation angle, *ang1*, rotates the original Y axis (principal direction) in the horizontal plane: this angle is measured in degrees clockwise.
- The second rotation angle, *ang2*, rotates the principal direction from the horizontal: this angle is measured in negative degrees down from horizontal.
- The third rotation angle, *ang3*, leaves the principal direction, defined by *ang1* and *ang2*, unchanged. The two directions orthogonal to the principal direction are rotated clockwise relative to the principal direction when looking toward the origin. The rotation of the Third Step in Figure 7 appears as counterclockwise because the view is away from the origin.

Zonal anisotropy can be considered as a particular case of a geometric anisotropy (see Isaaks and Srivastava, 1989, p. 385-386). This situation can be handled by entering the anisotropy parameter *anis* as a very large number, which causes the implicit range in the minor direction to infinity; the particular variogram structure is then added only to the major direction.

Note that, whether in 2-D or 3-D, the anisotropy directions need not be the same for each nested structure, allowing for a great flexibility in modeling experimental anisotropy. However, the more complicated the variogram model, the longer it takes to construct each kriging matrix; hence, the longer the kriging or simulation program will take. For an excellent discussion on variogram modeling refer to Chapter 16 of Isaaks and Srivastava (1989).

4.1.3.3 A Straightforward 2-D Variogram Example

Consider the semivariogram shown on Figure 8. The dots are the experimental semivariogram points in two orthogonal directions. The semivariogram that reaches the sill first (at about 10-15 distance units) is in the north-south direction (an azimuth of 0.0) and the variogram with the longer range is in the east-west direction (an azimuth of 90 degrees). The solid line in both directions is the fitted semivariogram model.

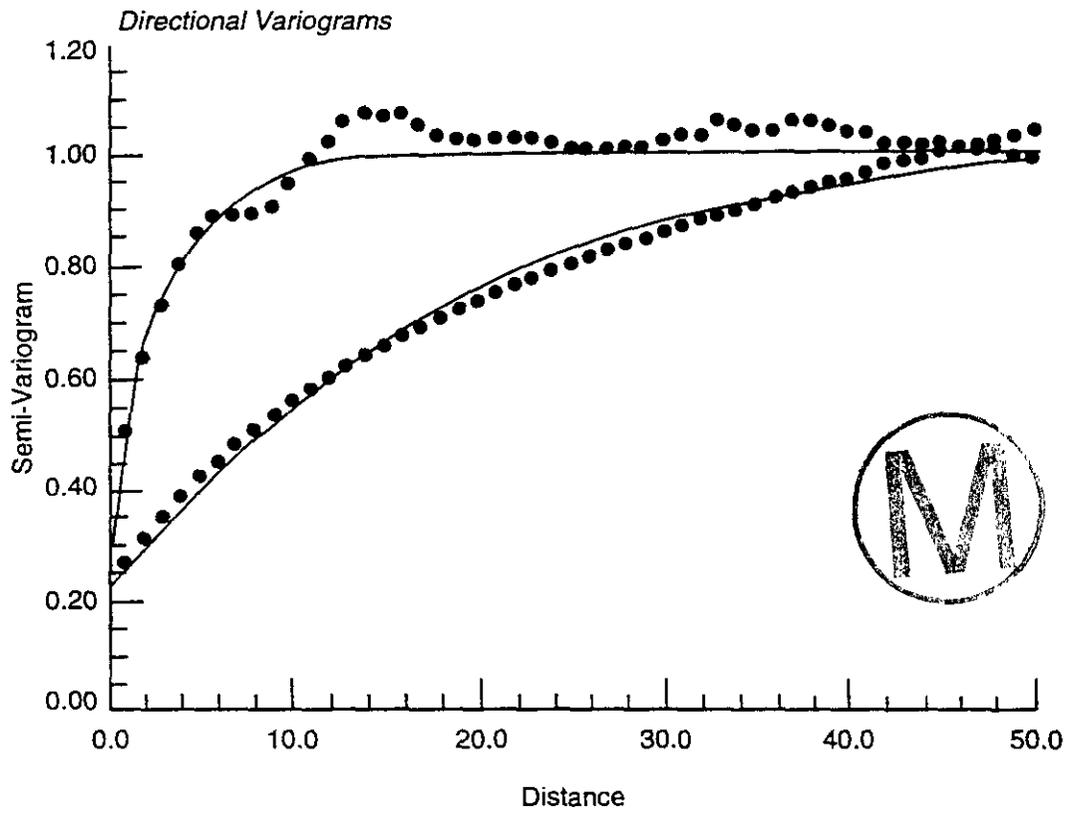
The north-south model was fitted with a nugget effect of 0.22, an exponential structure with contribution 0.53 and range parameter *a* of 1.6, and a spherical structure with contribution 0.25 and range 15.0. The east-west model was fitted with nugget effect of 0.22, an exponential structure with contribution 0.53 and range parameter *a* of 16.0, and a spherical structure with contribution 0.25 and range 50.0. The semivariogram parameters required by the kriging or simulation programs would be specified as follows:

c0 = nugget = 0.22.

nst = number of nested structures = 2.

it(1) = type of structure 1 = 2 (exponential).





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Figure 8. 2-D Variogram Example

azimuth(1) = 90 degrees (the east-west direction).

cc(1) = contribution of structure 1 = 0.53.

aa(1) = range of structure 1 in the direction **azimuth** = 16.0.

anis(1) = anisotropy of structure 1 = $1.6/16.0 = 0.10$.

it(2) = type of structure 2 = 1 (spherical).

azimuth(2) = 90 degrees (the east-west direction).

cc(2) = contribution of structure 2 = 0.25.

aa(2) = range of structure 2 in the direction **azimuth** = 50.0.

anis(2) = anisotropy of structure 2 = $15.0/50.0 = 0.30$.



4.1.4 CONSIM II: MultiGaussian Kriging

Although kriging was initially introduced to provide estimates for unsampled values, it is being used increasingly to build probabilistic models of uncertainty about these unknown values. In a nutshell, the kriging algorithm provides a minimum error-variance estimate of any unsampled value. Contouring a grid of kriging estimates is the traditional mapping application of kriging. Kriging used as a mapping algorithm is a low-pass filter that tends to smooth out details and extreme values of the original data set.

Because kriging is a minimum error variance estimation algorithm, it approximates, and in some cases is identical to, the conditional expectation of the variable being estimated. Thus, kriging can be used to estimate a series of posterior conditional probability distributions from which unsmoothed images of the attribute spatial distribution can be drawn. In the multiGaussian (MG) case, the conditional distribution is identified by the mean and variance obtained from simple kriging. In the indicator kriging (IK) approach, a series of conditional cumulative distribution function (CCDF) values are estimated directly.

The kriging principle, applied both as a mapping algorithm and as a tool to obtain conditional probability distributions, has been presented in numerous papers and textbooks (David, 1977; Issaks and Srivastava, 1989; Journel and Huijbregts, 1978).

4.1.4.1 Simple Kriging

All versions of kriging are elaborations on the basic linear regression algorithm and corresponding estimator:

$$[Z_{SK}^*(u) - m(u)] = \sum_{\alpha=1}^n \lambda_{\alpha}(u) [Z(u_{\alpha}) - m(u_{\alpha})] \quad (13)$$

where $Z(\mathbf{u})$ is the random variable, (RV) model at location \mathbf{u} , the \mathbf{u}_{α} 's are the n data locations, $m(\mathbf{u}) = E\{Z(\mathbf{u})\}$ is the location-dependent expected value of RV, $Z(\mathbf{u})$, and $Z_{SK}^*(\mathbf{u})$ is the linear regression estimator, also called the "simple kriging" (SK) estimator.

The SK weights $\lambda_{\alpha}(\mathbf{u})$ are given by the system of normal equations written in their more general non-stationary form as follows:

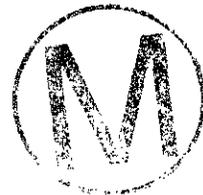
$$\sum_{\beta=1}^n \lambda_{\beta}(u) C(u_{\beta}, u_{\alpha}) = C(u, u_{\alpha}), \alpha = 1, \dots, n \quad (14)$$

The SK algorithm requires prior knowledge of the $(n + 1)$ means $m(\mathbf{u}), m(\mathbf{u}_{\alpha}), \alpha = 1, \dots, n$, and the $(n + 1)$ by $(n + 1)$ covariance matrix $[C(\mathbf{u}_{\alpha}, \mathbf{u}_{\beta}), \alpha, \beta = 0, 1, \dots, n]$ with $\mathbf{u}_0 = \mathbf{u}$. In most practical situations, inference of these means and covariance values requires a prior hypothesis (rather a *decision*) of stationarity of the random function $Z(\mathbf{u})$. If the random function (RF) $Z(\mathbf{u})$ is stationary with constant mean m , and covariance function $C(\mathbf{h}) = C(\mathbf{u}, \mathbf{u} + \mathbf{h}), \forall \mathbf{u}$, the SK estimator reduces to its stationary version:

$$Z_{SK}^*(u) = \sum_{\alpha=1}^n \lambda_{\alpha}(u) Z(u_{\alpha}) + \left[1 - \sum_{\alpha=1}^n \lambda_{\alpha}(u) \right] m \quad (15)$$

with the traditional stationary SK system:

$$\sum_{\beta=1}^n \lambda_{\beta}(u) C(u_{\beta} - u_{\alpha}) = C(u - u_{\alpha}), \alpha = 1, \dots, n \quad (16)$$



Stationary SK does not adapt to local trends in the data because it relies on the mean value m , assumed known and constant throughout the area. Consequently, SK is rarely used directly for mapping the z -values. Instead, it is the more robust ordinary kriging (OK) algorithm, discussed next, which is used.

According to strict stationary theory, it is SK that should be applied to algorithms such as sGs, which use the normal score transform. The OK algorithm, however, might be considered if enough data are available to re-estimate locally the normal score mean.

4.1.4.2 Ordinary Kriging

Ordinary kriging (OK) filters the mean from the SK estimator by requiring that the kriging weights sum to one. This results in the following OK estimator:

$$Z_{OK}^*(u) = \sum_{\alpha=1}^n v_{\alpha}(u)Z(u_{\alpha}) \quad (17)$$

and the stationary OK system:

$$\begin{cases} \sum_{\beta=1}^n v_{\beta}(u)C(u_{\beta} - u_{\alpha}) + \mu(u) = C(u - u_{\alpha}), \alpha = 1, \dots, n \\ \sum_{\beta=1}^n v_{\beta}(u) = 1 \end{cases} \quad (18)$$



where the $v_{\alpha}(u)$'s are the OK weights, and $\mu(u)$ is the Lagrange parameter associated with the constraint in the second expression in (18).

Comparing expression (16) and (18), note that the SK weights are different from the OK weights. It can be shown that ordinary kriging amounts to re-estimating, at *each* new location u , the mean m as used in the SK expression. Because ordinary kriging is most often applied within moving search neighborhoods, i.e., using different data sets for different locations u , the implicit re-estimated mean denoted $m^*(u)$ depends on the location u . Thus, the OK estimator (17) is, in fact, a simple kriging of type (13) where the constant mean value m is replaced by the location-dependent estimate $m^*(u)$:

$$\begin{aligned} Z_{OK}^*(u) &= \sum_{\alpha=1}^n v_{\alpha}(u)Z(u_{\alpha}) \\ &= \sum_{\alpha=1}^n \lambda_{\alpha}(u)Z(u_{\alpha}) + \left[1 - \sum_{\alpha=1}^n \lambda_{\alpha}(u) \right] m^*(u) \end{aligned} \quad (19)$$

Hence, ordinary kriging as applied within moving data neighborhoods is already a non-stationary algorithm, in the sense that it corresponds to a non-stationary RF model with varying mean but stationary covariance. This ability to rescale locally the RF model $Z(u)$ to a different mean value $m^*(u)$ explains the extreme robustness of the OK algorithm. Ordinary kriging has been and will remain the anchor algorithm of geostatistics.

4.1.5 CONSIM II: Indicator Kriging

Indicator kriging (IK) of a continuous variable provides a least-squares estimate of the conditional cumulative distribution function (CCDF) at cutoff z_k :

$$\begin{aligned} [i(u; z_k)]^* &= E\{I(u; z_k) | (n)\}^* \\ &= \text{Pr ob}^* \{Z(u) \leq z_k | (n)\} \end{aligned} \quad (20)$$

where (n) represents the conditioning information available in the neighborhood of location \mathbf{u} .

The IK process is repeated for a series of K cutoff values $z_k, k = 1, \dots, K$, which discretize the interval of variability of the *continuous* attribute z . The CCDF, built from assembling the K indicator kriging estimates of type (20), represents a probabilistic model for the uncertainty about the unsampled value $z(\mathbf{u})$.

If $z(\mathbf{u})$ is itself a binary categorical variable, e.g., set to 1 if a specific rock type prevails at \mathbf{u} , to 0 if not, then there is no need for any prior indicator transform. The direct kriging of $z(\mathbf{u})$ provides an estimate for the probability that $z(\mathbf{u})$ be one, i.e., for that rock type to prevail at location \mathbf{u} .

If $z(\mathbf{u})$ is a continuous variable, then the correct selection of the cutoff values z_k at which indicator kriging takes place is essential: with too many cutoff values, the inference and computation become needlessly tedious and expensive; too few, and the details of the distribution are lost.

4.1.5.1 Simple IK

The stationary mean of the binary indicator RF $I(\mathbf{u}; z)$ is the cumulative distribution function (CDF) of the RF $Z(\mathbf{u})$ itself; indeed:

$$\begin{aligned} E\{I(\mathbf{u}; z)\} &= 1 \cdot \text{Pr ob}\{Z(\mathbf{u}) \leq z\} + 0 \cdot \text{Pr ob}\{Z(\mathbf{u}) > z\} \\ &= \text{Pr ob}\{Z(\mathbf{u}) \leq z\} = F(z) \end{aligned} \tag{21}$$

The SK estimate of the indicator transform $i(\mathbf{u}; z)$ is thus written, according to expression (15):

$$\begin{aligned} [i(\mathbf{u}; z)]_{SK}^* &= [\text{Pr ob}\{Z(\mathbf{u}) \leq z | (n)\}]_{SK}^* \\ &= \sum_{\alpha=1}^n \lambda_{\alpha}(\mathbf{u}; z) i(\mathbf{u}_{\alpha}; z) + \left[1 - \sum_{\alpha=1}^n \lambda_{\alpha}(\mathbf{u}; z) \right] F(z) \end{aligned} \tag{22}$$



where the $\lambda_{\alpha}(\mathbf{u}; z)$'s are the SK weights corresponding to cutoff z . These weights are given by a SK system of type (16):

$$\sum_{\beta=1}^n \lambda_{\beta}(\mathbf{u}; z) C_I(\mathbf{u}_{\beta} - \mathbf{u}_{\alpha}; z) = C_I(\mathbf{u} - \mathbf{u}_{\alpha}; z), \alpha = 1, \dots, n \tag{23}$$

where $C_I(\mathbf{h}; z) = \text{Cov}\{I(\mathbf{u}; z), I(\mathbf{u} + \mathbf{h}; z)\}$ is the indicator covariance at cutoff z . If K cutoff values z_k are retained, simple IK requires K indicator covariances $C_I(\mathbf{h}; z_k)$ in addition to the K

CDF values $F(z_k)$. If the z -data are preferentially clustered, the sample CDF values should be declustered before being used (see program `declus` in Deutsch and Journel, 1992).

4.1.5.2 Ordinary IK

Just like any simple kriging, simple IK is dependent on the stationarity decision and on the CDF values $F(z)$ interpreted as mean indicator values. When data are abundant, ordinary indicator kriging within moving data neighborhoods may be considered; this amounts to re-estimating locally the prior CDF values $F(z)$. Both simple and ordinary kriging are implemented in CONSIM II.

4.1.5.3 Exactitude of the E-type Estimate

Because the CCDF returned by IK honors both hard z -data and constraint intervals, the corresponding E-type estimate (see below) also honors that information. More precisely, at a datum location \mathbf{u}_α , $[z(\mathbf{u}_\alpha)]^*_E = z(\mathbf{u}_\alpha)$, if the z -datum is hard, and $[z(\mathbf{u}_\alpha)]^*_E \in (a_\alpha, b_\alpha)$, if the information at \mathbf{u} is the constraint interval $z(\mathbf{u}_\alpha) \in (a_\alpha, b_\alpha)$. In practice, the exactitude of the E-type estimate is limited by the finite discretization into K cutoff values z_k . For example, in the case of a hard z -datum, the estimate is: $[z(\mathbf{u}_\alpha)]^*_E \in (z_{k-1}, z_k)$, with z_k being the upper bound of the interval containing the datum value $z(\mathbf{u}_\alpha)$. Thus, the E-type estimate attached to IK provides a straightforward solution to the difficult problem of constrained interpolation; as opposed to the quadratic programming solution which would limit the estimate $z^*(\mathbf{u}_\alpha)$ to either bound a_α or b_α if the constraint interval is active.

4.1.5.4 Correcting for Order Relation Problems

Regardless of the estimation algorithm used, it is imperative to correct order relation deviations. CONSIM II performs these corrections and provides a detailed report of the number and magnitude of corrections at each cutoff. The program performs within-class interpolation, as described in Section 4.1.2, to provide any required quantile value or probabilities of exceeding any given threshold value. CONSIM II also returns the mean of the CCDF, called the "E-type" estimate of $z(\mathbf{u})$, and defined as:

$$\begin{aligned}
 [z(\mathbf{u})]^*_E &= \int_{-\infty}^{+\infty} z \, dF(\mathbf{u}; z | (n)) \\
 &= \sum_{k=1}^{K+1} z'_k [F(\mathbf{u}; z_k | (n)) - F(\mathbf{u}; z_{k-1} | (n))]
 \end{aligned}
 \tag{24}$$

where $z_k, k = 1, \dots, K$ are the K cutoffs retained, and $z_0 = z_{min}, z_{K+1} = z_{max}$ are the minimum and maximum of the z -range, to be entered as input parameters. The conditional mean value z_k



within each class, (z_{k-1}, z_k) , is obtained by the interpolation procedure specified as input to CONSIM II.

The IK algorithm itself does not ensure that the resulting probability estimates (CCDF's for continuous variables or discrete probabilities for categorical variables), verify the order relations for legitimate probabilities, i.e., for CCDF's of continuous variables $z(\mathbf{u})$:

$$\begin{aligned} \text{Prob}\{Z(\mathbf{u}) \leq z|(\mathbf{n})\} &= F(\mathbf{u}; z|(\mathbf{n})) \in [0,1] \\ \text{and : } F(\mathbf{u}; z_{k'}|(\mathbf{n})) &\geq F(\mathbf{u}; z_k|(\mathbf{n})), \forall z_{k'} > z_k \end{aligned} \quad (25)$$

For conditional probabilities of an exhaustive set of mutually exclusive categorical variables $I_k(\mathbf{u})$, $k = 1, \dots, K$:

$$\begin{aligned} \text{Prob}\{I_k(\mathbf{u}) = 1|(\mathbf{n})\} &= F(\mathbf{u}; k|(\mathbf{n})) \in [0,1] \\ \text{and : } \sum_{k=1}^K F(\mathbf{u}; k|(\mathbf{n})) &= 1 \end{aligned} \quad (26)$$



The indicator $i_k(\mathbf{u})$ is set to 1 if category k prevails at location \mathbf{u} , to zero if not.

The flexibility of the IK approach is obtained at the cost of order relation problems. IK-derived conditional probabilities may not verify the order relations conditions (Eq. 25 or 26). In any particular study one would expect to meet at least one order relation deviation for up to one-half or two-thirds of the IK-derived CCDF's. Fortunately, the average magnitude of the probability corrections is usually on the order or 0.01, much smaller than shown in Figure 9. CONSIM II provides statistics of the order relation problems encountered, if desired.

In the case of categorical probabilities, the first constraint (Eq. 25) is easily met by resetting the estimated value $F^*(\mathbf{u}; z|(\mathbf{n}))$ to the nearest bound, 0 or 1, if originally valued outside the interval [0,1]. This resetting corresponds exactly to the solution provided by quadratic programming.

The second constraint (26) is tougher because it involves K separate krigings. One solution consists of kriging only $(K - 1)$ probabilities leaving aside one category k_0 , chosen with a large enough prior probability p_{k_0} , so that:

$$F^*(\mathbf{u}; k_0|(\mathbf{n})) = 1 - \sum_{k \neq k_0} F^*(\mathbf{u}; k|(\mathbf{n})) \quad (27)$$

Another solution, applied after the first constraint (Eq. 25) has been met, is to restandardize each estimated probability $F^*(\mathbf{u}; k|(\mathbf{n})) \in [0,1]$ by the sum $\sum_k F^*(\mathbf{u}; k|(\mathbf{n})) < 1$.

Correcting for order relations of continuous variable CCDF's is more delicate, because of the ordering of the cumulative indicators. There are two sources of order relation problems:

1. Negative indicator kriging weights. One solution is to constrain the IK system to deliver only non-negative weights. One would have to forfeit, however, the sometimes beneficial properties of having a non-convex kriging estimate.
2. Lack of data in some classes; see hereafter.

Practice has shown that the majority of order relation problems are due to a lack of data, more precisely, to cases when IK is attempted at a cutoff z_k which is the upper bound of a class (z_{k-1} , z_k) that contains no z -data. In such case the indicator data set is the same for both cutoffs z_{k-1} and z_k and yet the corresponding indicator variogram models are likely different; therefore, the resulting CCDF values will likely be different with a good chance for order relation problems.

Figure 9 shows an example with the following order relation problems:

$$\begin{aligned}
 F(u; z_3 | (n)) &< F(u; z_2 | (n)) \\
 F(u; z_8 | (n)) &< F(u; z_7 | (n)) \\
 F(u; z_9 | (n)) &> 1
 \end{aligned}
 \tag{28}$$



4.1.6 CONSIM II: The Sequential Simulation Approach

The most straightforward algorithm for generating realizations of a multivariate Gaussian field is provided by the sequential principle described in this section. Each variable is simulated sequentially according to its normal CCDF fully characterized through an SK system of Eq. 22 for sequential Indicator Categorical Simulation or Eq. 15 for Sequential Gaussian Simulation. The conditioning data consist of all original data and all previously simulated values found within a neighborhood of the location being simulated. CONSIM II will first simulate the categorical variable using sequential indicator categorical simulation and will then conduct a sequential Gaussian simulation within each category to "fill in" the spatial variability.

The Sequential Simulation procedure may be summarized as follows. Consider the joint distribution of N random variables Z_i with N very large. The N RV's Z_i may represent the same attribute at the N nodes of a dense grid discretizing the field, or they can represent N different attributes measured at the same location, or they could represent a combination of K different attributes defined at the N' nodes of a grid with $N = KN'$.

Next, consider the conditioning of these N RV's by a set of n data of any type symbolized by the notation $l(n)$. The corresponding N -variate CCDF is denoted:

$$F_{(N)}(z_1, \dots, z_N | (n)) = \text{Prob}\{Z_i \leq z_i, i = 1, \dots, N | (n)\}
 \tag{29}$$

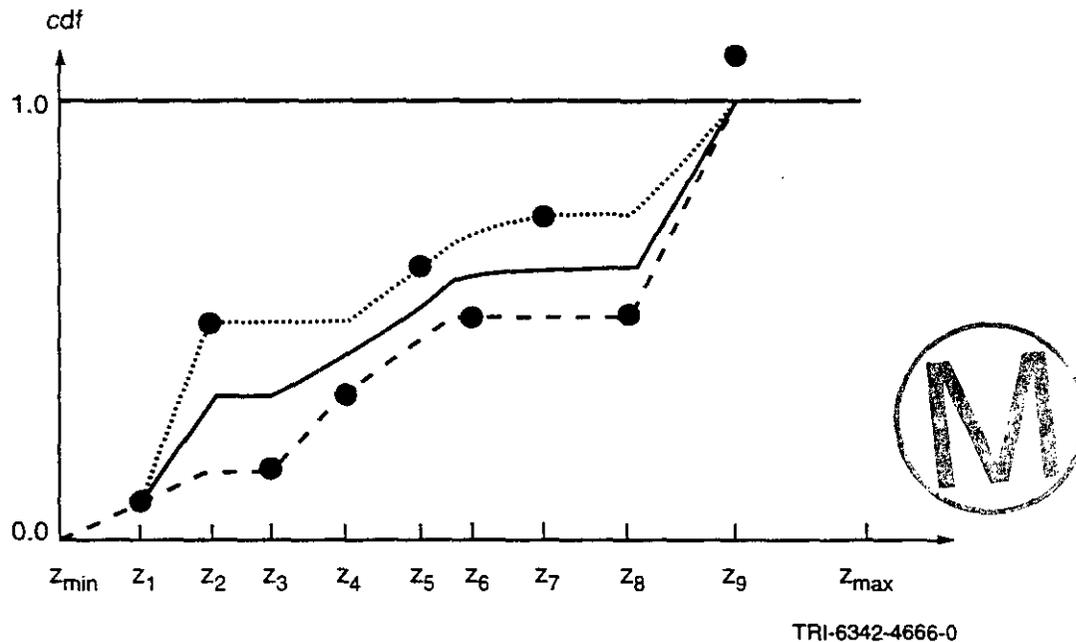


Figure 9. Order Relation Problems and Their Correction.
 (The dots are the CCDF values returned by IK. The corrected CCDF is obtained by averaging the forward and downward corrections.)

Expression (29) is completely general with no intrinsic limitations; some or all of the variables Z_i could be categorical.

Successive application of the conditional probability relation shows that drawing an N -variate sample from the CCDF (Eq. 29) can be done in N successive steps, each involving a univariate CCDF with increasing levels of conditioning:

- draw a value $z_1^{(1)}$ from the univariate CCDF of Z_1 given the original data (n). The value $z_1^{(1)}$ is now considered as a conditioning datum for all subsequent drawings; thus, the information set (n) is updated to $(n + 1) = (n) \cup \{Z_1 = z_1^{(1)}\}$.
- draw a value $z_2^{(1)}$ from the univariate CCDF of Z_2 given the updated data set ($n + 1$), then update the information set to $(n + 2) = (n + 1) \cup \{Z_2 = z_2^{(1)}\}$.

- sequentially consider all N RV's Z_i .

The set $\{z_i^{(1)}, i = 1, \dots, N\}$ represents a simulated joint realization of the N dependent RV's Z_i . If another realization is needed, $\{z_i^{(l)}, i = 1, \dots, N\}$, the entire sequential drawing process is repeated.

This sequential simulation procedure requires the determination of N univariate CCDF's, more precisely:

$$\begin{aligned}
 & \text{Prob}\{Z_1 \leq z_1 | (n)\} \\
 & \text{Prob}\{Z_2 \leq z_2 | (n + 1)\} \\
 & \text{Prob}\{Z_3 \leq z_3 | (n + 2)\} \\
 & \dots \\
 & \text{Prob}\{Z_N \leq z_N | (n + N - 1)\}
 \end{aligned}
 \tag{30}$$

The sequential simulation principle is independent of the algorithm or model used to establish the sequence (Eq. 30) of univariate CCDF's. In sGs, all CCDF's Eq. 30 are assumed Gaussian and their means and variances are given by a series of N simple kriging systems. In iCs, the CCDF's are obtained directly by indicator kriging.

4.1.6.1 Indicator Categorical Simulation (iCs)

CONSIM II begins by assuming that the observed data $T(\mathbf{u})$ can be divided into mutually exclusive categories $s_k, k = 1, \dots, K = \text{cat}$.

$$i_k(\mathbf{u}) = \begin{cases} 1 & \text{if } T(\mathbf{u}) \in s_k \\ 0 & \text{otherwise} \end{cases}
 \tag{31}$$

Note that each $T(\mathbf{u})$ can only fit into one category s_k . Also note that at any location \mathbf{u} we can define a probability of the $T(\mathbf{u})$ falling into a category s_k as

$$p_k(\mathbf{u}) = p\{T(\mathbf{u}) \in s_k\}
 \tag{32}$$

The field $T(\mathbf{u})$ is simulated as follows:

1. Code all observed $T(\mathbf{u})$ into categories, i.e.,

$$\begin{array}{ccccc} x_1 & y_1 & z_1 & T_1 & s(1) \\ x_2 & y_2 & z_2 & T_2 & s(2) \end{array}$$

$$x_\alpha \quad y_\alpha \quad z_\alpha \quad T_\alpha \quad s(\alpha)$$

where $s(\alpha) = 1, 2, \dots, k$ as input; also provide: variograms for s_k and global p_k (for simple kriging).

2. Select a category s_k , indicator transform using

$$i_k(u_\alpha) = \begin{cases} 1 & \text{if } s(\alpha) \in s_k \\ 0 & \text{otherwise} \end{cases} \quad (33)$$



3. Krige

$$[i_k(u|u_\alpha)]^* = \text{Prob}\{T(u) \in s_k | s(u_\alpha)\} = p_k^*(u|\alpha) \quad (34)$$

that is, krige the indicator of category s_k , which is the estimated probability of category s_k at the unknown location.

4. Repeat 2 and 3 for the $k = 1, 2, \dots, K$ categories, correct for order relations so that

$$\sum_{k=1}^K p_k^*(u|s_k(u_\alpha)) = 1 \quad (35)$$

5. Use the $p_k^*(\mathbf{u})$ as an empirical CDF $F_{s_k}(s_k)$ of $P\{s(\mathbf{u}) \in s_k\}$; generate a random $\mathbf{u}[0,1]$ and invert $F_{s_k}(s_k)$ to get a simulated s_k as S_k^* .
6. Go to a new random location u , and repeat steps 2 through 5.

Within each simulated category we can now simulate $T^*(u) = T(u)|s(u)s_k$ using the sGs algorithm as described in Section 4.1.6.2.

Figure 10 illustrates an example of a categorical simulation over a model domain using two categories.

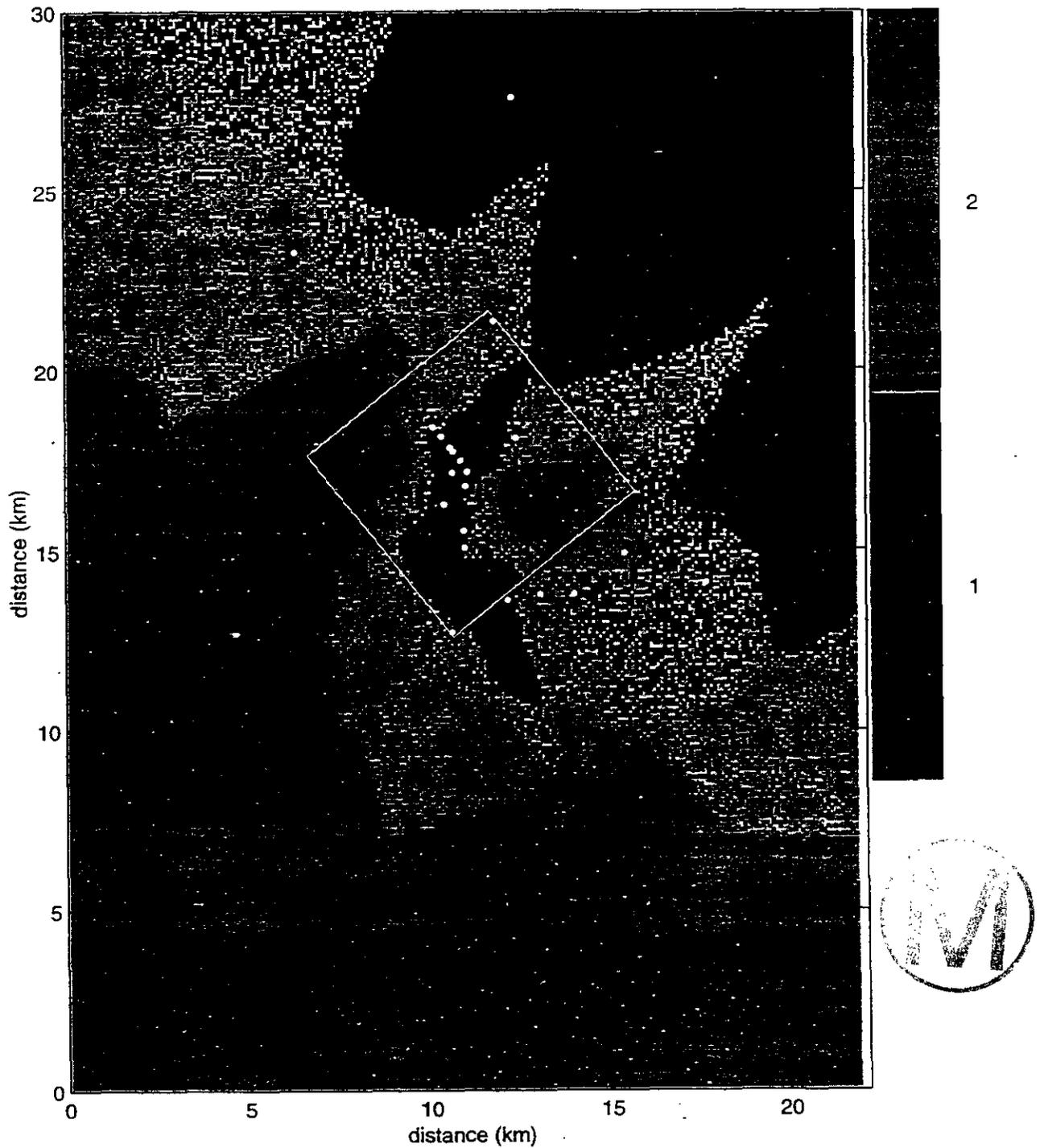


Figure 10. Example of Categorical Simulation over a Model Domain using Two Categories. Black dots indicate boreholes associated with Category 1; white dots are boreholes associated with Category 2.

4.1.6.2 Sequential Gaussian Simulation (sGs)

The conditional simulation (CS) of a *continuous* variable $T(\mathbf{u})$ modeled by a Gaussian-related stationary RF $T(\mathbf{u})$ proceeds as follows:

1. Determine the univariate CDF $F_z(T)$ representative of the entire study area and not only of the t-sample data available. Declustering may be needed if the T-data are preferentially located.
2. Using the CDF $F_z(T)$ perform the normal score transform of T-data into y-data with a standard normal CDF.
3. Check for bivariate normality of the normal score y-data. If the multivariate Gaussian model can not be retained, then consider an indicator-based algorithm for the stochastic simulation.
4. If a multivariate Gaussian RF model can be adopted for the y-variable, proceed with program `sgsim` and sequential simulation, i.e.,
 - Define a random path that visits each node of the grid (not necessarily regular) once. At each node \mathbf{u} , retain a specified number of neighboring conditioning data including both original y-data and previously simulated grid node y-values.
 - Use SK with the normal score variogram model to determine the parameters (mean and variance) of the CCDF of the RF $y(\mathbf{u})$ at location \mathbf{u} .
 - Draw a simulated value $y^{(1)}(\mathbf{u})$ from that CCDF.
 - Add the simulated value $y^{(1)}(\mathbf{u})$ to the data set.
 - Proceed to the next node, and loop until all nodes are simulated.
5. Backtransform the simulated normal values $\{y^{(1)}(\mathbf{u}), \mathbf{u} \in A\}$ into simulated values for the original variable $\{T^{(1)}(\mathbf{u}) = \varphi^{-1}(y^{(1)}(\mathbf{u}), \mathbf{u} \in A)\}$. Within-class interpolations and tail extrapolations are usually called for; see Section 4.1.2.



Figure 11 and 12 illustrate the sGs for the categorical simulation shown in Figure 10. Note that each sGs is independent of the other. Combining Figures 11 and 12 produces one CS field for a two-categorical problem. The grey scale in Figures 11 and 12 is presented in $\log_{10} \text{m}^2/\text{s}$ units.

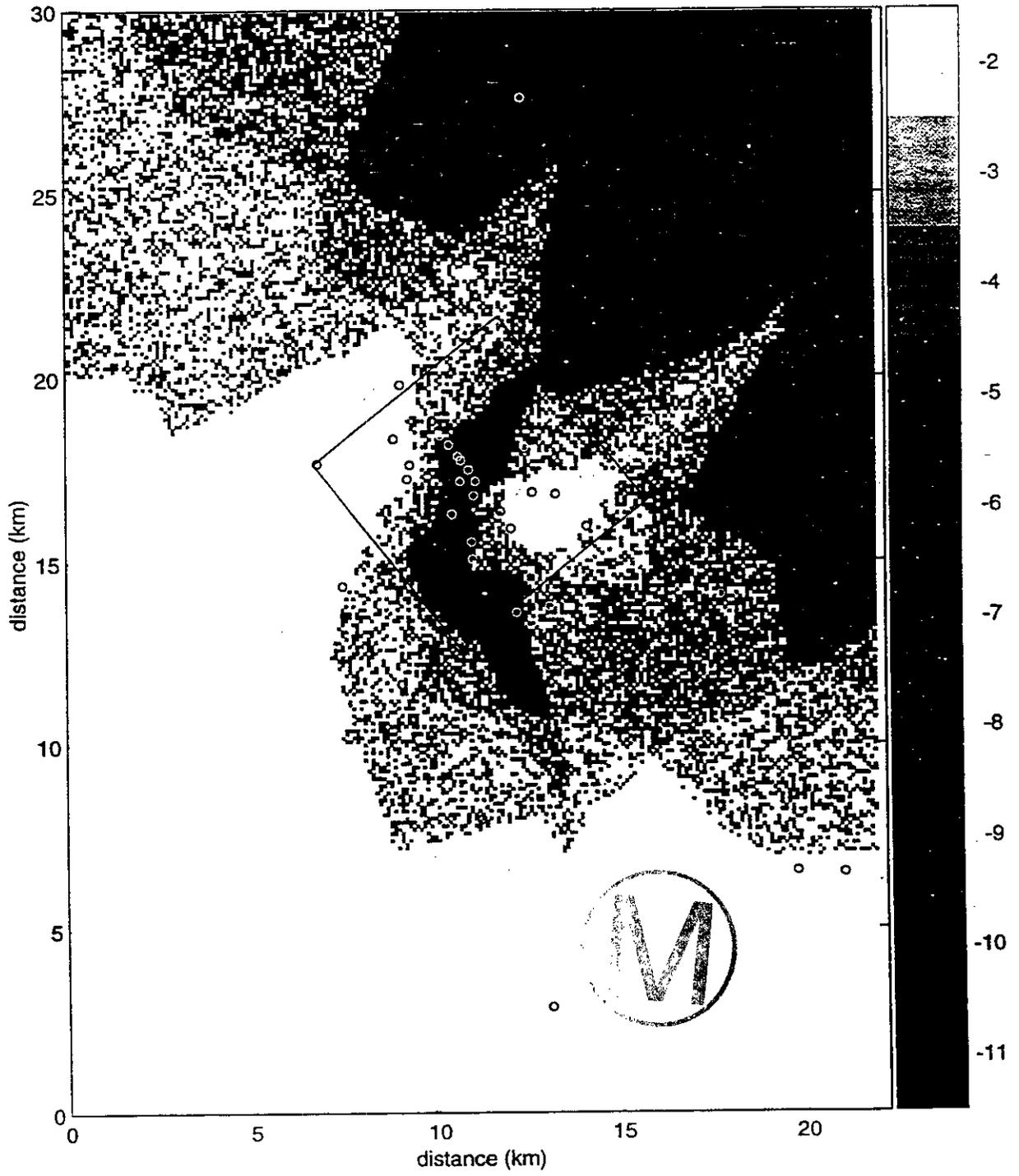


Figure 11. Sequential Gaussian Simulation (sGs) for Category 1.



Figure 12. Sequential Gaussian Simulation (sGs) for Category 2.

4.1.6.3 Implementation Considerations

Strict application of the sequential simulation principle calls for the determination of more and more complex CCDFs, in the sense that the size of the conditioning data set increases from (n) to $(n + N - 1)$. In practice, the argument is that the closer data screen the influence of more remote data; therefore, only the closest data are retained to condition any of the N CCDFs (Eq. 35). Because the number of previously simulated values may become overwhelming as i progresses from 1 to $N \gg n$, one may want to give special attention to the original data (n) even if they are more remote.

The neighborhood limitation of the conditioning data entails that statistical properties of the $(N + n)$ set of RV's will be reproduced only up to the maximum distance found in the neighborhood. For example, the search must extend at least as far as the distance to which the variogram is to be reproduced; this requires extensive conditioning as the sequence progresses from 1 to N . Gomez-Hernandez and Wen (1993) have suggested that sequential algorithms such as sGs can fail to adequately reproduce the long-range spatial correlations of some fields; this problem may be particularly pronounced for covariance functions models with zonal anisotropy. This situation can occur when the random sequence of simulated locations fails to populate the field at long distances early enough in the sequence so that the simulated values do not reflect the effects of the long distance correlations.

To circumvent this situation, **CONSIM II** uses a multigrid approach, a type of stratified random sampling, to force the sequential simulation to visit widely separated locations early in the sequence (Gomez-Hernandez and Cassiraga, 1994). The multigrid approach involves setting up an initial coarse grid, each point of which is visited randomly in the sequential simulation. Subsequent finer grids are superimposed and simulated until the grid spacing is reduced to the desired resolution. Because the multigrid approach requires the sequential simulation algorithms to visit widely-spaced locations first, it helps the simulations retain the long distance spatial correlation structure specified as input.

Theory does not specify the sequence in which the N nodes should be simulated. Practice has shown, however, that it is better to consider a random sequence. Indeed, if the N nodes are visited row-wise, any departure from rigorous theory may entail a corresponding spread of artifacts along rows.

4.1.7 CONSIM II: Connection to SWIFT II

Once the simulation (i.e., generation) of the transmissivity field is complete by **CONSIM II**, information concerning the transmissivity field is passed to the **SWIFT II** flow model finite difference grid. The details for each **SWIFT II** block that are passed from **CONSIM II** to **SWIFT II** include

1. The simulated (estimated) log transmissivity
2. A lower bound for the log transmissivity

3. An upper bound for the log transmissivity
4. The category for the block
5. A flag that can prohibit the block from being selected as a pilot point

CONSIM II generates items 1 through 4 for every point on the simulation grid as discussed in the previous sections. It then generates the same four items for every block on the SWIFT II grid by averaging. After the averaging is done, the simulation grid is effectively discarded, i.e., not used further by GRASP-INV.

To find transmissivities and a category for a SWIFT II grid block, the block must contain at least one simulated point. If not, a large negative (e.g. -99) value is assigned to the log transmissivity and its bounds, and the category for the block is set to 0. Subsequently, SWIFT II will *not* overwrite the values read from its input file for the conductivities for the block.

If there is at least one refined point within a SWIFT II grid block, simulated transmissivity values from each contained point are averaged to find a value for the SWIFT II block. There are two different approaches taken depending on the type of refined grid. If the refined grid is irregular, the geometric mean of the simulated transmissivities is calculated. If the refined grid is regular, an analog to resistance computations for an electrical circuit is used.

For an irregular grid (this includes the Gauss points used by the previous version of GRASP-INV) the arithmetic mean of the logarithms of the transmissivities for the included points is found. This is equivalent to finding the geometric mean of the transmissivities themselves. The arithmetic mean is found by summing the log transmissivities contained in the block and dividing by their number.

For a regular grid the first assumption is that each refined point has equal weight, i.e., comprises an equal volume within the SWIFT II grid block. A principal direction is selected and the SWIFT II grid block is partitioned into a sequence of slices, where each slice is perpendicular to that direction. Fluid entering the block must traverse each slice. If there is more than one refined point within a slice, the fluid has more than one path through the slice. This is analogous to resistance in parallel in an electrical circuit. Resistors in parallel have a total resistance found by the inverse of the sum of the inverses of the individual resistors. Since transmissivity is inversely proportional to resistance, the transmissivity for a slice is found from the sum of the transmissivities for the refined points within the slice. Each slice must be traversed in sequence. This is analogous to resistance in series. Resistors in series have total resistance equal to the sum of the individual resistors. Again applying the inverse relation between resistance and transmissivity, the average transmissivity across all slices is the inverse of the sum of the inverses of the individual slice transmissivities.

In two dimensions, a slice is a row or column of refined points. In three dimensions a slice is comprised of points in a plane. CONSIM II finds the directional transmissivity for each SWIFT II grid block in the x and y directions (T_x and T_y) using the electrical analogue. The equivalent



horizontal conductivity is then the geometric mean, $T_h = (T_x T_y)^{1/2}$. The calculations conducted are illustrated below for a two-dimensional problem.

4.1.7.1 Upscaling Example - Electrical Analog

Consider a geostatistical simulation grid of 25 x 25 (x,y), with 1m grid spacing in each direction. Assume the SWIFT II grid is 7 x 7 (x,y), with grid spacing equal to 3.6 m in the x and y directions. This example will illustrate the method used to upscale the results of the geostatistical simulation to the SWIFT grid. This example is designed such that each SWIFT II grid block will contain 3 or 4 simulation points in the x-direction and 3 or 4 in the y-direction. The simulation points that reside within a SWIFT II grid block will be averaged together to determine a transmissivity value assigned to the SWIFT II grid block. In this example, the simulation grid is created internally by CONSIM II. This grid is created by specifying the location option as zero (in catg and sgsim input files) and providing the number of blocks and their (equal) size in each direction. (See Sections 7.5.5, 7.5.6, and Appendix C.)

When the simulation grid is generated internally, i.e., the grid is equally spaced, CONSIM II finds an average horizontal transmissivity using the analogue of electrical resistance. The electrical analogue approach to finding the average horizontal transmissivity considers flow through slices in each direction. To traverse a single slice, fluid has a choice of paths, which is analogous to resistance in parallel. To traverse all slices, fluid must cross each slice, which is analogous to resistance in series.

As an example, assume the simulated log transmissivities falling within a SWIFT II grid block have the transmissivity and category values listed in Table 1 below.

Table 1. Simulated Log₁₀ Transmissivities and Categories Falling Within a SWIFT II Grid Block for Upscaling Example

x	y	Value	Category*
1.5	1.5	1.0	1
2.5	1.5	1.0	1
3.5	1.5	1.0	1
1.5	2.5	0.0	2
2.5	2.5	0.0	2
3.5	2.5	0.0	2
1.5	3.5	-1.0	2
2.5	3.5	-1.0	2
3.5	3.5	-1.0	2

*1=High transmissivity
 2=Low transmissivity



CONSIM II makes the assumption that each simulated point comprises an equal portion of the volume of the SWIFT II grid block that contains it. So for a SWIFT II grid block that has nine simulated points falling within it, the weights assigned to these points would be the same. Table 2 depicts the locations of the transmissivity values listed above within the SWIFT II grid block.

Table 2. Simulated Transmissivities Lying Within a SWIFT II Grid Block For Upscaling Example

0.1	0.1	0.1
1.	1.	1.
10.	10.	10.



As mentioned above, the electrical analogue approach to finding the average horizontal transmissivity considers flow through slices in each direction. Traversing a single slice is analogous to resistance in parallel. Traversing all slices is analogous to resistance in series. In this example, the x-direction is analyzed first, where flow is assumed from left to right in Table 2. Each slice is a column in Table 2. The transmissivity for a slice is found by adding its transmissivities. Calling the three columns slice 1, slice 2, and slice 3, their transmissivities are

$$\text{Slice 1 transmissivity} = 11.1$$

$$\text{Slice 2 transmissivity} = 11.1$$

$$\text{Slice 3 transmissivity} = 11.1$$

To traverse all three slices (analogous to encountering resistance in series), each slice transmissivity is inverted, the sum is found, and the result is inverted. Thus, the transmissivity in the x-direction, T_x , is given by

$$T_x = [(1/11.1) + (1/11.1) + (1/11.1)]^{-1} = 3.7$$

For the y-direction the same approach is taken only this time each slice is a row of Table 2. The slice transmissivities for the rows are:

$$\text{Slice 1 transmissivity} = 0.3$$

$$\text{Slice 2 transmissivity} = 3.0$$

$$\text{Slice 3 transmissivity} = 30.$$

Thus, the transmissivity in the y-direction, T_y , is given by

$$T_y = [(1/0.3) + (1/3.0) + (1/30.)]^{-1} = 0.27027$$

Horizontal transmissivity, T_h , is then estimated by the geometric mean of T_x and T_y . Thus,

$$T_h = (T_x T_y)^{1/2} = 1.0$$

The \log_{10} of T_h is 0.0.

The other variable that is upscaled to the SWIFT II grid block is the category variable. The category that is assigned to the SWIFT II grid block is the most frequent among the simulation points within the block. In case of ties, the lowest category number involved in the tie is selected and assigned to the block. In the example above, category 2 would be assigned to the SWIFT II grid block because of the larger number of category 2 values falling within the block.

CONSIM II does not calculate the vertical direction transmissivity because it is assumed that conditioning data is based on horizontal transmissivities. SWIFT II will calculate vertical conductivity by converting the horizontal transmissivity computed here to horizontal conductivity and multiplying by the nominal value of anisotropy (Section 7.4).

4.1.7.2 Upscaling Example - Geometric Mean

Consider the same grid used in the previous example of Section 4.1.7.1. The geostatistical simulation grid is 25 x 25 (x, y), with 1 m grid spacing in each direction. The SWIFT II grid is 7 x 7 (x, y), with grid spacing equal to 3.6 m in the x and y directions. The example is designed such that each SWIFT II grid block will contain 3 or 4 simulation points in the x-direction and 3 or 4 in the y-direction. The simulation points that reside within a SWIFT II grid block will be averaged together to determine a transmissivity value assigned to the SWIFT II grid block. In this example, the simulation grid is read from a text file. This is done by specifying the location option as 1 (in *catg* and *sgsim* input files) and providing the name of the text file and the columns to use on the file. When the simulation grid is provided on a text file, the geometric average of transmissivities found within a SWIFT II block is used as demonstrated below.

Assume the simulated log transmissivities falling within a SWIFT II grid block have the transmissivity and category values as listed in the previous example (Table 1). The geometric mean transmissivity taken over all the simulation values within the block is equivalent to calculating the arithmetic mean of the log transmissivities. Summing all values listed in Table 1 and dividing by 9 gives a mean $\log_{10} T_h$ value of 0.0. (Note: The example used gave equivalent values between the electric analog and geometric mean upscaling calculations, which is not usually the case.)

4.1.7.3 Summary

The steps used to upscale the geostatistical simulation results to the SWIFT grid are summarized as follows:



1. Use the electrical current analog to groundwater flow to find average transmissivity in the x-direction, T_x ,
2. Use the electrical current analog to groundwater flow to find average transmissivity in the y-direction, T_y ,
3. Find the equivalent horizontal isotropic transmissivity, $T_h = (T_x T_y)^{1/2}$,
4. Convert T_h to conductivity K_h by dividing by block thickness,
5. Estimate vertical conductivity K_v by multiplying K_h by the nominal anisotropy factor, and
6. Use K_h for both K_x and K_y in SWIFT II and use K_v for K_z .



Note the following with regard to block thickness in Step 4. Initially all blocks in a horizontal layer have the same thickness. Nonuniform thicknesses can be provided to SWIFT II either through the R1-21 cards or the R1-26 cards (see Appendix D). The grid block thickness used above is the thickness established after the R1-21 cards are read but before the R1-26 cards are read. So in GRASP-INV it is recommended that thicknesses *not* be modified using the SWIFT II R1-26 cards.

CONSIM II uses the same approach, depending on the type of simulation grid, to find minimum and maximum values for transmissivity in each block. Instead of simulated values it substitutes the minimum and maximum bounds for each simulated point during the averaging process. This substitution produces a minimum and maximum log transmissivity for the SWIFT II grid block. Note that the bounds were originally symmetric when simulation was being performed on the normal scores. Symmetry is generally lost during back transformation to original data, and can be further diminished during the averaging processes described above.

In the GRASP-INV scheme, the simulated SWIFT II grid is used as an initial estimate for the calibration process. At each step of the calibration, a pilot point(s) is found and its transmissivity is modified, along with that of grid blocks "nearby". Pilot point locations are selected from the set of SWIFT II grid block centers. If the location of a conditional data point coincides with a SWIFT II grid block center, the center should *not* be an eligible pilot point. That is, the transmissivity at such a point must be honored and therefore must not be modified.

Each conditioning data point is located on the SWIFT II grid (Section 7.5.2). Its distance to the center of the block is computed, wd . The diagonal distance from the block center to a block corner is also computed, cd . If the ratio wd / cd is less than a specified fraction, the data point is considered to fall on the grid block center. Currently, the specified fraction is 0.2. Note that this test and restriction apply only if the data point and the grid block are of the same category.

4.2 SWIFT II

The groundwater flow model of the Culebra Dolomite was developed using the computer code SWIFT II. SWIFT II (Sandia Waste Isolation, Flow, and Transport code) is a fully transient, three-dimensional, finite difference code that solves the coupled equations for single-phase flow and transport in porous and fractured geologic media, where the mass per unit volume, ρ , is a function of the concentration of the transported constituents. The SWIFT II code is supported by comprehensive documentation and extensive testing. The theory and implementation of SWIFT II are given by Reeves et al. [1986a] and the data input guide is given by Reeves et al. [1986b]. Finley and Reeves [1981] and Ward et al. [1984] present the verification-validation tests for the code.

The transient flow equation solved by SWIFT II is given by

$$\nabla \cdot \left[\frac{(\rho k)}{\mu} (\nabla p - \rho g \nabla z) \right] + q = \frac{\partial(\phi \rho)}{\partial t} \quad (36)$$

where $k = k(\mathbf{x})$ is permeability tensor, $p = p(\mathbf{x}, t)$ is pressure, z is the vertical coordinate and is considered positive downward, $\rho = \rho(\mathbf{x})$ is fluid density, q is flux sources or sinks, g is the gravitational constant, μ is fluid viscosity, ϕ is rock porosity, \mathbf{x} is the position vector, and t is time. Discretized, (36) becomes a matrix equation of the form

$$[A]\{p\}^n = [B]\{p\}^{n-1} + \{f\}^n \quad (37)$$

where, for the fully implicit scheme of time integration in SWIFT II, $[A] = [C] + [S]/\Delta t_n$, $[B] = [S]/\Delta t_n$, $[C]$ is the conductance matrix, $[S]$ is the storativity matrix, $\{f\}$ is the load vector, $\Delta t_n = t^n - t^{n-1}$, t is time, n is the time level (e.g., 1, 2, ..., L) is the maximum time level of the simulation.

4.3 GRASP II

Adjoint Sensitivity Analysis and Kriging

The GRASP II (groundwater adjoint sensitivity program) code computes measures of the behavior of a groundwater system typically based on pressures or heads at one or several locations. GRASP II then calculates the sensitivities of these measures to system parameters (e.g. permeabilities and prescribed pressure values at the boundaries). The computed measures are referred to as "performance measures" and may include weighted spatial sums of groundwater pressures at selected locations or weighted squared deviations of computed and observed pressures at selected locations (or boreholes).

The sensitivities are computed by the adjoint method [Chavent, 1971] and are derivatives of the performance measures with respect to the parameters for the modeled system, taken about the

assumed parameter values. The system parameters available for use with GRASP II are (1) \log_{10} transmissivity assigned to a pilot point (see below), (2) grid block permeabilities or transmissivities, (3) prescribed pressure values at the boundaries, (4) recharge, and (5) source/sink rates. In the application to be used by WIPP PA, weighted sums of the squared differences between calculated and observed groundwater pressures at selected boreholes will be the chosen performance measures, and transmissivities assigned to pilot points will be the chosen system parameter used during model calibration.

GRASP II presumes either steady state or transient state saturated groundwater flow conditions and postprocesses the results from a SWIFT II flow simulation. The theory and verification for the steady state flow sensitivity equations used in GRASP II are presented by Wilson et al. [1986], while those for the transient flow sensitivity equations are presented by RamaRao and Reeves [1990]. For completeness, a brief presentation of the pertinent equations solved by GRASP II during this study is given below.

A conventional approach to the evaluation of sensitivity coefficients is defined by the expression

$$J = f(\alpha, p) \quad (37)$$

where J is a performance measure and α is a vector of sensitivity parameters. Let α_1 be the parameter for which a sensitivity coefficient is sought. Then

$$dJ/d\alpha_1 = \partial J/\partial\alpha_1 + \partial J/\partial p \cdot \partial p/\partial\alpha_1 \quad (38)$$

The first term on the right-hand side of Eq. 38 represents the sensitivity resulting from the explicit dependence of J on α_1 and is called the direct effect. The second term represents an indirect effect due to the implicit dependence of J on α_1 through the system pressures, $p(\alpha)$. While the computation of the direct effect is a trivial step, that of the indirect effect involves the evaluation of the state sensitivities; $\partial p(x, t)/\partial\alpha_1$. State sensitivities may be calculated by the "parameter-perturbation approach" [Yeh, 1986] or by solution of the partial differential equation for state sensitivity [Sykes et al., 1985; Yeh, 1986]. However, these approaches require the state sensitivities to be recomputed whenever a new parameter is considered. In a numerical model with a large number of grid blocks/elements and different system parameters, this represents an enormous computational effort of the same order as in the multiple simulation approach to parameter sensitivity.

The adjoint sensitivity approach circumvents the need to compute state sensitivities. This is done by expressing the performance measure as the sum of two distinct terms, one containing, exclusively, the partial variations with respect to the pressure function and the second containing partial variations with respect to α_1 [RamaRao and Reeves, 1990]. Both terms include a function referred to as the adjoint state. The adjoint state is computed such that it greatly facilitates the



evaluation of the second term on the right-hand side of Eq. 38. The adjoint state vector λ is obtained by solving the following equation:

$$[A]\{\lambda\}^{n-1}=[B]\{\lambda\}^n + [\partial J/\partial\{p^n\}^T]^T \quad (39)$$

where T denotes the transpose of the matrix, A and B are the same matrices used in the primary problem (i.e., pressure solution) solved by SWIFT II, and J is the performance measure (e.g., the cumulative sum of squared pressure deviations between calculated and observed pressures). The solution of Eq. 39 permits the evaluation of parameter sensitivities by the following expression:

$$\frac{dJ}{d\alpha_i} = \frac{\partial J}{\partial \alpha_i} + \sum_{n=1}^L \{\lambda^n\}^T \left[\frac{\partial [A]}{\partial \alpha_i} \{p\}^n - \frac{\partial [B]}{\partial \alpha_i} \{p\}^{n-1} - \frac{\partial \{f^n\}}{\partial \alpha_i} \right] \quad (40)$$

The fact that there are not state sensitivity terms in the above expression leads to one important feature of the adjoint method, namely, the separation of the relatively time-intensive calculation of the adjoint state vector λ in Eq. 39 from the relatively non-time-intensive calculation of the sensitivity derivative Eq. 40. In general, this separation permits the calculation of sensitivity derivatives for all of the system parameters using the same adjoint state vector $[\lambda]$, a major advantage over the perturbation approach.

4.3.1 GRASP II: Objective Function

The objective function that is minimized during calibration is a weighted least square error criterion function which is a model fit criterion. The model fit criterion is a weighted sum of the squared deviations between the computed and measured pressures taken over all points in spatial and temporal domains where pressure measurements have been made.

For a purely steady state simulation, the objective function (also called performance measure) is given by

$$J_s(\underline{u}) = \sum_{i=1}^n w_i (P_i - P_{ob,i})^2 \quad (41)$$



where

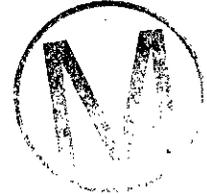
- $J_s(\underline{u})$ = objective function for steady state,
- n = number of boreholes,
- i = suffix for the borehole,
- P = calculated pressure,
- $P_{ob,i}$ = observed pressure, and
- w_i = weight assigned to the borehole.

For transient simulation, similarly

$$J_t(\underline{u}) = \sum_{t_1}^{t_2} \sum_{i=1}^n w_{i,t} (P_{i,t} - P_{ob,i,t})^2 \quad (42)$$

where

- $J_t(\underline{u})$ = objective function for transient state,
- t_1 = the beginning of the time window,
- t_2 = the end of the time window, and
- w = weight assigned to selected borehole for a given time t .



The transient performance measure may consist of short transient events during which a response is observed only at a single location or long-term events during which responses are observed at several locations.

In practice, the steady state calibration is undertaken first. Subsequently, the transient calibration is taken up. It is necessary to ensure that the fit between calculated and observed pressures be improved during transient calibration without degrading the fit to the steady state calibration. From experience, it has been found that this requires that the contributions from the steady state and the transient state to the combined performance measure should be approximately equal. Because transient performance measures can be generally much larger than the steady state performance measures (because values are summed up in the time window), an additional factor f is used to ensure that the steady state performance measure and the transient performance measure are approximately equal in the combined performance measure $J(\underline{u})$.

$$J(\underline{u}) = f J_s(\underline{u}) + J_t(\underline{u}) \quad (43)$$

where

- $J(\underline{u})$ = combined steady and transient objective function, and
- f = weight factor for steady state objective function.

Also,

$$f J_s(\underline{u}) \approx J_t(\underline{u}) \quad (44)$$

$$f \approx \frac{J_t(\underline{u})}{J_s(\underline{u})}$$

4.3.2 GRASP II: Adjoint Sensitivity Analysis

Adjoint sensitivity analysis provides an extremely efficient algorithm for computing sensitivity coefficients between a given objective function J and a large number of parameters (permeabilities in thousands of grid blocks as is the case here).

Let the groundwater flow model be represented by the following matrix equation:

$$\underline{A} \underline{p}^n = \underline{B} \underline{p}^{n-1} + \underline{f}^n \quad (45)$$

where for a fully implicit scheme of time integration adopted here:

- \underline{p} = vector of gridblock pressures,
- $\underline{A} = \underline{C} + \underline{B}$,
- $\underline{B} = \underline{S}/\Delta t$,
- \underline{C} = conductance matrix,
- \underline{S} = storativity matrix,
- \underline{f}^n = vector of source terms,
- $\Delta t = t^n - t^{n-1}$,
- t = time,
- n = time level (1,2,3...L), and
- L = maximum time level of the simulation.



First, an adjoint state vector $\{\lambda\}$ is obtained by the solution of the following equation:

$$\underline{A} \underline{\lambda}^{n-1} = \underline{B} \underline{\lambda}^n + \left[\frac{\partial J}{\partial \underline{p}^n} \right]^T \quad (46)$$

where T denotes the transpose of the matrix.

Eq. 46 is solved backwards in time, from $n = L$ to $n = 1$ with

$$\underline{\lambda}^L = 0 \quad (47)$$

If a_i is a generic sensitivity parameter in the gridblock i , the sensitivity coefficient dJ/da_i is evaluated by the expression:

$$\frac{dJ}{da_i} = \frac{\partial J}{\partial a_i} + \sum_{n=1}^L \underline{\lambda}^{nT} \cdot \left[\frac{\partial \underline{A}}{\partial a_i} \underline{p}^n - \frac{\partial \underline{B}}{\partial a_i} \underline{p}^{n-1} - \frac{\partial \underline{f}^n}{\partial a_i} \right] \quad (48)$$

Here, Eq. 48 is evaluated with $\alpha_i = K_i$, the permeability in the grid block.

4.3.3 GRASP II: Locating Pilot Points

De Marsily et al. (1984) pioneered the concept of pilot points as parameters of calibration. He assigned their locations based on some considerations. In GRASP-INV, LaVenue and Pickens' (1992) approach to location of pilot points is followed. Pilot points are placed at grid-block center locations where their potential for reducing the objective function is the highest. This potential is quantified by the sensitivity coefficients (dJ/dY_p) of the objective function J , with respect to Y_p , the logarithm (to base 10) of pilot-point transmissivity. A large number of candidate pilot points are considered (as specified by the user), usually the centroids of all the grid blocks in the flow model grid. Each potential pilot point is initially described by an x,y,z location (grid block center) and a category type. The variograms for each category represented by the candidate pilot points and the number of neighboring grid blocks with the same category type is considered in the sensitivity equations.

Coupled adjoint sensitivity analysis and kriging is used to compute the required derivatives and the procedure is documented in RamaRao and Reeves (1990). It is described briefly here.

The user specifies the maximum number of pilot point locations to consider (e.g., 50, 100). The code will then determine the grid blocks with the highest derivative $\frac{dJ}{dY_m}$ (see below) and then

calculates $\frac{dJ}{dY_p}$ (see below) for these grid blocks only. It then re-ranks these grid blocks' $\frac{dJ}{dY_p}$

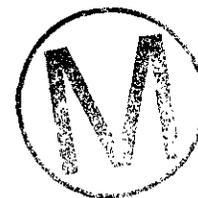
sensitivities and places a pilot point in the grid block with the highest sensitivity value. GRASP-INV then sends this new pilot point location to PAREST to optimize the pilot point's transmissivity value.

Let P be a pilot point added to a set of N observed transmissivity values within a particular category. Let T_p be the transmissivity assigned to pilot point P . Kriging is done using Y_p , where

$$Y_p = \log_{10} T_p \quad (49)$$

The kriged estimate (Y^*) at the centroid of a grid block m for this category is given by

$$Y_m^* = \sum_{k=1}^N \gamma_{m,k} Y_k + \gamma_{m,p} Y_p \quad (50)$$



where k is the subscript for an observation point, p is the subscript for pilot point, $\gamma_{m,k}$ is the kriging weight between the interpolation point m and data point k , and $\gamma_{m,p}$ is the kriging weight between interpolation point m and pilot point p .

When a pilot-point transmissivity is perturbed, the kriged transmissivities and hence the conditionally simulated (CS) values in the neighboring grid blocks having the same category of the pilot point are altered, causing the objective function J to change. If a neighboring grid block belongs to another category, its CS value will not be affected by the addition of a nearby pilot point belonging to another category. Let Y_m^* represent the CS value assigned to grid block m . Using the chain rule,

$$\frac{dJ}{dY_p} = \sum_{m=1}^M \frac{\partial J}{\partial Y_m} \frac{\partial Y_m}{\partial Y_p} \quad (51)$$

where M is the total number of grid blocks in the flow model.

$$\frac{\partial Y_m}{\partial Y_p} = \gamma_{m,p} \quad (52)$$

where $\gamma_{m,p}$ is the linear weight between a pilot point and the finite-difference grid block centroid. This result is valid for a CS field also, because the kriging error is independent of the kriged values.

$$\frac{dJ}{dY_p} = \sum_{m=1}^M \frac{dJ}{dY_m^*} \cdot \gamma_{m,p} \quad (53)$$

$$Y_m^* = \log_{10}(T_m^*) \quad (54)$$

$$T_m^* = k_m \frac{\rho_m}{\mu_m} g b_m \quad (55)$$

$$\frac{dJ}{dY_m} = \ln(10) k_m \frac{dJ}{dK_m} \quad (56)$$

where T^* is the CS transmissivity, k is the CS permeability, ρ is fluid density, μ is fluid viscosity, g is acceleration due to gravity, b is grid block thickness, and m is the subscript denoting grid block.

Combining Equations 51, 52, and 53 yields

$$\frac{dJ}{dY_p} = \ln(10) \sum_{m=1}^M \gamma_{m,p} k_m \frac{dJ}{dk_m} \quad (57)$$

The sensitivity coefficient, dJ/dk_m of the objective function with respect to the permeability in a grid block m , is obtained by adjoint sensitivity analysis.

4.4 PAREST

PAREST comprises the optimization code used to assign transmissivities to selected pilot point locations. The optimization is essentially conducted in a two step process. Given the parameter to be optimized, determine which direction to adjust its initial value (i.e., increase or decrease). Once the direction is chosen, determine the optimal change or "step length" in this direction. Details concerning these two parts of the optimization process are discussed below.

4.4.1 PAREST: Parameters of Calibration

The pilot-point transmissivities are the parameters that are adjusted for calibration. However, in the mathematical implementation, the logarithms (to base 10) of the transmissivities (and not the transmissivity) are treated as parameters. The calibration parameters are given by

$$Y_p = \log_{10} T_p \quad (58)$$

where T_p is the transmissivity at a pilot point (suffix p denotes pilot point).



4.4.2 PAREST: Optimizing Pilot Point Transmissivity

The transmissivities at pilot points are assigned by an unconstrained optimization algorithm and a subsequent imposition of constraints. The optimization algorithm chosen here belongs to a class of iterative search algorithms. It involves a repeated application of the following equation until convergence is achieved:

$$\underline{Y}_{i+1} = \underline{Y}_i + \beta_i \cdot \underline{d}_i, \quad (59)$$

where i is the iteration index, \underline{d}_i is the direction vector, β_i is the step length (a scalar), and \underline{Y}_i is the vector of parameters to be optimized (i.e., logarithms of pilot-point transmissivities to base 10).

The steps in the implementation of this algorithm are as follows:

1. For the selected number of pilot points, use the initial estimates of the pilot-point \log_{10} transmissivity ($Y_p = \log_{10} T_p$), i.e., the kriged values in the gridblocks where pilot points are located.

2. Compute the direction vector, \underline{d}_i , as per one of the three algorithms discussed below (Fletcher-Reeves, Broyden's, or Davidon-Fletcher-Powell). The direction vector constitutes a direction in the hyperspace of the parameters. By advancing along the direction vector, the new values of the parameters are obtained. The step length β determines the actual advance along this direction.
3. Determine the optimal step length β , which minimizes the objective function.

$$\beta_i J(\underline{Y}_{i+1}) = \min J(\underline{Y}_i + \beta_i \underline{d}_i)$$

4. Update the parameters:

$$\underline{Y}_{i+1} = \underline{Y}_i + \beta_i \underline{d}_i$$

Impose the constraints.

5. Check for convergence.
6. If convergence is achieved, the optimization algorithm is completed and the pilot points are added to the data and passed to the CONSIMX code to modify the grid block transmissivity values which are then sent to SWIFT II
7. If convergence is not achieved, iterate within the optimization routine: using the augmented data set, modify the grid block transmissivities with the CONSIMX code, derive the corresponding pressure field, and recompute the gradient vector using the already selected pilot point locations. (The pilot point selection process will be skipped. Go to Step 2 above.)

4.4.2.1 Direction Vector: \underline{d}_i

Three options for the computation of the direction vector \underline{d}_i are considered. They are the algorithms due to (1) Fletcher-Reeves, (2) Broyden, and (3) Davidon-Fletcher-Powell (Luenberger, 1973; Gill et al., 1981; Carrera and Neuman, 1986). These methods are well-known in classical literature and are not described here. The details with respect to pilot point methodology are given by LaVenue and RamaRao (1992).

4.4.2.2 Step Length: β_i

The step length β_i , (a scalar) is determined by:

(60)

$$\beta_i J(\underline{Y}_{i+1}) = \min J(\underline{Y}_i + \beta_i \underline{d}_i)$$

Thus, β_i is obtained by solving

$$\frac{\partial J(\underline{Y}_{i+1})}{\partial \beta_i} = 0 . \quad (61)$$



The solution of Eq. 61 follows from Carrera and Neuman (1986) and Neuman (1980). The details in respect to pilot points, are presented in LaVenue and RamaRao (1992) and are not repeated here.

4.4.2.3 Constraints

It is possible that the optimization algorithms may dictate large changes in the transmissivities assigned to pilot points and bring about a reduction in the objective function. Such recommended large changes may be viewed as undesirable for several reasons. At any point in the field, one can obtain a kriged estimate of transmissivity and its variance (kriging variance). One may construct a confidence interval (assuming a normal distribution of kriging errors) for the transmissivity. It is reasonable to expect the calibrated value to be within the confidence band. A constraint may be imposed to achieve this.

There also may be situations where the confidence band is large. A large change in a pilot-point transmissivity value, even if contained within the confidence band, can cause a large change in the spatial correlation structure of the transmissivity field. One objective in calibration can then be to limit the maximum change to a specified value so that the geostatistical structure of the transmissivity field is not altered significantly.

Consider the k th parameter, whose value is Y_k (k th element in the vector of parameters, \underline{Y}). Then,

$$\begin{aligned} \Delta Y_{k,i} &= (Y_{k,i+1} - Y_{k,i}) \\ &= \beta_i \cdot d_{k,i} \end{aligned} \quad (62)$$

where i is an iteration index.

Constraint 1: The parameter value should lie within the confidence band.

$$Y_k - m\sigma_y \leq Y_{k,i+1} \leq Y_k + m\sigma_y \quad (63)$$

Thus Y_k gives the kriged value at the location of k (the pilot point), σ gives the kriging variance at the same location, and m is the multiplier of the standard deviation, which gives the semi-width of the confidence band. GRASP-INV uses a 95% confidence band, which is obtained from CONSIM II during the simulation of the transmissivity field (Section 4.1.7). The 95% confidence interval values are sent to PAREST as grid block minimum and maximum values and are therefore used as constraints during pilot point transmissivity optimization.

Constraint 2: The change in any parameters must be limited to ΔY_{\max} .

$$\Delta Y_{k,i} \leq \Delta Y_{\max} \quad (64)$$

After the optimization, these constraints are implemented for each parameter. If a constraint becomes active (imposed), the optimal step length computed is reduced; however, the direction is preserved.

4.4.2.4 Convergence Criteria

Distinction Between Inner and Outer Iterations

There are two levels of iteration, designated as inner and outer iterations. During an outer iteration, optimal location of a set of pilot points is calculated using coupled kriging and adjoint sensitivity analysis. Subsequently, the transmissivities are optimized by a sequence of inner iterations. An inner iteration relates to the iterations needed to optimize the transmissivities of the pilot points once they have been located. Thus, if an inner iteration is repeated, the pilot point locations remain fixed and the optimization conducts a second iteration on the pilot-point transmissivity values. When the convergence of an inner iteration is achieved, the selected pilot points are added to the transmissivity data set. This then sets the stage for another outer iteration.

Convergence Criteria: Inner Iterations

The following criteria may be used to define convergence when optimizing the transmissivities assigned to a set of pilot points. These criteria are very similar to those employed by Carrera and Neuman (1986).

1. The performance measure (J) drops below a prescribed minimum value (J_{\min}):

$$J \leq J_{\min}.$$

2. The number of iterations (N_{ITER}) equals a prescribed maximum number of iterations, for the inner iterations ($I_{\text{TERM}1}$):



$$NITER \geq ITERMX1 .$$

3. The ratio of the norm of the gradient to the initial gradient norm reduces below a prescribed value (GRNR):

$$\frac{\|g\|}{\|g_0\|} \leq \begin{matrix} GRNR \\ \text{(gradient norm ratio)} \end{matrix}$$

4. The gradient norm $\|g\|$ is less than a prescribed minimum (GRMIN):

$$\|g\| \leq GRMIN$$

5. The relative change in objective function is defined, as $\Delta J/J$, where ΔJ is the change in the objective function during one iteration. Iterations are terminated if this relative change falls below a prescribed value (RELCJ):

$$\frac{\Delta J}{J} \leq RELCJ$$

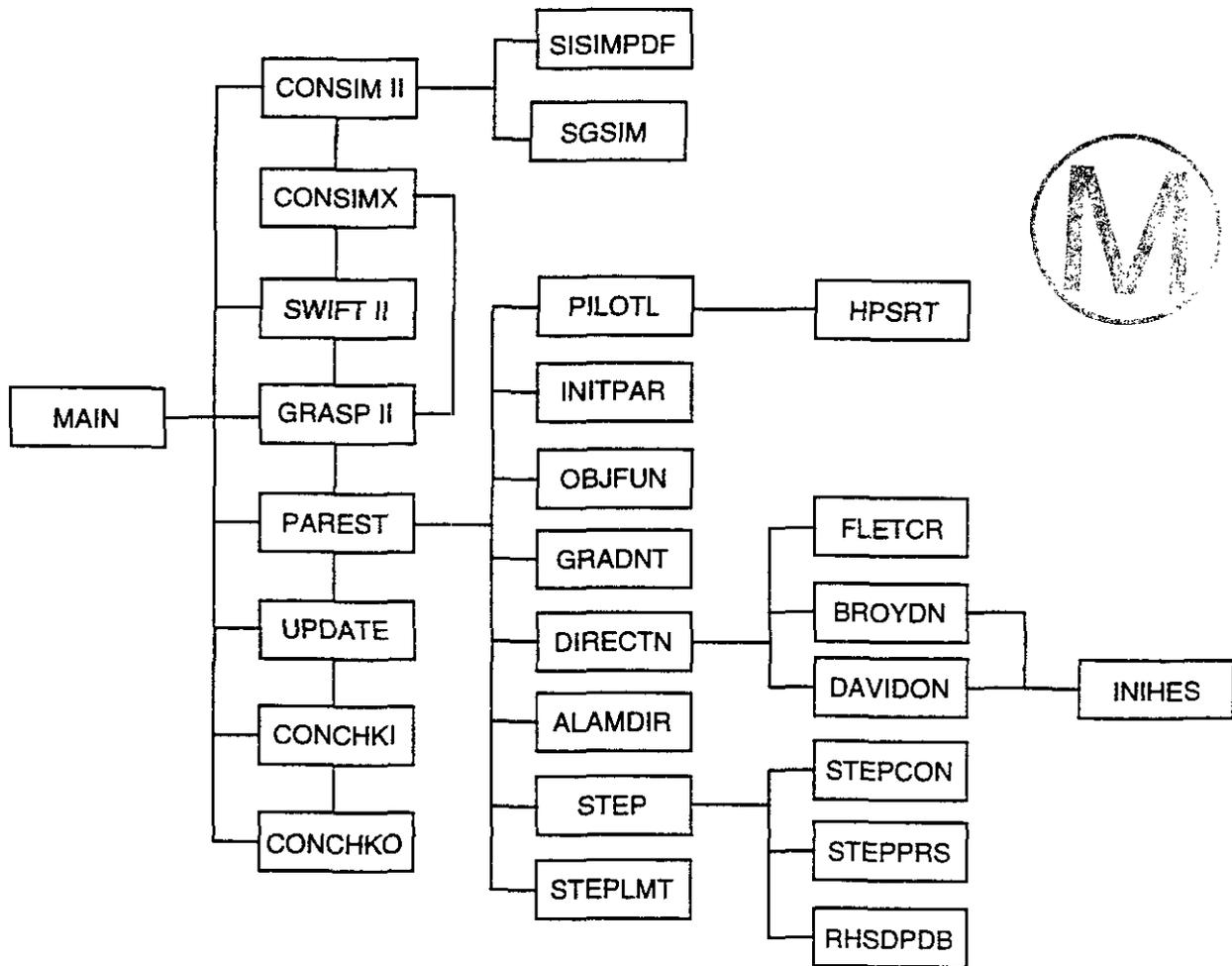
Convergence Criteria: Outer Iterations

Outer iterations are terminated essentially on criteria (1) and (2) of inner iterations.

4.5 Code Organization

Figure 13 illustrates the overall code organization. Table 3 lists the important subroutines and their functions.





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Figure 13. GRASP-INV Code Organization

Table 3. GRASP-INV Subroutines and Their Functions

<u>Name of Subroutine</u>	<u>Purpose</u>
MAIN	Driver Program for this code package.
SWIFT II	Simulation of pressures.
GRASP II	Sensitivity derivatives of performance measure with reference to model parameters.
SISIMPDF	Conditional simulation of categorical variables such as lithologic types.
CONSIM2	Conditional simulation of transmissivities (calls SISIMPDF and SGSIM) and averaging of simulated transmissivity values to the SWIFT II grid blocks.
CONSIMX	Modifies grid block conductivity values after a pilot point is added to the observed data set and sends this information to SWIFT II.
SGSIM	Conditional simulation of continuous variables such as transmissivities
PAREST	Assigns pilot-point transmissivities by optimization
PILOTL	Selects the pilot-point locations based on sensitivity analysis
INITPAR	Initializes pilot-point transmissivities and their covariance matrix for the first iteration in calibrations
READ3	Reads input related to pilot-point transmissivity optimization
OBJFUN	Compute weighted least squares objective function
GRADNT	Computes gradients of objective function to pilot-point transmissivities
DIRECTN	Computes directions in search algorithm
STEP	Computes step length in search algorithm



Table 3. GRASP-INV Subroutines and Their Functions (continued)

UPDATE	Updates the pilot-point transmissivities at the end of an iteration
HPSRT	Sorts absolute gradients in descending order
BROYDN	Computes direction per Broyden algorithm
FLETCH	Computes direction per Fletcher-Reeves (conjugate gradients) algorithm
INIHER	Computes initial approximate inverse Hessian matrix
STEPCON	Computes transmissivities-dependent constant in step-length formula.
STEPPRS	Computes pressure-dependent expressions in step-length formula.
ALAMDIR	Computes expressions involving Kriging weights and directions (to be used in solving sensitivity of pressure to step length)
RHSDPDB	Computes right-hand column vector for solving the equation for sensitivity of pressure to step length
STEPLMT	Implements constraints on step length after optimization
CONVCKI	Checks convergence of inner iterations
CONVCKO	Checks convergence of outer iterations



5.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE

The GRASP-INV code can solve one-, two-, or three-dimensional groundwater flow calibration problems to either steady-state or transient-state conditions. It is computationally intensive and therefore must be run on at least a powerful personal computer with a minimum of 16 MB of RAM, 300 MB of disc space, and an operating frequency of at least 66 MHz.

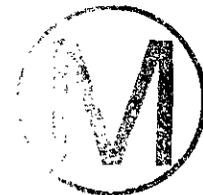


6.0 USER INTERACTIONS WITH THE SOFTWARE

The code GRASP-INV (Version 2.01) is designed to perform automated calibration of a conditionally simulated (or kriged) transmissivity field by an iterative procedure. The code was written in FORTRAN 77 and is designed for use on a DEC Alpha workstation running the Open VMS operating system. To run the code, the user should go to the directory WPSPRODROOT:[GRLEXE]. The user should then type "run graspinv_PA96.exe" and the code will begin to execute.

The code performs the following series of operations in an iterative cycle:

- Step 1: Generate conditionally simulated transmissivity field. Initially, the fields are based on the measured transmissivity data. During subsequent iterations in the calibration, they are based on measured transmissivity augmented by synthetic pilot point transmissivities.
- Step 2: Simulate the pressures in the groundwater flow system.
- Step 3: Compute the sensitivity coefficients of a weighted least square error function with respect to pilot point transmissivity.
- Step 4: Select the location of pilot points based on the results of Step 3.
- Step 5: Determine the optimal transmissivity at the selected locations of pilot points.
- Step 6: Test for convergence.
- Step 7: If convergence is achieved, stop. If not, augment the measured transmissivity data with the pilot point data. GO TO STEP 1.



7.0 DESCRIPTION OF INPUT FILES

The input to the GRASP-INV code consists of several separate input files, each relating to one or more distinct steps. The names of the input files and the relevant codes that read them are given below in Table 4.

Table 4. Names of Input Files and Relevant Codes

NO.	INPUT FILE	RELEVANT CODE
1	MAIN.INP	MAIN (DRIVER)
2	RAND.INP	MAIN (DRIVER)
3	PARAM.INP	PAREST
4	DXDYDZ.INP	CONSIM II
5	CONSIM.INP	CONSIM II
6	CATG.INP	CONSIM II
7	COND.DAT	CONSIM II
8	XYZ.DAT	CONSIM II
9	SGSIM.INP	CONSIM II
10	SWIFT.INP	SWIFT II
11	GRASP.INP	GRASP II & PAREST
12	OBSGRASP.DAT	GRASP II

The construction of each of the separate input files in the table is described here. A separate subsection is used for each input file. Example data sets for CONSIM II, SWIFT II, GRASP II, and PAREST are contained in Appendix C to aid the user in setting up the input to GRASP-INV.

Input File Descriptions:

MAIN.INP contains information regarding which of the four components of the code (CONSIM II, SWIFT II, GRASP II, or PAREST) the user wants to run.

RAND.INP contains the random number to be used in the calibration run. (Note: n number of rand.inp files are needed for n number of calibrated fields desired.)

PARAM.INP	contains information regarding the optimization options used during the calibration process.
DXDYDZ.INP	contains the NX,NY,NZ,DX,DY,DZ for each of the SWIFT II finite difference grid blocks, scaling factors in the x, y, and z directions, offset values for the origin of the geostatistical simulation grid relative to the SWIFT II grid in the x, y, and z directions, and information regarding the manner in which to assign the vertical conductivity anisotropy value and range (either by category or by specified zones).
CONSIM.INP	contains information concerning the number of categories and the type of simulation to be performed for each category and the input file names for CONSIM II for each category and the name of the dxdydz.inp file.
CATG.INP	input file for categorical indicator simulation routine of CONSIM II, contains information concerning the indicator variograms, the conditioning data file, the simulation points, the number of neighbors to use in the simulation routine, etc.
COND.DAT	input file for CONSIM II containing the observed categorical and transmissivity data.
XYZ.DAT	optional input file for CONSIM II containing x, y, z locations of geostatistical simulation grid.
SGSIM.INP	input file for sequential Gaussian simulation routine of CONSIM II. A SGSIM.INP file is needed for each category. Thus SGSIM1.INP will be used for category 1 and SGSIM2.INP will be the input file used for category 2, etc. The information contained in this file concerns the variogram used for the spatial variability within the category, the conditioning data file name, the number of neighbors to be used in the simulation process, the range of the simulated variable.
SWIFT.INP	contains input to SWIFT II such as aquifer properties, groundwater properties, boundary conditions, and time step information.
GRASP.INP	contains input to GRASP II such as the type of performance measure, the number of pilot points to add, the locations to select as potential pilot-point locations, the transient time windows used in calibration.
OBSGRASP.DAT	contains the observed pressure data at each of the boreholes at each SWIFT II time step.



7.1 Input File - MAIN.INP

This file contains only one record with four variables. It may be recalled that GRASP-INV contains four principal segments:

1. CONSIM II
2. SWIFT II
3. GRASP II
4. PAREST

This input file enables the user to start from any one segment and end up on any other segment. For example, if one wishes to use SWIFT II only, one should start on segment 2 and finish on segment 2. Similarly, if one wants to use CONSIM II, SWIFT II, and GRASP II, but not PAREST, then one should start on segment 1 and end on segment 3. However, if one uses GRASP-INV for calibration purposes, one should start on segment 1 and end on segment 4.

- List: IBOPT, IEOPT, NSTAGES, NSTDAT
- Format: (4I5)
- IBOPT: Segment number from which the execution should start (≤ 4 ; see above).
- IEOPT: Segment number at the end of which the execution should stop (≤ 4 ; see above).
- NSTAGES: = 1: if purely steady state or purely transient state calibration is to be done.
= 2: if two-stage calibration is done. First steady-state calibration is done. Then, after its convergence, transient-state calibration is done. Under this option, SWIFT II data set is constructed for a transient run. However, GRASP-INV can interpret the same data set for steady-state simulation during the steady-state calibration phase.
- NSTDAT: 1 This variable is not used now. Use 1 for input.
- RSTFLAG: = 1: A restart run is desired (Not Used for WIPP Application)
= 0: A normal run is desired.

7.2 Input File - RAND.INP

Record 1:

- List: NUMFLDS

Format: (List directed, i.e., free)

NUMFLDS: The number of transmissivity fields to be generated and calibrated.
(Should be 1 for WIPP Application)

Record 2:

List: RANDNUM (I) for I=1, NUMFLDS

Format: (List directed, i.e., free)

RANDNUM: a five-digit odd integer

7.3 Input File - PARAM.INP

This file contains three records. They all relate to the inner iterations for the optimization of the transmissivity values at the pilot points.

Record 1:

List: XLATR

Format: (List directed, i.e., free)

XLATR: A coefficient for the plausibility criterion
(η in Equation 3-13, Lavenue and RamaRao, 1992)
For this version, set to 0.0.
Plausibility criterion is ignored.



Record 2:

List: ITER1, ITERB, KSTPFLG, NCONF

ITER1: Number of iterations for which Fletcher-Reeves Conjugate Gradients (FRCG) Algorithm is used. After the number of iterations, either Broyden algorithm (if ITERB=1) or Davidon-Fletcher-Powell (DFP) algorithm (if ITERB=0) is used, if the total number of iterations (ITERMX) required are more than ITER1.

ITERB: 1: Broyden algorithm will be used for subsequent iterations after "ITER1" number of FRCG iterations
0: DFP algorithm will be used for subsequent iterations after "ITER1" number of FRCG iterations

- KSTPFLG: 1: Optimal step length based on Newton's method will be computed and then constraints will be imposed.
0: Ad hoc step length, based on constraints only, will be used. (This option may not lead to convergence, but saves time if successful.)
- NCONF: =0: Use min and max \log_{10} transmissivity values as determined by CONSIM II as constraints for each grid block.
=-1: Ignore min and max values determined by CONSIM II.

Record 3:

- List: IGRAD, ITERMX, DMXMIN, MXCHMN, GRMIN, GRPCT, OBJPCT, MXPENA, PCT, PCX, IPACE
- Format: (List directed, i.e., free)
- IGRAD = 1 for this version
- ITERMX: Maximum number of inner iterations in the optimization of pilot point transmissivity
- DMXMIN: Not used now; set to 0.0
- MXCHMN: Not used now; set to 0
- GRMIN: Iterations stop if the norm of the gradient becomes smaller than this value (default value = 10^{-3})
- GRPCT: Iterations stop if the percentage of the gradient norm with respect to that at the first iteration becomes smaller than this value (default value = 10^{-3})
- OBJPCT: Iterations stop if the percent reduction in the objective function is smaller than this value; in MXPENA number of iterations
- MXPENA: Maximum number of iterations allowed without significant reduction in the objective function (see above)
- PCT: Maximum change per iteration for $\log_{10}T$ value at pilot point
- PCX: Not used now; set to 0.0



PACE: Number of iterations between the "pacer" iterations in the FRCG algorithm (a default value equals the number of pilot points used in that iteration).

7.4 Input File - DXDYDZ.INP

This input file is necessary to overlay the CONSIM II simulation grid onto the SWIFT II grid. Note that CONSIM II can be executed essentially as a stand-alone program. However, to avoid abnormal termination of GRASP-INV, this input file should be provided. Its contents need not be realistic for such a run, but it must be present.

Output from CONSIM II is passed to SWIFT II and GRASP II through common blocks. The four items that are passed in general terms are

1. Details for each SWIFT II grid block
2. The conditional data
3. Variogram information
4. Anisotropy ratios for horizontal-to-vertical conductivities.



Each item depends in some way on the contents of file corgrid (see Section 7.5.4). Thus, they are discussed below.

The following data are read as List directed, i.e., free format.

Record 1:

- **Skalex, Skaley, Skalez:** scaling factor for each direction used to overlay the simulation grid onto the SWIFT II (coarse) grid. For example, the CONSIM II input data used to condition the field may have x,y,z locations in kilometers and the SWIFT II grid may be described in meters. In this case the three variables above would be 1000. each. Thus, these variables simply relate the difference in scale used in the geostatistical simulation grid to the SWIFT grid.

Record 2:

- **OffSetx, OffSety, OffSetz:** offset for each direction used to overlay the simulation grid onto the SWIFT II grid. The same concept as above but for the origin of the two grids.

Record 3:

- **nxsw, nysw, nzsw:** number of grid blocks in each direction for the SWIFT II grid.

Record 4:

- **dxsw_i, i = 1,...,nxsw:** grid block sizes in the x-direction SWIFT II grid.

Record 5:

- **dysw_j, j = 1,...,nysw:** grid block sizes in the y-direction SWIFT II grid.

Record 6:

- **dzsw_k, k = 1,...,nzsw:** grid block sizes in the z-direction SWIFT II grid.

Record 7:

- **UseZone:** must be 0 (anisotropy by category) or 1 (anisotropy by zone)

If UseZone = 0, then using a separate line for each category, enter Record 7a

Else if UseZone ≠ 0, then enter Records 7b,7c, and 7d.

Record 7a:

- **aninom, animin, animax:** the nominal, minimum, and maximum value to be used for the vertical-to-horizontal anisotropy ratio for the category.

Record 7b:

- **NumZone:** the number of zones having similar anisotropy. Then for each zone n, two lines are required

Record 7c:

- **izone(n, 1), izeone(n, 2), jzone(n, 1), jzone(n, 2), kzone(n, 1), kzone(n, 2):** starting and ending index delimiting the zone in the x, y, and, z directions

Record 7d:

- **aninom, animin, animax:** the nominal, minimum, and maximum value to be used for the vertical-to-horizontal anisotropy ratio for the zone.



7.4.1 Comments

As stated above, anisotropy ratios can be provided either by category or by zone. Both require a nominal value and a range (minimum and maximum) over which the nominal is allowed to vary. Currently, only the nominal is being used. The range will become important for 3-dimensional problems where vertical conductivity is to be calibrated.

If anisotropies are input by category, then for each SWIFT II block its category is noted. If the category is zero, then the value for z-direction conductivity read from the SWIFT II input is used. If the category is positive, then the nominal value for the category is multiplied by the horizontal conductivity simulated for the block to get z-direction conductivity.

If anisotropies are input by zone, then each SWIFT II block is checked to see if it belongs to a zone. If not, then the value for z-direction conductivity read from the SWIFT II input is used. If it does belong to a zone, then the nominal value for the zone is multiplied by the horizontal conductivity simulated for the block to get z-direction conductivity.

The SWIFT II grid is input the same way as for a SWIFT II input file. That is, the number of grid blocks (nxsw, nyaw, nzsw) is given followed by the sizes:

$dxsw_i$ for $i = 1, \dots, nxsw$
 $dysw_j$ for $j = 1, \dots, nyaw$
 $dzsw_k$ for $k = 1, \dots, nzsw$



To superimpose the simulation grid onto the SWIFT II grid requires scaling factors and offsets. Simulation point (x_s, y_s, z_s), it is located on the SWIFT II grid using:

$S_x = x_s * Skalex + OffSetx$
 $S_y = y_s * Skaley + OffSety$
 $S_z = z_s * Skalez + OffSetz$

Then the point (S_x, S_y, S_z) is located on the SWIFT II grid by finding the block index that contains these coordinates. The scaling factors are useful if there is a change in distance units. For example, the conditioning data coordinates may be given in kilometers whereas SWIFT II requires distance in meters. Thus, Skalex and Skaley would each be 1000.

7.5 CONSIM II Input

7.5.1 Data Files

For input, there is a primary data file for CONSIM II that provides some run-type flags and the names of other input files for iCs and sGs. One input file is required for iCs. Each category requires an input file for sGs. Files containing conditional data and simulation locations are optional, depending on the type of run parameters the user specifies. Their names are found in

the input file for iCs. In the usual case where output from CONSIM II is to provide input for the other GRASP-INV modules, a file containing information for this connection is required. Finally, if a restart run is being implemented, a file containing the last field generated is required. These last two file names are found in the primary input file.

On output, CONSIM II writes the results from iCs and each sGs to different files, both standard results and debug results. It also writes the data required to back-transform normal scores to the original conditioning data, if the forward step was required. The names for all these files are found in the input files for iCs and sGs. CONSIM II combines all simulation results onto the SWIFT II grid and writes them to a file name specified in the primary input file.

CONSIM II reads and writes data with a format similar to the menu-driven packages Geo-EAS (Englund and Sparks, 1988) and GSLIB (Deutsch and Journel, 1992). The format, described below and as shown in Appendix A, is a simple ASCII format with no special allowance for data compression. The data file format is a simplified Geo-EAS format, hence with no allowance for the user to specify explicitly the input format. The data values are always read with free format.

When reading conditional data or gridding, the following conventions are used by the "simplified Geo-EAS format":

1. The first line in the file is taken as a title and is transferred to output files.
2. The second line should be a numerical value specifying the number of numerical variables *nvar* in the data file.
3. The next *nvar* lines contain character identification labels and additional text (optional) that describe each variable.
4. The following lines, from *nvar* +3 until the end of the file, are considered as data points and must have *nvar* numerical values per line. If there are several measured variables and there are locations where all of these values are not available, a large negative or positive numbers (e.g., less than $-1.0e21$ or greater than $1.0e21$) may be used in the data set in place of a missing value. A data trimming limit may then be specified in the CONSIM II input file to ignore this missing variable at the location. The number of data will be the number of lines in the file minus *nvar* +2 minus the number of missing values. The programs read numerical values and *not* alphanumeric characters; alphanumeric variables may be transformed to integers or the source code modified.



7.5.2 Grid Definition

There are three grids of interest when running CONSIM II within GRASP-INV: The CONSIM II simulation grid, the SWIFT II grid, and a "super block" multigrid. Normally the simulation grid is more refined than the SWIFT II grid. The simulation and SWIFT II grids can have different length units, but *the coordinates of the conditioning data must be given relative to the simulation*

grid. CONSIM II estimates or simulates a value at each refined grid point and then averages the values onto the SWIFT II grid, as described in Section 4.1.7. The super block grid is used internally by CONSIM II to help ensure that simulations retain the long distance spatial correlation structure defined in the input (Section 4.1.6.3).

The simulation grid can be regularly- or irregularly-spaced. An irregular grid must be read in from a file that has every point defined. Output that is grid-dependent will be written in the same order that the grid is read. A regular grid can come from an input file or can be generated internally by CONSIM2. In the latter case the user supplies a number of blocks (nxr, nyr, nzz) and block size (dxr, dyr, dzr) in each direction. CONSIM II generates a set of coordinates corresponding to grid block centers.

An internally generated regular grid is ordered the same way SWIFT II stacks its grid block properties. That is, x cycles fastest, then y, then z. The index location of any particular node i_x , i_y , i_z can be located by:

$$loc = (i_z - 1) * nxr * nyr + (i_y - 1) * nxr + i_x \quad (65)$$

Given the above one-dimensional index location of a node the three coordinate indices can be calculated as:

$$i_z = 1 + \text{int} \left(\frac{loc - 1}{nxr * nyr} \right) \quad (66)$$

$$i_y = 1 + \text{int} \left(\frac{loc - 1 - (i_z - 1) * nxr * nyr}{nxr} \right) \quad (67)$$

$$i_x = loc - (i_z - 1) * nxr * nyr - (i_y - 1) * nxr \quad (68)$$



Program CONSIM II applies a two-tiered approach to simulating heterogeneous spatially correlated media. The algorithm first simulates the occurrence of discrete categories, using the iCs algorithm. Within each category, the continuous variable of interest is simulated by sGs algorithm.

7.5.3 Variogram Transformation

Variogram information is input for iCs and sGs as described in Sections 4.1.6.1 and 4.1.6.2, respectively, where the available models are described in Section 4.1.3. There is a length component to each of the models and this component must conform to the length units of the simulation grid (and conditioning data). For the spherical, exponential, and Gaussian models, the a parameter has units length (L). The c parameter of the power model has units L^{-2} . If there is a nonunit horizontal scaling factor, the parameters for sGs must be scaled for subsequent use by GRASP-INV in order to correctly determine kriging weights.

The horizontal scaling factors are Skalex and Skaley (Section 7.4). Normally their use will be for units conversion. If these two factors are not equal, the task of converting the a or c parameter appears daunting. Thus, for this effort it is assumed that they are equal and Skalex is used to convert the parameters for each category and nested structure.

For the spherical, exponential, and Gaussian models, the a parameter is converted by

$$a_{\text{new}} = a * \text{Skalex}$$

and for the power model, parameter c is converted by

$$c_{\text{new}} = c / (\text{Skalex})^a$$



7.5.4 Input File - CONSIM.INP

The primary input file for CONSIM II is in ASCII format and contains a list of file names and operational flags. There is a minimum of nine items on the file (more if there is more than one indicator category) and each item exists on a separate line. The lines are identified here by the item's variable name within the code as follows:

Format: (List Directed, i.e., free)

- **parfile:** the name of the file containing input for Indicator Categorical Simulation (iCs) (e.g., CATG.INP).
- **state:** *estimation* or *simulation*, indicating whether mean kriged values or simulated values should be produced at each point, respectively.
- **smeth(1):** *sgsim*, which means Sequential Gaussian Simulation (sGs) will be used for category 1. (Sequential indicator simulation is not available in this version of CONSIM II.)
- **strpar(1):** the name of the file containing input for sGs for category 1 (e.g., SGSIM1.INP).
- **corgrid:** the name of the file containing SWIFT II gridding, scaling factors, and vertical-to-horizontal conductivity anisotropy ratios (e.g., DXDYDZ.INP).
- **coresult:** the name of the file where categories and transmissivities generated by CONSIM II are written for each SWIFT II grid block (e.g., OUT.DAT).

- **coresult2:** the name of the file where categories and *calibrated* transmissivities are written for each SWIFT II grid block. This file is written at a frequency of the user's choosing and can be used for restarting GRASP-INV (e.g., OUT2.DAT).
- **r121:** the name of the file where calibrated conductivities are written for each SWIFT II grid block. This file is written at a frequency of the user's choosing and is written in a format compatible with that required for reading SWIFT II R1-21 cards (e.g., SWIFT121.DAT).
- **rstfile:** the name of the file containing categories and transmissivities for each SWIFT II grid block to be used as an initial field for a restart run. This is a copy of a coresult2 file from a previous run (e.g., RESTART.DAT). **This feature is not needed for the WIPP PA application.**

If there is more than one indicator category, then *smeth* and *strpar* are repeated as a pair, once for each additional category. Files **parfile**, **strpar(i)**, and **corgrid** must exist for every run. File **rstfile** is only required to exist for a restart run.

To execute properly CONSIM II requires two additional items, both provided through labeled common by the main GRASP-INV driver. First is a restart flag, **rstflag**, a logical variable that when true indicates that this is a restart run. It is read from the MAIN.INP file. Nearly all of the CONSIM II functions are skipped in this case; instead the initial field is assumed to be that read from file **rstfile**. However, all the input files that were used to generate the field that exists on **rstfile** must be accessible for the restart run.

The second item is a seed for the random number generator used by CONSIM2, **seed**. The seed must be a positive integer. It is read by the GRASP-INV driver program from the data file RAND.INP described above.

7.5.5 Input File - CATG.INP

The *sisimpdf* subroutine is for the simulation of integer-codes categorical variables. The following parameters are required; see also Appendix A:

datafl: the input data is a simplified Geo-EAS formatted file (e.g., COND.DAT).

ixl, iyl, izl, and ivrl: the column numbers for the *x*, *y*, and *z* coordinates and the variable to be simulated. Any or all of the coordinate column numbers can be set to zero which indicates that the simulation is 2-D or 1-D.

tmin and tmax: all data values strictly less than *tmin* and strictly greater than *tmax* are ignored.



locopt: if 0 then internally generate a regularly-spaced simulation grid, if 1 read the simulation grid from a file.

If **locopt** = 0, then provide

- **nxr, nyr, nzs:** the number of grid blocks in each direction
- **dxr, dyr, dzr:** the grid block size in each direction

Else if **locopt** = 1, then provide

- **locafl:** file name for the simulation grid in Geo-EAS format (e.g., XYZ.DAT)
- **ixloc, iyloc, izloc:** column numbers for x, y, z coordinates on file **locafl**

outfl: the output grid is written to this file. The output file will contain the results, cycling fastest on *x*, then *y*, then *z*, then simulation by simulation.

idbg: an integer debugging level between 0 and 3. The larger the debugging level the more information written out.

dbgfl: the file for the debugging output.

nsim: the number of simulations to generate.

ipower: the number of multigrids to use (see Section 4.1.6).

sstrat: 0/1 don't use /use buffer locations in multigrid strategy (see Section 4.1.6)

noct: the number of original data to use per octant. If this parameter is set to 0 then it will not be used; otherwise, the closest *noct* data in each octant will be retained for the simulation of a grid node.

radius: the search radius. This radius can be made anisotropic with the following parameters:

sang1, sang2, sang3, sanis1, and sanis2: parameters defining the 3-D anisotropy of the search ellipsoid. A detailed interpretation of these parameters is given in Section 4.1.3.

ndmin and ndmax: the minimum and maximum number of original data that will be used to simulate a grid node. If there are fewer than *ndmin* data points the node is not simulated.



nodmax: the maximum number of previously simulated nodes to use for the simulation of another node.

mik and **mikcat:** if *mik* is set to 0, then a full indicator kriging will be performed at each grid node location to establish the conditional distribution. If *mik* is set to 1, then the median approximation will be used, i.e., a single variogram is used for all categories; therefore, only one kriging system needs to be solved and the computer time is significantly reduced. The variogram corresponding to category *mikcat* will be used.

ktype: the kriging type (0 = simple kriging, 1 = ordinary kriging) used throughout the loop over all nodes. SK is required by theory, only in cases where the number of original data found in the neighborhood is large enough can OK be used without the risk of spreading data values beyond their range of influence (Isaaks, 1990). The global pdf values (specified with each category) are used for simple kriging.

ncut: the number of categories.

The following set of parameters are required for each category:

cut, CDF, nst, and c0: the integer category, the global pdf value, the number of semivariogram structures, and the isotropic nugget constant.

For each of the **nst** nested structures one must define **it** the type of structure, **aa** the a parameter, and **cc** the c parameter on one line and **ang1, ang2, ang3, anis1** and **anis2**, the geometric anisotropy parameters on another. A detailed description of these parameters is given in Section 4.1.3. Each semivariogram model refers to the corresponding indicator transform, Gaussian variogram with a small nugget constant is not a legitimate variogram model for a discontinuous indicator function. There is no need to standardize the parameters to a sill of one since only the relative shape affects the kriging weights.

7.5.6 Input File - SGSIM.INP

datafl: the input data in a simplified Geo-EAS formatted file (e.g., COND.DAT).

ixl, iyl, izl, ivrl, and iwt: the column numbers for the *x*, *y* and *z* coordinates, the variable to be simulated and the declustering weight. Any of all of the coordinate column numbers can be set to zero which indicates that the simulation is 2-D or 1-D. If the declustering weight is unavailable then *iwt* may be set to zero.

tmin and **tmax:** all data values strictly less than *tmin* and strictly greater than *tmax* are ignored.

itrans: if set to 1 then the variable is already standard normal (the simulation results will be left unchanged); if *itrans*=0, transformation is required. Note that for post-auditing

purposes, the user may wish to compute the variogram of the simulation. The experimental variogram should agree with the input variogram, within statistical fluctuations. In such a case, the user might need to suppress the back transform of the simulated field. This can be accomplished by setting $itrans = 2$.

transfl: output file for the transformation table if transformation is required ($itrans = 0$).

zmin and **zmax:** the minimum and maximum allowable data values. These are used in the back transformation procedure.

ltail and **ltpar** specify the back transformation implementation in the lower tail of the distribution: $ltail = 1$ implements linear interpolation to the lower limit $zmin$ and $ltail = 2$ implements power model interpolation, with $w = ltpar$, to the lower limit $zmin$.

The middle class interpolation is linear.

utail and **utpar** specify the back transformation implementation in the upper tail of the distribution: $utail = 1$ implements linear interpolation to the upper limit $zmax$, $utail = 2$ implements power model interpolation, with $w = utpar$, to the upper limit $zmax$, and $utail = 4$ implements hyperbolic model extrapolation with $w = utpar$. The hyperbolic tail extrapolation is limited by $zmax$.

locopt: if 0, then internally generate a regularly-spaced simulation grid; if 1, read the simulation grid from a file.

If $locopt = 0$, then provide

- **nxr, nyr, nzz:** the number of grid blocks in each direction
- **dxr, dyr, dzr:** the grid block size in each direction



Else if $locopt = 1$, then provide

- **locagl:** file name for the simulation grid in Geo-EAS format (e.g., XYZ.DAT)
- **ixloc, iyloc, izloc:** column numbers for x, y, z coordinates on file locagl

outfl: the output grid is written to this file. The output file will contain the results, cycling fastest on x, then y, then z, then simulation by simulation.

estfl: the output estimation file, containing the kriged estimates at each location (same format as outfl).

idbg: an integer debugging level between 0 and 3. The larger the debugging level the more information written out.

dbgfl: the file for the debugging output.

ktype: the kriging type (0 = simple kriging, 1 = ordinary kriging) used throughout the loop over all nodes. SK is required by theory, only in cases where the number of original data found in the neighborhood is large enough can OK be used without the risk of spreading data values beyond their range of influence (Isaaks, 1990).

nsim: the number of simulations to generate.

ipower: number of multigrids to us (see Section 4.1.6).

sstrat: 0/1 don't use/use buffer locations in multigrid strategy (see Section 4.1.6).

noct: the number of original data to use per octant. If this parameter is set to 0, then it will not be used; otherwise, it will override the *ndmax* parameter and the data will be partitioned into octants and closest *noct* data in each octant will be retained for the simulation of a grid node.

radius: the search radius. This radius can be made anisotropic with the following parameters:

sang1, sang2, sang3, sanis1, and sanis2: parameters defining the 3-D anisotropy of the search ellipsoid. A detailed interpretation of these parameters is given in Section 4.1.3.2.

ndmin and ndmax: the minimum and maximum number of original data that should be used to simulate a grid node. If there are fewer than *ndmin* data points the node is not simulated.

nodmax: the maximum number of previously simulated nodes to use for the simulation of another node.

nst and c0: the number of semivariogram structures and the isotropic nugget constant.

For each of the **nst** nested structures one must define **it** the type of structure, **aa** the **a** parameter, and **cc** the **c** parameter on one line and **ang1, ang2, ang3, anis1** and **anis2**, the geometric anisotropy parameters on another. A detailed description of these parameters is given in Section 4.1.3. The semivariogram model refers to the normal scores. The kriging variance is directly interpreted as the variance of the conditional distribution;



consequently, the nugget constant c_0 and c (sill) parameters should add to 1.0. Recall that the power model is not a legitimate model for a multiGaussian phenomenon.

7.6 SWIFT II Input

The theory found within the SWIFT II code may be found in Reeves et al. (1986a). Examples of the SWIFT II code application may be found in Reeves et al. (1986b). Due to the size of the SWIFT II User's Manual, it is located in Appendix D.

7.7 GRASP II Input

7.7.1 Input File - GRASP.INP

The following is a listing of all input data cards for the GRASP code:



AD-1: Run Title

List: TITLE (I), I=1, 40
Format: (20A4/20A4)
Note: 160 column-long (2 cards) alphanumeric data to serve as title for the GRASP-INV run.

AD-2: Title Cards from the File SWIFT.INP

List: TITLE2 (I), I=1, 40
Format: (20A4/20A4)
Note: The two title cards required for this input must be exactly the same as the M-1 card used in the associated SWIFT II input-data set. Any discrepancy will terminate the job, so transfer the cards from SWIFT II data set by split screen editing.

AD-3: Option Type

List: IOPT
Format: I5
IOPT: 0 Both adjacent states and the sensitivity coefficients are to be evaluated.
Use 0 for this version

AD-4: Performance Measure Type Definition

List: IPMTYP, NPROB, LOUT, IPRT, ISTWTFL, ELSTWT, NOITER, OBJMIN
Format: (I5) F10.0, I5, E10.0

- IPMTYP Performance measure type.
- 2 Weighted sum of squared deviations between computed and observed pressures at elevation.
 - 0 Terminates execution of the run (a blank card can be used).
- NPROB Equals 1, for this version
- LOUT Option for output of adjoint state (unit source influence function)
- 1 Output suppressed
 - 1 Output activated at every time step
 - n Output activated at every nth time step
- IPRT Option for printing the grid block sensitivity coefficient (marginal and/or dimensionless values)
- Note: This variable is the same as the PRT (on M-3 card) in a SWIFT II run.
- 1 Print output arrays as areal layers (x-y), block numbers increase from left to right and decrease down the computer page in the y-direction
 - 1 Similar to the above, except that the y-direction (J-block) numbers increase down the computer page.
 - 2 Print output arrays as vertical sections (x-z).
- Note: The code uses a default value of 1 for IPRT.
- ISTWTFL:
- 0 Steady state calibration
 - 1 Transient state calibration
- RELSTWT: Relative weight to be given to the steady-state calibration field while performing transient state calibration (usually 0.45 to 0.55), preferably 0.50
- NOITER: Number of outer iterations to be performed (each outer iteration selects a new set of pilot points).
- OBJMIN: Minimum value of the objective function at which iterations can be stopped.



AD-5-B:

This group of cards relates to the modification to the default weight of unity assigned by the code for each observation. If no modifications are needed, insert one blank card. Otherwise, read as many cards as required, terminating with one blank card at the end.

List: II, JJ, KK, LSET1, LSET2, U1

Format: 5(I5), E10.0

II x-direction index I of the grid block
JJ y-direction index J of the block
KK z-direction index K of the grid block
LSET1 The first and the last observation data set numbers
LSET2 (LL in Group 1, List 1) to which the modified weights apply
U1 modified weight

AD-6: Sensitivity Parameter Type and Output Options

List: ISPTYP, MSOUT, NDSOUT, IPRT
Format: (4I5)
ISPTYP 8 Pilot point observation of Log₁₀ of transmissivity
MSOUT 0 The grid-block values of

$$\lambda \frac{dJ}{d(\log_{10} T)}$$

are not output.

1 The grid-block values of

$$\lambda \frac{dJ}{d(\log_{10} T)}$$

are printed for the zone of influence of the pilot point.

2 In addition to the output in option 1, the grid-block values of dJ/dK , where K = permeability, will be printed over the zone of influence of the pilot point.

3 In addition to the output under options 1 and 2 above, the grid block permeabilities will be output in the zone of influence of the pilot point.



- 4 All of the output of 3 and grid-block permeabilities will be written to GRASPXXX.DAT. DJ/DK will be written to GRASPDKH.DAT

NDSOUT

- 0 the pilot point over each grid block in the zone of influence of the pilot point **will not** be printed.
- 1 the pilot point over each grid block in the zone of influence of the pilot point **will be printed**. Dimensionless sensitivity of $dJ/d\log T_p$ written to GRASPDLP.DAT; kriging lamdas written to GRASPLAM.DAT

AD-7-E1:

List: XORIGIN, YORIGIN, SCALE

Format: (3FI5.0)

XORIGIN: X-coordinate of the outer corner of the SWIFT II grid block (1,1) with respect to the kriging data origin for distances. (Units: SWIFT II units; meters.)

YORIGIN: Y-coordinate: of the above.

SCALE: Kriging data length (distance units) divided by SWIFT II data length units (e.g., If kriging data is the km and SWIFT II data is in meters, SCALE = 1000).



AD-7-E2: Pilot Point Grid Definition

List: I1P, I2P, J1P, J2P, K1P, K2P, IOKRIG, KRIGOPT, IRANGE, NPS1, IINC, JINC, NPSB

Format: (13I5)

I1P, I2P The lower and upper limits on the index I (x-direction) over the grid of candidate pilot points

J1P, J2P The lower and upper limits on the index J (y-direction) over the grid of candidate pilot points

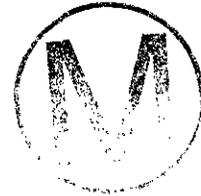
K1P, K2P The lower and upper limits on the index K (z-direction) over the grid of candidate pilot points

IOKRIG Output control for kriging results

- 0 Minimal output from kriging computations will be printed, overriding the output options in the kriging data set
- 1 Output from kriging computations will be printed, subject, however to the options in the kriging data set

KRIGOPT

- 1 No longer used.



IRANGE

- 0 Pilot point regions are not the same (read AD-7-E3 for each pilot point)
- 1 Pilot point regions are the same (read AD-7-E3 only once)

NPS1

Number of pilot points to be selected from the candidate pilot point locations

IINC

- ≥ 0 Centroid of every grid block in the range defined will be considered as a potential pilot point
- 2 Starting from I1P, the I index of potential pilot points is taken as I1P, I1P + 2, I1P + 4, etc., until I2P is reached or exceeded. This in effect causes only alternate grid block centroids to be treated as potential pilot points. Similarly, if IINC = -3, every third grid block centroid will be treated as a potential pilot point.

JINC

Similar to IINC, in the J-direction.

NPSB

- > 0 Number of candidate Pilot Point Locations to be considered.

AD-7-E3: Definition of the Zone of Influence of Pilot Point

- List: I1, I2, J1, J2, K1, K2
- Format: (6I5)
- I1, I2 The lower and upper limits on the Index I (x-direction) over the region of influence of the pilot point
- J1, J2 The lower and upper limits on the Index J (y-direction) over the region of influence of the pilot point
- K1, K2 The lower and upper limits on the Index K (z-direction) over the region of influence of the pilot point

Read one card per pilot point if $IRANGE = 0$, or only read one card for all the pilot points if $IRANGE > 0$. If $IRANGE = 0$, then the first card refers to the pilot point 1, the second card refers to the pilot point 2, and so on. No blank card is needed at the end of this set of cards.

Note:

- (1) The set of AD-7-E2 and AD-7-E3 may be repeated for the appropriate number of regions (should be ≤ 9).
- (2) A blank card for AD-7-E2 is required to terminate this set for pilot point grid(s). This blank card denotes that there are no more pilot point grids for the chosen performance measure.
- (3) The set of cards, from AD-4 to AD-7 cards, can be repeated for different events in calibration. For example, one may calibrate the transmissivity field first by using steady state heads and then calibrating to one long-term pumping test, using the pilot points in an appropriate region and then repeating the procedure for another long-term pumping test, and so on. Such data sets would then contain the repetition of the records of AD-4 through AD-7.
- (4) The data set GRASPINP is terminated by a blank card for AD-4, denoting that no more performance measures exist.

7.7.2 Input File - OBSGRASP.DAT

This group of records relates to the observed pressures in the boreholes. The code assigns a (default) weight of 1.0 for each observation.

Note: This group of data cards comprises several sets, each set corresponding to one time step in the SWIFT II simulation at which the pressure in a borehole was observed. Each set consists of several cards, each card relating to one borehole location and the observed pressure at that time step. One blank card terminates the entry of this data relating to the boreholes for the assigned time. Then the data relating to the next time is entered. When all the time steps at which observations are made are exhausted, another blank card signifies the end of all sets.

Thus, one card from List 1, followed by as many cards as required from List 2, are used for one time step. Repeat the sequence of input as many times as required. (This input should thus have two blank cards at the end.)

List 1: LL, LTIME

Format: (2I5)



-
- LL Observation Data Set Number. (Starts from one and increases sequentially.) Zero terminates all input from Unit 36.
- LTIME The time step, at the end of which the pressure observations in boreholes are made.
- List 2: II, JJ, KK, OBS
- Format: (3I5, 5X, E12.0)
- Note: Read as many cards as required. One card corresponds to one borehole. Terminate this list with a blank card.
- II x-direction index I of the grid block
- JJ y-direction index J of the grid block
- KK z-direction index at elevation K of the grid block
- OBS observed pressure at elevation, in Pascals



8.0 ERROR MESSAGES

Error messages will be printed only for the SWIFTINP data file for the SWIFT II portion of the GRASP-INV model. These error messages will be located at the bottom of the SWIFTOUT file and should be cross-referenced to the Error Message Listing located in the SWIFT II Users Manual (Appendix D).



9.0 DESCRIPTION OF OUTPUT FILES

MAIN.OUT

The main output file for GRASP-INV. It contains a summary of the code's execution and presents information concerning the pilot point locations and the objective function values during the calibration run. This file contains:

1. Echoprint of CONSIM II Input Files.
2. Performance measure.
3. For all pilot points selected:

(x,y) Location
 $Y = \text{Log}_{10}T$
 σ_Y

4. Search directions
5. Step length as computed by Newton's method.
6. Step length as modified by constraints.
7. Updated pilot point $Y = \text{Log}_{10}T$.
8. Revised performance measure.

Items 2 through 8 are printed for every iteration.

SUMRY.OUT

An output file for GRASP-INV that contains information concerning the number of fields calibrated.

CAMDAT.OUT

Output file written at the end of the GRASP-INV run, which contains the model grid information, boundary conditions, and final conductivity values for each SWIFT grid block. Written in CAMDAT Data Base Binary format. This file is used as input to the SECOFLOW code.

CATG.OUT

Output file from CONSIM2 containing the x, y, z, and category number for the simulation grid

SGSSIM.OUT

Output file from CONSIM2 containing x, y, z, and sequential Gaussian simulated values for category 1 points. Note each category will have its own file, thus SGSSIM1.OUT will be used for category 1 and





SGSSIM2.OUT will be the input file used for category 2, etc. The information contained in this file concerns the variogram used for the spatial variability within the category, the conditioning data file name, the number of neighbors to be used in the simulation process, the range of the simulated variable.

OUT.DAT

Output file containing information concerning the simulated field being input to the SWIFT grid; the x, y, z coordinates of the SWIFT grid block centers, the category assigned to the grid block, its simulated value, and the range (minimum and maximum) of the simulated value that is used by the optimization routine PAREST.

OUT2.DAT

Output file containing information concerning the final calibrated transmissivity field; the x, y, z coordinates of the SWIFT grid block centers, the category assigned to the grid block, its simulated value, and the range (minimum and maximum) of the simulated value that is used by the optimization routine PAREST and the pilot point locations.

SWIFT.OUT

The output file from the SWIFT II code that contains information on the specifics of the gridded domain used to solve the groundwater flow equation. In addition, it contains the calculated groundwater flow velocities for each grid block.

SWIFT121.DAT

The output file from the GRASP-INV code that contains the final (i.e., post-calibration) conductivity field written in a SWIFT II code R-121 card format.

SWIFTWEL.DAT

An optional output file from the SWIFT II code that contains pressure information for wells specified in the SWIFT code for each time step.

SWIFTVEC.DAT

An optional output file from the SWIFT II code that contains groundwater velocities for each grid block in the model domain.

GRASP.OUT

The output file from the GRASP II code that contains the calculated WLS objective function and the grid-block sensitivities of the objective function to changes in the grid-block conductivities.

GRASPDKH.DAT

An optional output file from the GRASP II code that contains sensitivities of an objective function to changes in grid block conductivities for each grid block of the flow model.

GRASPDPB.DAT

An optional output file from the GRASP II code that contains sensitivities of an objective function to changes in model boundary pressures.



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11.0 APPENDIXES

Appendix A: CONSIM II Common Notation



\forall : for all

a : range parameter or power (for the power variogram)

a_l : coefficient of component number l of the trend model

$B(z)$: Markov-Bayes calibration parameter

c : contribution to the nugget or slope (for the power variogram)

$C(0)$: covariance value at separation vector $\mathbf{h} = 0$ It is also the stationary variance of random variable $Z(\mathbf{u})$

$C(\mathbf{h})$: stationary covariance between any two random variable $Z(\mathbf{u})$, $Z(\mathbf{u} + \mathbf{h})$ separated by vector \mathbf{h}

$C(\mathbf{u}, \mathbf{u}')$: non-stationary covariance of two random variable $Z(\mathbf{u})$, $Z(\mathbf{u}')$

$C_k(\mathbf{h})$: nested covariance structure in the linear covariance model

$$C(\mathbf{h}) = \sum_{k=1}^K C_k(\mathbf{h})$$

$C_I(\mathbf{h}; z_k, z_{k'})$: stationary indicator cross covariance for cutoffs $z_k, z_{k'}$; it is the cross covariance between the two indicator random variables $I(\mathbf{u}; z_k)$ and $I(\mathbf{u} + \mathbf{h}; z_{k'})$

$C_{ZY}(\mathbf{h})$: stationary cross-covariance between the two random variables $Z(\mathbf{u})$ and $Y(\mathbf{u} + \mathbf{h})$ separated by lag vector \mathbf{h}

$Circ(\mathbf{h})$: circular semivariogram function of separation vector \mathbf{h}

$E\{\cdot\}$: expected value

$E\{Z(\mathbf{u}) (n)\}$: conditional expectation of the random variable $Z(\mathbf{u})$ given the realizations of n other neighboring random variables (called data)

$Exp(\mathbf{h})$: exponential semivariogram model, a function of separation vector \mathbf{h}

$F(\mathbf{u}; z)$: non-stationary cumulative distribution function of random variable $Z(\mathbf{u})$

$F(\mathbf{u}; z(n))$: non-stationary conditional cumulative distribution function of the continuous random variable $Z(\mathbf{u})$ conditioned by the realizations of n other neighboring random variable (called data)

$F(\mathbf{u}; k(n))$: non-stationary conditional probability distribution function of the categorical variable $Z(\mathbf{u})$

$F(\mathbf{u}_1, \dots, \mathbf{u}_K; z_1, \dots, z_K)$: K -variate cumulative distribution function of the K random variables $Z(\mathbf{u}_1), \dots, Z(\mathbf{u}_K)$

$F(z)$: cumulative distribution function of a random variable Z , or stationary cumulative distribution function of a random function $Z(\mathbf{u})$

$F^{-1}(p)$: inverse cumulative distribution function or quantile function for the probability value p $[0,1]$

$\gamma(\mathbf{h})$: stationary semivariogram between any two random variables $Z(\mathbf{u})$, $Z(\mathbf{u} + \mathbf{h})$ separated by lag vector \mathbf{h}

$\gamma(\mathbf{h}; z)$: stationary indicator semivariogram for lag vector \mathbf{h} and cutoff z : it is the semivariogram of the binary indicator random function $I(\mathbf{u}; z)$

$\gamma(\mathbf{h}; p)$: same as above, but the cutoff z is expressed in terms of p -quantile with $p = F(z)$

$\gamma_{ZY}(\mathbf{h})$: stationary cross semivariogram between the two random variables $Z(\mathbf{u})$ and $Y(\mathbf{u} + \mathbf{h})$ separated by lag vector \mathbf{h}

$G(y)$: standard normal cumulative distribution function

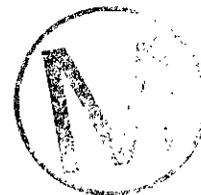
$G^{-1}(p)$: standard normal quantile function such that $G(G^{-1}(p)) = p \in [0,1]$

\mathbf{h} : separation vector

$I(\mathbf{u}; z)$: binary indicator random function at location \mathbf{u} and for cutoff z

$i(\mathbf{u}; z)$: binary indicator value at location \mathbf{u} and for cutoff z

$j(\mathbf{u}; z)$: binary indicator transform arising from constraint interval



$f_1(\cdot)$: function of the coordinates used in a trend model

$\lambda_\alpha, \lambda_\alpha(\mathbf{u})$: kriging weight associated to datum α for estimation at location \mathbf{u}

M : stationary median of the distribution function $F(z)$

m : stationary mean of the random variable $Z(\mathbf{u})$

$m(\mathbf{u})$: mean at location \mathbf{u} , expected value of random variable $Z(\mathbf{u})$; trend component model in the decomposition $Z(\mathbf{u}) = m(\mathbf{u}) + R(\mathbf{u})$, where $R(\mathbf{u})$ represents the residual component model

$m^*_{KT}(\mathbf{u})$: estimate of the trend component at location \mathbf{u}

$\mu, \mu(\mathbf{u})$: Lagrange parameter for kriging at location \mathbf{u}

$N(\mathbf{h})$: number of pairs of data values available at lag vector \mathbf{h}

$\prod y_i = y_1 \cdot y_2 \dots y_n$: product

$q(p) = F^{-1}(p)$: quantile function, i.e., inverse cumulative distribution function for the probability value, $p \in [0,1]$

$R(\mathbf{u})$: residual random function model in the decomposition $Z(\mathbf{u}) = m(\mathbf{u}) + R(\mathbf{u})$, where $m(\mathbf{u})$ represents the trend component model

ρ : correlation coefficient $[-1, +1]$

$\rho(\mathbf{h})$: stationary correlogram function $\in [-1, +1]$

$\sum_{i=1}^n y_i = y_1 + y_2 + \dots + y_n$: summation

$\Sigma(\mathbf{h})$: matrix of stationary covariances and cross-covariances

σ^2 : variance

$\sigma^2_{OK}(\mathbf{u})$: ordinary kriging variance of $Z(\mathbf{u})$

$\sigma^2_{SK}(\mathbf{u})$: simple kriging variance of $Z(\mathbf{u})$



$Sph(\mathbf{h})$: spherical semivariogram function of separation vector \mathbf{h}

\mathbf{u} : coordinates vector

$Var\{\cdot\}$: variance

$Y = \varphi(Z)$: transform function $\varphi(\cdot)$ relating random variables Y and Z

$Z = \varphi^{-1}(Y)$: inverse transform function $\varphi(\cdot)$ relating random variables Z and Y

Z : generic random variable

$Z(\mathbf{u})$: generic random variable at location \mathbf{u} , or a generic random function of location \mathbf{u}

$Z^*_{COK}(\mathbf{u})$: cokriging estimator of $Z(\mathbf{u})$

$Z^*_{KT}(\mathbf{u})$: estimator of $Z(\mathbf{u})$ using some form of prior trend model

$Z^*_{OK}(\mathbf{u})$: ordinary kriging estimator of $Z(\mathbf{u})$

$Z^*_{SK}(\mathbf{u})$: simple kriging estimator of $Z(\mathbf{u})$

$\{Z(\mathbf{u}), \mathbf{u} \in A\}$: set of random variables $Z(\mathbf{u})$ defined at each location \mathbf{u} of a zone A

$z(\mathbf{u})$: generic variable function of location \mathbf{u}

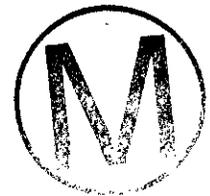
$z(\mathbf{u})$: z -datum value at location \mathbf{u}

z_k : k -th cutoff value

$z^{(l)}(\mathbf{u})$: l -th realization of the random function $Z(\mathbf{u})$ at location \mathbf{u}

$z_c^{(l)}(\mathbf{u})$: l -th realization conditional to some neighboring data

$z^*(\mathbf{u})$: an estimate of value $z(\mathbf{u})$



$[z(\mathbf{u})]^*_E$: E -type estimate of value $z(\mathbf{u})$, obtained as an arithmetic average of multiple simulated realizations $z^{(l)}(\mathbf{u})$ of the random function $Z(\mathbf{u})$



Appendix B: Program CONSIM II Dimensioning Parameters

Dimensioning parameters for CONSIM II can be found in three different include files: CDP.INC, TIEC2S.INC, and CONSIM.INC. File CDP.INC is included in nearly every subprogram in GRASP-INV. TIEC2S.INC is used to tie CONSIM II to SWIFT II. CONSIM.INC is used primarily within CONSIM II.

The parameters within CDP.INC that are used by CONSIM II are

- MAXCUT:** maximum number of cutoffs for an indicator-based method, which serves as the maximum number of categories.
- MAXDAT:** maximum number of conditioning data points.
- MAXNST:** maximum number of structures defining a variogram model.
- MAXXSW:** maximum number of SWIFT II blocks in the x-direction.
- MAXYSW:** maximum number of SWIFT II blocks in the y-direction.
- MAXZSW:** maximum number of SWIFT II blocks in the z-direction.
- MAXBSW:** maximum total number of SWIFT II blocks, the product of MAXXSW, MAXYSW, and MAXZSW.

Note that the SWIFT II code is dimensioned independent of the number of grid blocks in each direction, but CONSIM II requires arrays dimensioned in each of the principal directions.

The parameters within TIEC2S.INC are

- MAXLX:** maximum number of simulation points in the x-direction found within a single SWIFT II block (regular simulation grid).
- MAXLY:** maximum number of simulation points in the y-direction found within a single SWIFT II block (regular simulation grid).

MAXLZ: maximum number of simulation points in the z-direction found within a single SWIFT II block (regular simulation grid).

MAXZONE: maximum number of zones used to delineate anisotropies.

The parameters within CONSIM.INC are

MAXLOC: maximum number of points on the simulation grid

MAXX: maximum number of super block grid refinements in the x-direction, $(2)^{\text{ipower}} + 1$, ipower described in section 7.5.5.

MAXY: maximum number of super block grid refinements in the y-direction, $(2)^{\text{ipower}} + 1$, ipower described in section 7.5.5.

MAXZ: maximum number of super block grid refinements in the z-direction, $(2)^{\text{ipower}} + 1$, ipower described in section 7.5.5.

MAXSBX: maximum number of super blocks in the x-direction.

MAXSBY: maximum number of super blocks in the y-direction.

MAXSBZ: *maximum number of super blocks in the z-direction.*

MAXNOD: maximum number of previously simulated nodes used to simulate the current point.

MAXSAM: maximum number of data points used to simulate the current point.

The variable ipower (Section 7.5.5) is not allowed to exceed 7 so that MAXX, MAXY, and MAXZ need not exceed 129. If a direction (e.g., z-direction) is not being simulated, then the maximum (e.g., MAXZ) can be set to one. Parameter MAXXYZ is set to their product.



Typically only one super block is used so that **MAXSBX**, **MAXSBY**, and **MAXSBZ** can all be set to one. Parameter **MAXSB** is set to their product. The definitions for two other parameters depend on the above: $\mathbf{MXSX} = 2 \cdot \mathbf{MAXBSX}$ and $\mathbf{MXSXY} = 4 \cdot \mathbf{MAXSBX} \cdot \mathbf{MAXSBY}$.

Parameter **MAXKR1** is set to $\mathbf{MAXNOD} + \mathbf{MAXSAM} + 1$. This defines the maximum number of simultaneous equations to be solved to simulate a point. $\mathbf{MAXKR2} = \mathbf{MAXKR1} \cdot (\mathbf{MAXKR1} + 1) / 2$ is the maximum size of the matrix to be solved.

Parameter $\mathbf{MAXROT} = \mathbf{MAXCUT} \cdot \mathbf{MAXNST} + 1$ is used to dimension the maximum number of rows in the rotation matrix used for distance calculations. Parameter $\mathbf{MXCUT} = \mathbf{MAXCUT} + 1$ is also used for dimensioning. Recall that both **MAXCUT** and **MAXNST** are defined in **CDP.INC**.

Appendix C: Example Data Sets for GRASP-INV

C.1 CONSIM II Example Problem 1

Consider that there are three observed transmissivity data points and we wish to obtain the kriging estimate at a fourth location. Assuming the variogram is represented well by an exponential model, the simple kriging estimate may be obtained as follows:

Known values: $z_1 = 0.1$ at (0, 1)
 $z_2 = 0.0$ at (1, 1)
 $z_3 = 0.2$ at (1, 0)
 Unknown values: $z_0 = ?$ at (0, 0)

Simple Kriging Estimate by hand calculation

(a) Variogram Model (exponential)

$$\gamma(h) = c \left[1 - \exp\left(-\frac{|h|}{a}\right) \right] + c_0 \quad (C-1)$$

where:

c_0 = nugget effect,
 c = contribution,
 $c_0 + c$ = sill,
 a = range,
 h = distance between two points.



(b) Simple Kriging Procedure

SK estimates the expected value of z_0 as weighted sum of known values z_1 , z_2 , and z_3 .

$$z_0 = \sum_{i=1}^3 \lambda_i z_i \quad (C-2)$$

where λ_i ($i = 1, 2, 3$) can be derived by solving the following equation

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} c_{01} \\ c_{02} \\ c_{03} \end{bmatrix} \quad (C-3)$$

where

c_i ($i, j = 1, 2, 3$) is covariance between points with known values, and
 c_0 ($j = 1, 2, 3$) is covariance between the point with unknown value and other points.

(c) Relationship between $\gamma(h)$ and $c(h)$

$$c_{ij}(|h|) = \sigma^2 - \gamma_{ij}(|h|) \quad (C-4)$$

where σ^2 is the sill or variance of the variable (assumed to equal 1.0).

(d) Calculation of z_0 .

Assume;

- $c_0 = 0.0$ (nugget effect),
- $c = 1.0$ (contribution),
- $c_0 + c = 1.0$ (sill),
- $a = 0.6667$ (range).

By making use of equations (1), (3) and (4), we get equation (5)

$$\begin{bmatrix} 1 & 0.2231 & 0.1199 \\ 0.2231 & 1 & 0.2231 \\ 0.1199 & 0.2231 & 1 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} 0.2231 \\ 0.1199 \\ 0.2231 \end{bmatrix} \quad (C-5)$$

and

$$(\lambda_1, \lambda_2, \lambda_3) = (0.1925, 0.0340, 0.1925)$$

Therefore, the kriged estimate is equal to:

$$z_0 = \lambda_1 z_1 + \lambda_2 z_2 + \lambda_3 z_3$$

$$z_0 = 0.1925 \times 0.1 + 0.0340 \times 0.0 + 0.1925 \times 0.2$$

$$z_0 = 0.057746 \text{ (calculated using a spread sheet for more accuracy)}$$



The GRASP-INV input files needed to set up and solve this problem are listed in Figure C-1.

Figure C.1. Input Files for CONSIM II Example 1
(Page 1 of 4)

(a) MAIN.inp

1 1 1 1

(b)DXDYDZ.inp

1. 1. 1.
0.0 0.0 0.0
2 2 1
1.0 1.0 /
1.0 1.0 /
1.0 /
-1
1
1 2 1 2 1 1
0.1 0.01 1.0

(c)RAND.inp

1
123812

(d) XYZ.dat

xyz.dat: 2-d Simple Kriging Example - Gauss

3
x
y
z
0.000000 0.000000 0.000000
1.000000 0.000000 0.000000
1.000000 1.000000 0.000000
0.000000 1.000000 0.000000

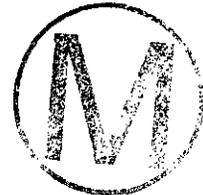


Figure C.1. Input Files for CONSIM II Example 1

(Page 2 of 4)

(e) CONSIM.inp

catg.inp
estimation
sgsim
sgsim.inp
dxdydz.dat
out.dat
out2.dat
swift.121
restart.rec

contents of file

1. pdf input parameter file
 2. must either be "simulation" or "estimation"
 3. ... records then occur in pairs, one pair per category method for the category, must currently be "sgsim"
input parameter file for the category
- 5th from last line. file where coarse grid info can be found (input)
4th from last line. file where initial coarse field is written (restart form)
3rd from last line. file for writing final calibrated field (restart form)
2nd from last line. file for writing final calibrated field (R1-21 form)
Last line. file containing restart record (input)

Figure C.1. Input Files for CONSIM II Example 1
(Page 3 of 4)

(f) CATG.inp

Parameters for SISIMPDF

START OF PARAMETERS:

cond.dat	\hard data file
1 2 0 3	\column: x,y,z,vr
-20. 20.	\data trimming limits
1	\simulation grid regular(0)or not(1)
xyz.dat	\0=>dimensions, 1=>location file
1 2 0	\0=>spacing, 1=>x,y,z coordinates
catg.out	\output file for simulation
1	\debugging level: 0,1,2,3
catg.dbg	\output File for Debugging
1	\number of simulations
1	\number of nested grids
1	\0=no buffer locations, 1=yes
4	\max per octant(0 -> not used)
5.0	\maximum search radius
0.0 0.0 0.0 1.0 1.0	\sang1,sang2,sang3,sanis1,2
3 3	\min, max data for simulation
0	\number simulated nodes to use
0 2	\0=full IK, 1=med approx(cat #)
0	\0=SK, 1=OK
1	\number of categories
1 1.00 1 0.00	\cat # , global pdf, nst, nugget
1 5.0 1.0	\it, aa, cc
0.0 0.0 0.0 1.0 1.0	\ang1,ang2,ang3,anis1,2

(g) COND.dat

SK-Gauss Example: Conditioning data $c1=N(0,1)$

4
x
y
cat
cat1
0.0 1.0 1 0.1
1.0 0.0 1 0.2
1.0 1.0 1 0.0



Figure C.1. Input Files for CONSIM II Example 1
(Page 4 of 4)

(h) SGSIM.inp

Parameters for SGSIM (for SK-Gauss example)

START OF PARAMETERS:

cond.dat	
1 2 0 4 0	\column: x,y,z,vr,wt
-98 1.0e21	\data trimming limits
1	\0=transform the data, 1=don't
sgtr1.out	\output transformation table
-4.0 4.0	\zmin,zmax(tail extrapolation)
2 2.0	\lower tail option, parameter
2 0.5	\upper tail option, parameter
1	\0=regular, 1=not regular grid
xyz.loc	\location file name
1 2 0	\0=>spacing, 1=>x,y,z coordinates
sgsim.out	\output File for simulation
sgest.out	\output File for estimation
4	\debugging level: 0,1,2,3,4
sgsim.dbg	\output File for Debugging
0	\kriging type (0=SK, 1=OK)
1	\number of simulations
1	\number of nested grids
0	\0=no_buffer_locations 1=yes
0	\max per octant(0 -> not used)
40.0	\maximum search radius
0.0 0.0 0.0 1.0 1.0	\sang1,sang2,sang3,sanis1,2
0 8	\min, max data for simulation
8	\number simulated nodes to use
1 0.0	\nst, nugget effect
2 0.6667 1.0	\it, aa, cc
0.0 0.0 0.0 1.0 1.0	\ang1,ang2,ang3,anis1,anis2:



C.2 CONSIM II Example Problem 2

This example presents the GRASP-INV files needed to generate a two-dimensional unconditional simulation for an ensemble of random fields. Two categories will be considered in this case. One indicator realization will be generated and 50 sequential Gaussian realizations for two continuous variables will be generated with the following semi-variogram models.

Categorical simulation: exponential variogram model:

$$\gamma(h) = c \left[1 - \exp\left(-\frac{|h|}{a}\right) \right] + c_0$$

where

c_0 = nugget effect = 0.0,
 c = contribution = 0.25,
 a = range = 2.0,
 h = distance between two points.

Continuous variable simulation for category 1: exponential variogram model

$$\gamma(h) = c \left[1 - \exp\left(-\frac{|h|}{a}\right) \right] + c_0$$



where

c_0 = nugget effect=0.2,
 c = contribution=0.8,
 $c_0 + c$ = sill=1.0,
 a = range=1.0,
 h = distance between two points.

Continuous variable simulation for category 2: spherical variogram model

$$\begin{aligned} \gamma(h) &= c \left[1.5 \frac{h}{a} - 0.5 \left(\frac{h}{a} \right)^3 \right] + c_0, \text{ if } h \leq a \\ &= c + c_0, \text{ if } h \geq a \end{aligned}$$

where

c_0 = nugget effect = 0.0,
 c = contribution = 1.0,
 a = range = 3.0,
 h = distance between two points.

The GRASP-INV needed to set up and generate the realizations described above are presented in Figure C.2.



Figure C.2. Input Files for CONSIM II Example 2
(Page 1 of 5)

(a) MAIN.inp

1 1 1 1

(b) DXDYDZ.inp

1. 1. 1.
0.0 0.0 0.0
100 100 1
100*1.0/
100*1.0 /
1.0 /
-1
1
1 100 1 100 1 1
0.1 0.01 1.0

(c) RAND.inp

1
123812



Figure C.2. Input Files for CONSIM II Example 2

(Page 2 of 5)

(d) CONSIM.inp

catg.inp
simulation
sgsim
sgsim1.inp
sgsim
sgsim2.inp
dxdydz.inp
out.dat
out2.dat
swift.121
restart.rec

contents of file

1. pdf input parameter file
 2. must either be "simulation" or "estimation"
 3. ... records then occur in pairs, one pair per category method for the category, must currently be "sgsim"
input parameter file for the category
- 5th from last line. file where coarse grid info can be found (input)
4th from last line. file where initial coarse field is written (restart form)
3rd from last line. file for writing final calibrated field (restart form)
2nd from last line. file for writing final calibrated field (R1-21 form)
Last line. file containing restart record (input)



Figure C.2. Input Files for CONSIM II Example 2
(Page 3 of 5)

(e)CATG.inp

Parameters for SISIMPDF (for sGs example)

START OF PARAMETERS:

1 2 3 0	\hard data file
-1.0e21 1.0e21	\column: x,y,z,vr
0	\data trimming limits
100 100 1	\simulation grid regular(0) or not(1)
1.0 1.0 1.0	\nx,ny,nz or location file (if 1 above)
catg.out	\0=>spacing, 1=>x,y,z coordinates
1	\output file for simulation
catg.dbg	\debugging level: 0,1,2,3
1	\output File for Debugging
3	\number of simulations
0	\number of nested grids
0	\0=no buffer locations, 1=yes
20.0	\max per octant(0 -> not used)
0.0 0.0 0.0 1.0 1.0	\maximum search radius
0 10	\sang1,sang2,sang3,sanis1,2
10	\min, max data for simulation
0 1	\number simulated nodes to use
0	\0=full IK, 1=med approx(cat #)
2	\0=SK, 1=OK
1 0.50 1 0.00	\number of categories
2 2.0 0.25	\cat # , global pdf, nst, nugget
0.0 0.0 0.0 1.0 1.0	\it, aa, cc
2 0.50 1 0.00	\ang1,ang2,ang3,anis1,2
2 2.0 0.25	\cat # , global pdf, nst, nugget
0.0 0.0 0.0 1.0 1.0	\it, aa, cc
	\ang1,ang2,ang3,anis1,2



Figure C.2. Input Files for CONSIM II Example 2
(Page 4 of 5)

(f) SGSIM1.inp

Parameters for SGSIM (for sGs example)

START OF PARAMETERS:

1 2 3 4 0	\column: x,y,z,vr,wt
-1.0e21 1.0e21	\data trimming limits
2	\0/1/2 = Transf/Don't/don't backtrn
sgstrn1.tab	\output transformation table
0.0 20.0	\zmin,zmax(tail extrapolation)
1 0.0	\lower tail option, parameter
2 0.5	\upper tail option, parameter
0	\simulation grid regular(0) or not(1)
100 100 1	\nx,ny,nz or location file (if 1 above)
1.0 1.0 1.0	\0=>spacing, 1=>x,y,z coordinates
sgssim1.out	\output File for simulation
sgsest1.out	\output File for estimation
1	\debugging level: 0,1,2,3
sgssim1.dbg	\output File for Debugging
0	\kriging type (0=SK, 1=OK)
50	\number of simulations
3	\number of nested grids
0	\0=no_buffer_locations 1=yes
0	\max per octant(0 -> not used)
20.0	\maximum search radius
0.0 0.0 0.0 1.0 1.0	\sang1,sang2,sang3,sanis1,2
0 4	\min, max data for simulation
8	\number simulated nodes to use
1 0.20	\nst, nugget effect
2 1.0 0.80	\it, aa, cc
0.0 0.0 0.0 1.0 1.0	\ang1,ang2,ang3,anis1,anis2:

Figure C.2. Input Files for CONSIM II Example 2
(Page 5 of 5)

(g) SGSIM2.inp

Parameters for SGSIM (for sGs example)

START OF PARAMETERS:

1 2 3 4 0	\column: x,y,z,vr,wt
-1.0e21 1.0e21	\data trimming limits
2	\0/1/2 = Transf/Don't/don't backtrn
sgstrn2.tab	\output transformation table
0.0 20.0	\zmin,zmax(tail extrapolation)
1 0.0	\lower tail option, parameter
2 0.5	\upper tail option, parameter
0	\simulation grid regular(0) or not(1)
100 100 1	\nx,ny,nz or location file (if 1 above)
1.0 1.0 1.0	\0=>spacing, 1=>x,y,z coordinates
sgssim2.out	\output File for simulation
sgsest2.out	\output File for estimation
1	\debugging level: 0,1,2,3
sgssim2.dbg	\output File for Debugging
0	\kriging type (0=SK, 1=OK)
50	\number of simulations
3	\number of nested grids
0	\0=no_buffer_locations 1=yes
0	\max per octant(0 -> not used)
20.0	\maximum search radius
0.0 0.0 0.0 1.0 1.0	\sang1,sang2,sang3,sanis1,2
0 4	\min, max data for simulation
8	\number simulated nodes to use
1 0.0	\nst, nugget effect
1 3.0 1.0	\it, aa, cc
0.0 0.0 0.0 1.0 1.0	\ang1,ang2,ang3,anis1,anis2:



C.3 SWIFT II/GRASP II Example Problem 1

Consider a one-dimensional homogeneous aquifer, discretized into 5 grid blocks each 200 m in length, permeability of $1.0193679E-07m^2$, porosity of 0.10, water viscosity of $1.0E-03$, gravity of $9.81 m/s^2$, fluid density of $1000 kg/m^3$, and subjected to prescribed pressures of $1.962E+06 Pa$ at the upgradient end and $9.81E+05 Pa$ at the downgradient end. The geometry, hydrogeologic and fluid properties and the prescribed pressures are shown in **Figure C-3** (at the end of this problem). The resulting pressure distribution of this one-dimensional problem is linear and the Darcy velocity is constant throughout the aquifer. The fluid and the aquifer properties presented above result in a hydraulic conductivity of $1.0 m/sec$. The hand calculated pressures and velocities for each grid block are listed below.

Pressure Distribution =

$$P_i = P_o(1 - \frac{x_i}{L}) + P_L(\frac{x_i}{L})$$

where;

$$P_o = 1.962E+06 Pa$$

$$P_L = 9.81E+05 Pa$$

$$L = 1000m$$

$$x_i = 100m, 300m, 500m, 700m, \text{ and } 900m \text{ for grid blocks 1 through 5 respectively}$$

thus, the pressure in

$$\text{Grid block 1} = 1.8639E+06 Pa$$

$$\text{Grid block 2} = 1.6677E+06 Pa$$

$$\text{Grid block 3} = 1.4715E+06 Pa$$

$$\text{Grid block 4} = 1.2753E+06 Pa$$

$$\text{Grid block 5} = 1.0791E+06 Pa$$

Darcy Velocities=

$$v = K\Delta h/L$$

where;

$$v = \text{Darcy velocity}$$

$$K = \text{hydraulic conductivity}$$

$$\Delta h = \text{hydraulic head difference (i.e., } h_1 - h_2)$$

$$L = \text{Length between points where } h_1 \text{ and } h_2 \text{ are located}$$

and

$$K = k \rho \frac{g}{\mu} \quad h = \frac{P}{\rho g} + z$$



where;

k = permeability
g = gravity
 ρ = fluid density
 μ = fluid viscosity
z = elevation of measuring point

With $z = 0$ m in this example, $k=1.0193679E-07m^2$, fluid viscosity of $1.0E-03$, gravity of 9.81 m/s², fluid density of 1000 kg/m³, and a hydraulic head gradient of 0.1 m/m, the calculated Darcy velocity of 0.1 m/s is obtained for each of the five grid blocks in the model domain.

Sensitivity to Grid Block Permeability

The sensitivity coefficients of a pressure at a selected grid block in the model domain to the grid block permeabilities and boundary pressures are obtained by direct differentiation of the above equation as shown below:

$$\frac{\partial p}{\partial k} = 0$$

$$\frac{\partial p}{\partial p_L} = x/L$$

$$\frac{\partial p}{\partial p_o} = (1 - x/L)$$

An interpretation of the first equation above is necessary. It shows that the variation of pressure at any point x is zero, when the homogeneous permeability (k) is altered throughout the aquifer by a constant amount. When applied to a finite difference model such as SWIFT II with N = grid blocks, this equation may be written as

$$\sum_{m=1}^N \frac{\partial p_i}{\partial k_m} = 0 \text{ for all } i$$

where

i, m = suffixes denoting grid block numbers
 N = total number of grid blocks in the system

Note that even in a homogeneous aquifer, the individual sensitivity coefficients, dp/dk_m , are not zero. The above equation is used to verify the sum of sensitivity coefficients dp/dk_m rather than the individual values. Expressions for the individual sensitivity coefficients were not available in published literature, so they are derived below to aid in the verification of GRASP-INV.

The equations presented below are based on the following assumptions;

1. All k_m , permeability values will be independent of the suffix and are referred to herein without the suffix as simply k .

2. N = total number of grid blocks.

For a performance measure of pressure in grid block m , the sensitivity of the permeability in grid block m is given by:

$$\frac{\partial P_m}{\partial k_m} = \frac{1(P_o - P_L)}{2N} \left(\frac{N - 2m + 1}{N} \right) \frac{1}{k}$$

For a performance measure of pressure in grid block m , the sensitivity of the permeability in grid block l , where l is to the left of grid block m , is given by:

$$\frac{\partial P_m}{\partial k_l} = \frac{(P_o - P_L)(N - m + 0.5)}{N} \frac{1}{Nk}$$

For a performance measure of pressure in grid block m , the sensitivity of the permeability in grid block r , where r is to the right of grid block m , is given by:

$$\frac{\partial P_m}{\partial k_r} = \frac{(P_o - P_L)(m - 0.5)}{kN^2}$$

For a performance measure of pressure in grid block m , the sensitivity to the pressure at the boundary $x=0$ is given by;

$$\frac{\partial P_m}{\partial p_o} = \frac{(N - m + \frac{1}{2})}{N}$$



For a performance measure of pressure in grid block m , the sensitivity to the pressure at the boundary $x=L$ is given by;

$$\frac{\partial P_m}{\partial p_L} = \frac{(m - \frac{1}{2})}{N}$$

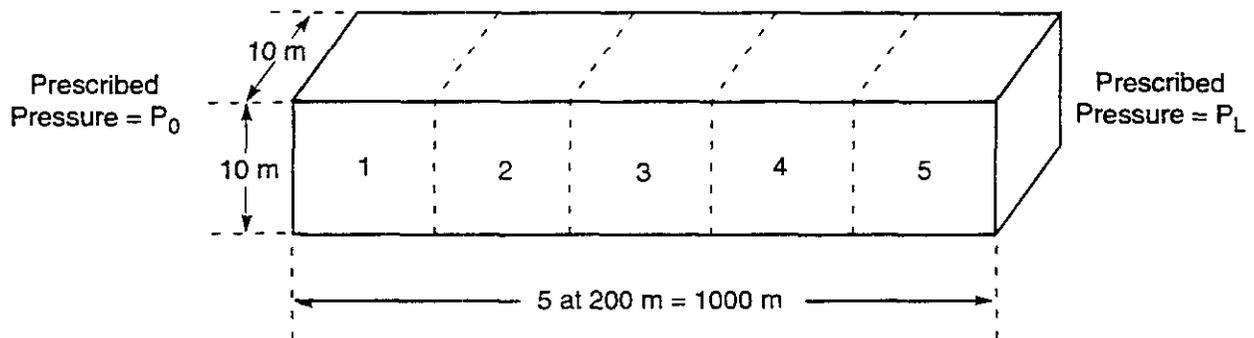
Using the above analytical expressions for the sensitivity of a pressure at grid block to grid block permeabilities and boundary pressures, the following results may be obtained for this example problem.

Sensitivity of Pressure in Grid Block 2 to:

<u>Grid Block</u>	<u>Grid Block Permeability</u>	<u>Boundary Pressure</u>
1	1.347305E12	0.7
2	3.849444E11	
3	-5.774166E11	
4	-5.774166E11	
5	-5.774166E11	0.3

The GRASP-INV input files to set up and solve this example problem are listed in Figure C-4.





Boundary Conditions

$$P_0 = 1.962 \times 10^6 \text{ Pa}$$

$$P_L = 9.810 \times 10^5 \text{ Pa}$$

Geohydrologic Parameters

$$k = 10^{-6} \text{ g m}^2 \text{ (g = 9.81)}$$

$$\rho = 10^3 \text{ kg/m}^3$$

$$\mu = 10^{-3} \text{ Pa sec}$$

(hydraulic conductivity = 1.0 m/sec)

Geometry

$$\Delta x = 200 \text{ m}$$

$$N = 5$$

$$\Delta y = \Delta z = 10 \text{ m}$$

TRI-6342-4684-0



Figure C-3. One Dimensional Flow Problem Used in SWIFT Example 1

Figure C-4. Input Files for SWIFT/GRASP Example 1
(Page 1 of 3)

(a) MAIN.inp

2 3 1 1

(b) PARAM.inp

0.0
1 1 1 3 (KSTPFLG,NCONF)
1 1 0.0 0 3*0.0 20 3.00000 0.0 1

(c) DXDYDZ.inp

1. 1. 1.
0.0 0.0 0.0
5 1 1
5*200.0/
10.0/
10.0/
-1
1
1 5 1 1 1 1
0.1 0.01 1.0

(d) RAND.inp

1
123812



Figure C-4. Input Files for SWIFT/GRASP Example 1
 (Page 2 of 3)

(e) SWIFT.inp

```

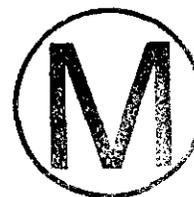
$NOECHO
ONE DIMENSIONAL FLOW PROBLEM WITH FIXED PRESSURES ON EACH END
QUALITY ASSURANCE TEST CASE FOR GRASP-INV
4 0 0 0 0 0 0 1 0 M1.1
5 1 1 1 0 1 3 -1 0 20 1 0 1 M2
0 0 0 0 0 0 0 M3-1
4.53 E-10 7.57 E-10 20.7 E-05 4.182 E+3 0.800 E+3 9.810 R1-1
0 0 0 0 0 0 0. 0. 0. R1-2
2500. 1.E+5 25. 1000.0 1300.00 R1-3
1 0 0 2 R1-6
25. 0.001 25. 0.0018 R1-7
0.25 0.0012 R1-8
000. 25. R1-11.1
-100. 25. R1-11.2
0 0 R1-12
25. 1.E+5 0. 0. R1-16
5*200.0 /
10.0 /
10.0 /
1.00E-00 1.00E-00 1.00E-00 0.10 0.0 0.0 0.0 R1-20
R1-BLK
R1-26.B
/R1-
4 1
27/
1 1 1 1 1 1 0
1.000E+00 1.962E+06
5 5 1 1 1 1 0
2.000E+00 9.810E+05
R1-28.E
R1-33.B
R1-27BLN
I-1
I-1-BL
R2-1
0 0 0
0 0 0 0 0 0 0 0 0 0
00.0 0.0
0 -1 0 -1 -1 1 011 0 0000 0 01 -1 -1 -1 R2-13-1
1 0111 0000 0000 0000 1 R2-13-2
1 5 1 1 1 1 0. -99.9 R2-16
1 5 1 1 1 1 0. -99.9 R2-16
1 5 1 1 1 1 0. -99.9 R2-16
0 0 0 1 0 0 0 0 0 0 R2-1
  
```



Figure C-4. Input Files for SWIFT/GRASP Example 1
(Page 3 of 3)

(f) GRASP.inp

097B-21C-001D	AD-1
* GRASP INPUT FOR ADJOINT SENSITIVITIES TO ONE DIMENSIONAL FLOW PROBLEM WITH FIXED PRESSURES ON EACH END	
	M1.1
QUALITY ASSURANCE TEST CASE FOR GRASP-INV	
0	IOPT
1 1 1 -1 0 1.00 01	AD-4
2 2 1 1 1 1 1.0	AD-5
1 1 1 1	AD-6
1 5 1 1 1 1 1	AD-7A
2 1 1 1	AD-6
1 1 1 1 1 1	AD-7A
5 5 1 1 1 1	AD-7A
0	end



C.4 SWIFT II /GRASP II Example Problem 2

This example problem employs the same horizontal, one-dimensional, homogeneous aquifer with pressure boundary conditions as used in the SWIFT/GRASP Example Problem 1. The difference in this test problem is that the sensitivity coefficients for a weighted least square (WLS) performance measure to the grid block conductivity and boundary pressures are obtained.

Consider a performance measure, J, consisting of a weighted least squares objective function of calculated and observed pressures:

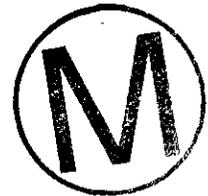
$$J = \sum w_i (p_i - p_{ob,i})^2$$

Then;

$$dJ/dk_m = 2 \sum w_i (p_i - p_{ob,i}) \delta p / \delta k_m$$

Assuming we consider the observed pressure at the location coinciding with grid block 3 (shown in the above example to be equal to 1.4715E+6 Pa) to represent the observed pressures at each of the other four grid block locations, the expression for the sensitivity of the WLS performance measure to the permeability of grid block 1 is (assuming an equal weight of 0.2 for each of the 5 observed pressures);

$$\begin{aligned} \frac{DJ}{Dk_1} = & 2 \cdot [0.2(1.8639E6 - 1.4715E6) \frac{\partial P_1}{\partial k_1} + 0.2(1.6677E6 - 1.4715E6) \frac{\partial P_2}{\partial k_1} \\ & + 0.2(1.4715E6 - 1.4715E6) \frac{\partial P_3}{\partial k_1} + 0.2(1.2753E6 - 1.4715E6) \frac{\partial P_4}{\partial k_1} \\ & + 0.2(1.0791E6 - 1.4715E6) \frac{\partial P_5}{\partial k_1}] \end{aligned}$$



The general expression used to determine the sensitivity of the WLS performance to the grid block permeabilities is;

$$\therefore \frac{DJ}{Dk_i} = 2 \cdot [78480 \frac{\partial P_1}{\partial k_i} + 39240 \frac{\partial P_2}{\partial k_i} + 0 - 39240 \frac{\partial P_4}{\partial k_i} - 78480 \frac{\partial P_5}{\partial k_i}]$$

To evaluate the expressions for the sensitivity of pressure, p, with respect to conductivity, k, one may use the expressions presented in Wilson et al. (1986);

The sensitivity of the pressure in grid block m to the conductivity in grid block m is given by:

$$\frac{\partial P_m}{\partial k_m} = \frac{1}{2} \frac{(P_o - P_L)}{N} \left(\frac{N - 2m + 1}{N} \right) \frac{1}{k}$$

The sensitivity of the pressure in grid block m to the conductivity in grid block l, where l is to the left of grid block m, is given by:

$$\frac{\partial P_m}{\partial k_l} = \frac{(P_o - P_L)(N - m + 0.5) l}{N N k}$$

The sensitivity of a pressure in grid m to the conductivity in grid block r, where r is to the right of grid block m, is given by:

$$\frac{\partial P_m}{\partial k_r} = - \frac{(P_o - P_L)}{k} \frac{(m - 0.5)}{N^2}$$

Thus, to verify that GRASP-INV provides the correct sensitivities, the values of DJ/Dk for each of the five grid blocks is presented below:

For k_1 :

$$\begin{aligned} \frac{\partial P_1}{\partial k_1} &= 7.698888E11 & \frac{\partial P_4}{\partial k_1} &= 5.774166E11 \\ \frac{\partial P_2}{\partial k_1} &= 1.347305E12 & \frac{\partial P_5}{\partial k_1} &= 1.924722E11 \\ \therefore \frac{DJ}{Dk_1} &= 1.510521E17 \end{aligned}$$

For k_2 :

$$\begin{aligned} \frac{\partial P_1}{\partial k_2} &= -1.924722E11 & \frac{\partial P_4}{\partial k_2} &= 5.774166E11 \\ \frac{\partial P_2}{\partial k_2} &= 3.849444E11 & \frac{\partial P_5}{\partial k_2} &= 1.924722E11 \\ \therefore \frac{DJ}{Dk_2} &= -7.552609E16 \end{aligned}$$

For k_3 :

$$\begin{aligned} \frac{\partial P_1}{\partial k_3} &= -1.924722E11 & \frac{\partial P_4}{\partial k_3} &= 5.774166E11 \\ \frac{\partial P_2}{\partial k_3} &= -5.774166E11 & \frac{\partial P_5}{\partial k_3} &= 1.924722E11 \end{aligned}$$

$$\therefore DJ/Dk_3 = -1.510521E17$$

For k_4 :

$$\frac{\partial P_1}{\partial k_4} = -1.924722E11 \quad \frac{\partial P_4}{\partial k_4} = -3.849444E11$$

$$\frac{\partial P_2}{\partial k_4} = -5.774166E11 \quad \frac{\partial P_5}{\partial k_4} = 1.924722E11$$

$$\therefore \frac{DJ}{Dk_4} = -7.552609E16$$

For k_5 :

$$\frac{\partial P_1}{\partial k_5} = -1.924722E11 \quad \frac{\partial P_4}{\partial k_5} = -1.347305E12$$

$$\frac{\partial P_2}{\partial k_5} = -5.774166E11 \quad \frac{\partial P_5}{\partial k_5} = -7.698888E11$$

$$\therefore \frac{DJ}{Dk_5} = 1.510521E17$$

$$\frac{DJ}{DP_B} = 2 \sum w_i (p_i - p_{ob,i}) \frac{\partial p_i}{\partial p_B}$$

Consider the sensitivity of the same WLS performance measure, J, to boundary pressures. The derivative, or sensitivity, of J with respect to boundary pressures, P_B may be expressed by;

To evaluate the expressions for the sensitivity of p with respect to boundary pressures, one must use the expressions developed in Section 9.12.4 (presented again below). For a performance measure of pressure in grid block m, the sensitivity to the pressure at the boundary $x=0$ is given by;

$$\frac{\partial p_m}{\partial p_0} = \frac{(N - m + \frac{1}{2})}{N}$$

For a performance measure of pressure in grid block m, the sensitivity to the pressure at the boundary x=L is given by;

$$\frac{\partial p_m}{\partial p_L} = \frac{(m - \frac{1}{2})}{N}$$

Thus, for the boundary at x=0, the sensitivity of the WLS performance measure to the boundary pressure at x=0 is;

$$\frac{DJ}{DP_0} = 2 \cdot [78480 \frac{\partial P_1}{\partial P_0} + 39240 \frac{\partial P_2}{\partial P_0} + 0 - 39240 \frac{\partial P_4}{\partial P_0} - 78480 \frac{\partial P_5}{\partial P_0}]$$

Since,

$$\begin{aligned} \frac{\partial P_1}{\partial P_0} &= 0.9 & \frac{\partial P_4}{\partial P_0} &= 0.3 \\ \frac{\partial P_2}{\partial P_0} &= 0.7 & \frac{\partial P_5}{\partial P_0} &= 0.1 \end{aligned}$$

$$\therefore \frac{DJ}{DP_0} = 1.56960E5$$

The sensitivity of the WLS performance measure to the boundary pressure at the X=L boundary is;

$$\frac{DJ}{DP_L} = 2 \cdot [78480 \frac{\partial P_1}{\partial P_L} + 39240 \frac{\partial P_2}{\partial P_L} + 0 - 39240 \frac{\partial P_4}{\partial P_L} - 78480 \frac{\partial P_5}{\partial P_L}]$$

Since:

$$\begin{aligned} \frac{\partial P_1}{\partial P_L} &= 0.1 & \frac{\partial P_4}{\partial P_L} &= 0.7 \\ \frac{\partial P_2}{\partial P_L} &= 0.3 & \frac{\partial P_5}{\partial P_L} &= 0.9 \end{aligned}$$

$$\therefore \frac{DJ}{DP_L} = -1.56960E5$$



The GRASP-INV files need to set up and solve this example problem are listed in Figure C-5.

Figure C-5. Input Files for SWIFT/GRASP Example Problem 2
(Page 1 of 2)

(a) MAIN.inp

same as SWIFT/GRASP Example Problem 1

(b) PARAM.inp

same as SWIFT/GRASP Example Problem 1

(c) DXDYDZ.inp

same as SWIFT/GRASP Example Problem 1

(d) RAND.inp

same as SWIFT/GRASP Example Problem 1

(e) SWIFT.inp

same as SWIFT/GRASP Example Problem 1



Figure C-5. Input Files for SWIFT/GRASP Example Problem 2
(Page 2 of 2)

(f) GRASP.inp

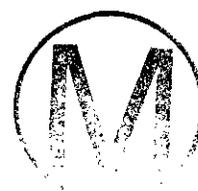
```
097B-21C-001D                                AD-1
* GRASP INPUT FOR ADJOINT SENSITIVITIES TO
ONE DIMENSIONAL FLOW PROBLEM WITH FIXED PRESSURES ON EACH END
QUALITY ASSURANCE TEST CASE FOR GRASP-INV
0                IOPT
2 1 1 -1 0 1.00 01                            AD-4
1 1 1 1 1 0.2
2 1 1 1 1 0.2
3 1 1 1 1 0.2
4 1 1 1 1 0.2
5 1 1 1 1 0.2

1 1 1 1                                        AD-6
1 5 1 1 1 1 1                                AD-7A

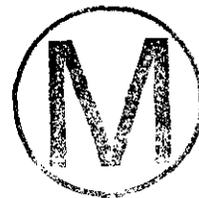
2 1 1 1                                        AD-6
1 1 1 1 1 1                                AD-7A
5 5 1 1 1 1                                AD-7A
0
0
```

(g) OBSGRASP.dat

```
1 1
1 1 1 1.4715E+06
2 1 1 1.4715E+06
3 1 1 1.4715E+06
4 1 1 1.4715E+06
5 1 1 1.4715E+06
0
0
```



Appendix D: SWIFT II Input Guide



REVISED DATA INPUT GUIDE* FOR SWIFT II

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February 1990

(*Adapted from NUREG/CR-3162 and SAND83-0242. Revisions correspond to code enhancements performed by INTERA, Inc. since code development in 1983.)

ABSTRACT

The data input guide is one of three documents that describe the SWIFT II computer code. The code SWIFT II is a fully transient three-dimensional finite-difference code that solves the coupled equations for transport in a fractured or non-fractured geologic media. The processes that SWIFT II considers are: fluid flow; heat transport; dominant species miscible displacement (brines); trace-specific miscible displacement (radionuclides), and matrix diffusion. The model features include fluid density as a function of pressure, temperature and salinity; fluid viscosity as a function of temperature and salinity; hydrodynamic dispersion as a tensor function of fluid viscosity; unconfined and confined aquifers; radioactive chains and decay; linear adsorption; anisotropy; heterogeneity; and choice of boundary conditions. This user's manual, which is an update of the original user's manual by Reeves et al. (1986a), should permit the analyst to use the code effectively by facilitating the preparation of input data. A second companion document, Reeves et al. (1986b), discusses the theory and implementation of the models employed by the SWIFT II code. A third document, Reeves et al. (1986c), provides illustrative problems for instructional purposes.

This report contains detailed descriptions of the input data along with an appendix of the input diagnostics. The use of auxiliary files, unit conversions, and program variable descriptors are also included in this document.



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PREFACE

This updated data input guide was prepared by INTERA Inc. to incorporate all changes to the model input as a consequence of model enhancements to SWIFT II since 1983. The original code documents for the computer code SWIFT II were published in Reeves et al. (1986a, b, c). The code enhancements have been developed and implemented in response to the varied applications of SWIFT II by INTERA staff. All enhancements have been designed, tested, and approved by either Dr. Mark Reeves who led the development team for SWIFT II, or by Dr. Suresh Pahwa who was a key member of the development teams for the predecessor codes SWIFT (Dillon et al., 1981) and SWIP (Intercomp, 1976).



1. INTRODUCTION

This report focuses upon the input data of the SWIFT II computer code and complements two other reports. Reeves et al. (1986b) gives the theory and formulation of the models employed by the SWIFT II code, whereas Reeves et al. (1986c) provides instruction problem sets, complete with listings of the data input and output. In addition, Finley and Reeves (1981) provide illustrative problems which, although designed for the SWIFT code, may be used for an initial orientation to SWIFT II. Verification and field comparison tests of the SWIFT code are presented by Ward et al. (1984). As a result of code enhancements, minor changes to the data sets presented in Finley and Reeves (1981) and Ward et al. (1984) are necessary in order to run them with the revised version of SWIFT II.

1.1 The SWIFT Models

The SWIFT model has been developed, maintained, and applied by Sandia National Laboratories. The Nuclear Regulatory Commission has sponsored this work under its high-level nuclear-waste program. The capability of SWIFT has been enlarged to include fractured media, a free-water surface, and additional boundary conditions. The new code is designated as SWIFT II. The two models, SWIFT and SWIFT II, are fully transient (with steady-state options), three-dimensional, finite-difference codes, which solve the coupled equations for flow and transport in geologic media. Both may be used for evaluation of repository site performance and repository design performance.

The processes considered are:

- Fluid flow,
- Heat transport,
- Brine migration, and
- Radionuclide-chain transport.



Flow, heat, and brine transport are coupled via fluid density, fluid viscosity, and porosity. Together they provide the velocity field on which the radionuclide transport depends.

The types of media considered are:

- Porous media (SWIFT and SWIFT II), and
- Fractured media (SWIFT II).

As discussed in Reeves et al. (1986b), the SWIFT II code permits local one-dimensional subsystems to be attached, as desired, to the grid blocks comprising the global system. The local units may be used either to characterize the second porosity of a fractured media or to extend the boundaries of the system in a relatively inexpensive manner.

1.2 Program Structure

The SWIFT II program consists of a main routine and about 70 supporting subroutines. A flow chart of the main routine is illustrated in Figure 1-1. The basic organization is focused upon the three global integration modules ITER, ITERS, and ITERC. Subroutine ITER solves the coupled partial differential equations for fluid flow, heat transport, and brine transport under transient condition; ITERS integrates the flow and brine equations under steady-state conditions; and ITERC solves the coupled partial differential equations for transport of radionuclide chain. All other routines provide support functions for the integration. The support function of interest in this report is data input.

1.3 Data Input Forms

Data input occurs in eight of the subroutines shown in Figure 1-1. Seven of the routines are positioned outside the recurrent time-step loop extending from READ2 to PRINT2. These routines read time-independent data. The other routine, READ2, is positioned inside the recurrent time-step loop. Therefore, it reads time-dependent data. Regarding the storage allocation function, the three routines SWIFT, READ0 and READ0D provide data that optimally partition the common-block arrays.

SWIFT reads information for the global-system arrays, READ0 for the radionuclide arrays, and READ0D for the local subsystem arrays. In regard to the dual-porosity function, routines READ0D and READ1D provide input pertaining specifically to the local porosity, whereas the other routines provide input pertaining to the global porosity. Finally, the data input cards divide naturally into groups depending upon the program unit in which they are read. The "shorthand" notation used by each group and a brief description of the function of each group is given in Table 1-1.

Conditions for Figure 1-1 are as follows:

1. Are plots desired for a previous run?
2. Is this a restart run?
3. Is dual porosity to be included?



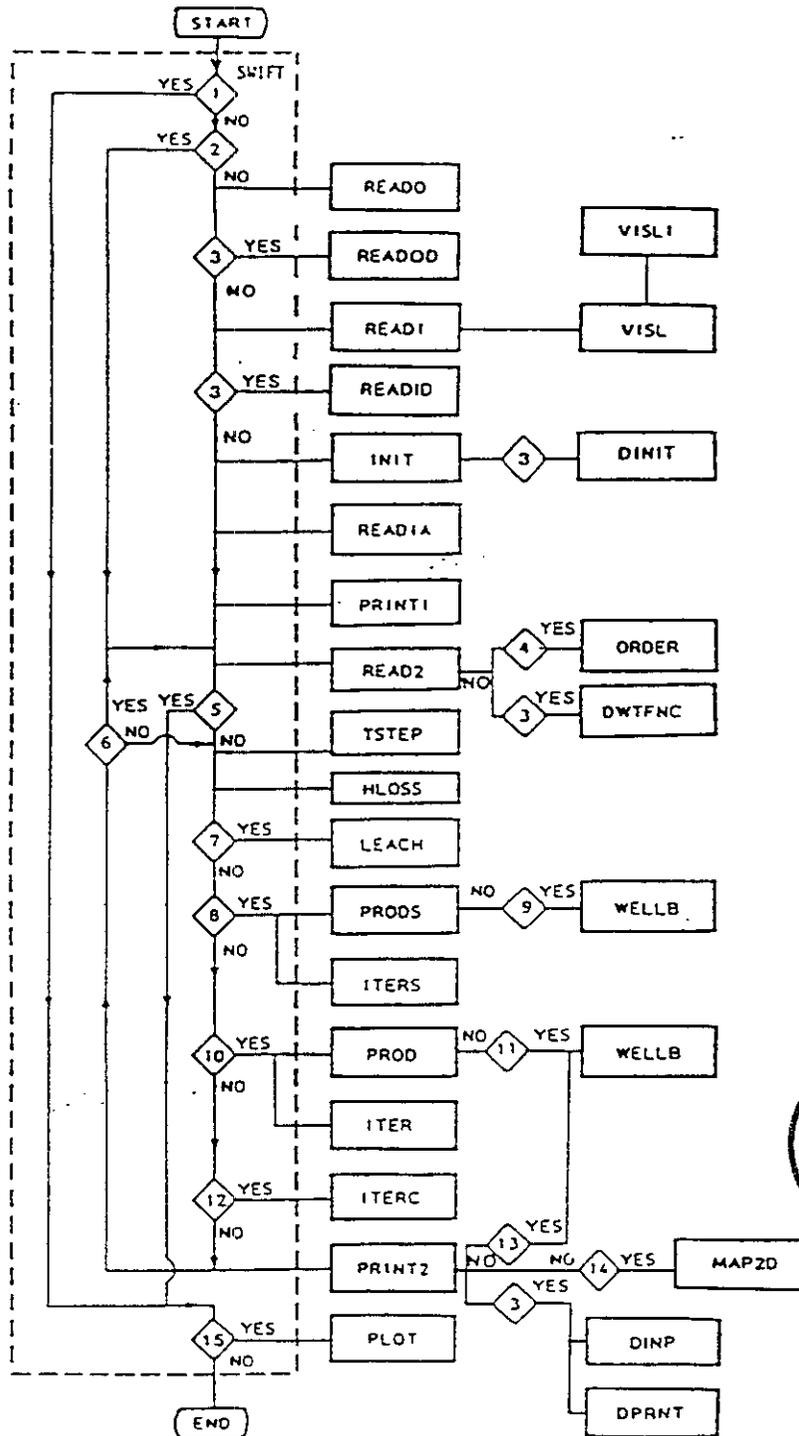
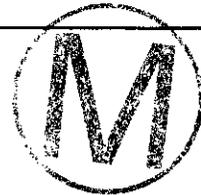


Figure 1-1. General Structure of SWIFT II.

4. Is the reduced-bandwidth direct method of solution used (multidimensional problems only)?
5. Is the run to be terminated at this time step?
6. Are the recurrent data to be read at this time step?
7. Is the waste-leach submodel employed?
8. Is the steady-state pressure solution sought?
9. Are steady-state wellbore calculations to be performed?
10. Is the transient pressure solution sought?
11. Are the transient wellbore calculations to be solved?
12. Are the radionuclide transport calculations to be performed?
13. In the transient wellbore calculations, are the well rates to be calculated semi-implicitly?
14. Are any two-dimensional contour maps desired?
15. Are any plots desired for this run?

Table 1-1

Data Input Groups



<u>Routine</u>	<u>Notation</u>	<u>Data Function</u>
SWIFT	M	General problem setup
READ0	R0	Radionuclide-chain information
READ0D	R0D	Dimensioning data of the local arrays
READ1	R1	Properties of the global system
READ1D	R1D	Properties of the local subsystems
INIT	I	Initialization data
READ1A	R1A	Specification of waste-leach submodel
NMONINP	N	Nuclide monitor block
READ2	R2	Time-dependent data
PRTPLT	P	Plotting Data

Input data is read from the file named SWIFTINP. Comments may be freely interspersed with the data in the data file. Any line with a "\$" (dollar sign) in column one is considered to be a comment and the entire line is ignored. By default, the input data is echoed to the beginning of the output file. The echo may be turned off by placing the following card at any point in the input file (columns 1-7):

\$NOECHO

Data following the above card will not be echoed to the output file. Data echoing may be turned back on with the following card (columns 1-5):

\$ECHO

Any number of \$ECHO/\$NOECHO cards may appear within an input file.

Chapters 2 through 9 define the data entered within each data group. Other useful items, such as auxiliary disc files, units of measurement, and a variable index are treated in a remaining chapter and in Appendices A, B, and C. However, for easy reference, the final appendix is reserved for the input-error diagnostics that are printed by the code.

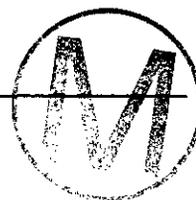


2.0 THE M, RO, AND ROD CARDS

2.1 The M Cards

The data supplied by the M cards provide general program control and storage allocation. These functions include:

- primary equations to be solved in the global systems,
- primary equations to be solved in the local subsystems,
- radionuclide solution control,
- restart control,
- printing and plotting control,
- number of grid blocks in the global system, and
- storage allocation for the coefficient matrix.



READ M-1 (20A4/20A4) Title.

LIST: TITLE

TITLE Any title up to 160 characters (80/card) in length may be used.

READ M-2 (10I5) Option Parameters.

LIST: NCALL, RSTRT, ISURF, IFREE, NPLP, NPLT, NPLC, IUNIT, LBIO, LBIOR

NCALL Control parameter for solving the primary partial differential equations within the global system. See Table 2-1.

RSTRT Control parameter for restarting the program.

-1- Map from restart. (Choose restart record on M-6.)

0 - A normal run starting from initial conditions.

> 0 - For a calculational restart, the number (ITIME) of the time step at which calculations are to resume.

Table 2-1

Global Solution Options for the Primary Equations*

<u>NCALL</u>	<u>Pressure</u>	<u>Temperature</u>	<u>Brine</u>
0	T	T	T
-2	T	T	
1	T		
2	T		T
3			
4	S		
5	S		S

 *"T" denotes a transient solution option.
 "S" denotes a steady-state solution option.

NOTE: For a calculational restart, a restart record from a previous run, corresponding to the specified time step, ITIME, must exist on the restart unit (filename SWIFTRSI). Parameter ITIME is printed each time a restart record is written. Furthermore, a restart record is written at the end of a recurrent data set providing RSTWR = 1 (READ R2-13).

ISURF Control parameter for the wellbore calculations.

- 0 - Rates and pressures will be specified at the reservoir formation level.
- 1 - Surface values will be specified. The wellbore model will calculate changes from the surface to the top of the completion zone.

IFREE Control parameter for the free-water surface.

- 0 - No free-water surface.
- 1 - Active free-water surface.

REFERENCE: The free-water surface option is described by Reeves et al. (1986b), Section 5.6.

- NPLP Control parameter for plotting pressures in the wells.
- 1 - Bottom-hole and, if wellbore calculations are performed, surface pressures are plotted. For an observation well (zero production rate) the bottom-hole pressure is the gridblock pressure.
 - 0 - No pressure plots are desired.
 - 1 - Pressure plots are desired for a previous run. Skip READ M-3 through R2-15 and proceed to READ P-2.
- NPLT Control parameter for plotting temperatures in the well.
- 1 - For an observation well the grid-block temperature is plotted. For an injection well the bottom-hole temperature is plotted if wellbore calculations are performed. For a production well the bottom-hole temperature is always plotted. In addition, the surface temperature is plotted if the wellbore calculations are performed.
 - 0 - No temperature plots are desired.
 - 1 - Temperature plots are desired for a previous run. Skip READ M-3 through READ R2-15 and proceed to READ P-2.
- NPLC Control parameter for plotting concentration in the well.
- 1 - The concentration in the well is plotted for both observation and production wells.
 - 0 - No concentration plots are desired.
 - 1 - Concentration plots are desired for a previous run. Skip READ M-3 through R2-15 and proceed to READ P-2.
- IUNIT Unit specification control.
- 0 - English Engineering System (lb, ft, d).
 - 1 - SI System (kg, m, s).
- LBIO Nuclide monitor block control.
- 0 - No action.



-
- 1 - Nuclide concentrations are written on file SWIFTNMD at each time step. (See Section 6.7.)

LIBOR Control parameter for specification of an internal nuclide discharge region.

- 0 - No action.

- 1 - Nuclide discharge rates across an internal region will be computed. This value will necessitate the input of N-2 cards which defines the internal discharge region(s).

NOTE: Skip to READ P-1 if NPLP, NPLT, or NPLC are negative.

NOTE: Skip to READ R2-1 if this is a restart run, i.e., if RSTRT > 0. Skip to READ M-6 if RSTRT < 0.

READ M-3-1 (14I5) Core Allocation and Control.

LIST: NX, NY, NZ, HTG, NCP, NRT, KOUT, PRT, NSMAX, NABLMX, NAQMAX, NRCHMX, METHOD, KOUTG

NX Number of grid cells in the x direction ($NX \geq 2$).

NY Number of grid cells in the y direction ($NY \geq 1$).

NZ Number of grid cells in the z direction ($NZ \geq 1$).

HTG Control parameter for input of reservoir description data.

- 1 - Homogeneous reservoir, Cartesian geometry.
- 2 - Heterogeneous reservoir, aquifer data entered on regional basis, Cartesian geometry.
- 3 - Cylindrical geometry. The reservoir may be heterogeneous in the vertical direction.

NCP Number of radioactive/trace components in the system.

NRT Number of global rock types.

NOTE: Freundlich coefficients, dispersivities, thermal conductivities, and a salt-dissolution coefficient are all functions of the global rock type. Rock types of all blocks are initialized to IRT

= 1. Changes of rock type to other values are entered in READ R1A-1.

KOUT Output control.

- 0 - All initialization output is activated.
- 1 - All initialization output except initial arrays (concentrations, pressures, etc.) is activated.
- 3 - No initialization output is activated. A value of KOUT = 3 can be used to omit printing of most initialization data.

PRT Output array orientation control.

- 1 - Print output arrays as areal layers (x-y). Block numbers in the x direction increase from left to right and in the y direction decrease down the computer page.
- +1 - Print output arrays as above except that y-direction block numbers increase down the computer page.
- 2 - Print output arrays as vertical x-z sections.

NSMAX Maximum number of radioactive/trace component sources.

NABLMX Maximum number of aquifer influence-function blocks. This data is used for dimensioning the influence-function arrays.

NAQMAX Control parameter defined by the number of times that the data input loop over cards R1-27 through R1-33. These cards specify the boundary conditions. This variable allows for the specification of multiple types of boundary conditions in one simulation. This variable allows for dynamic core storage allocation with respect to some boundary condition arrays.

NRCHMX Maximum number of surface recharge blocks.

NOTE: The following parameter, METHOD, is a flag that determines whether D4 ordering is to be performed in preparation for the direct-solution algorithm. Parameter METHOD may be changed in READ R2-2. Thus, for example, direct solution may be specified here, and L2SOR solution may be specified in READ R2-2. However, the converse is not true because in that case, the coefficient matrix would not be properly ordered.

METHOD Matrix solution technique.

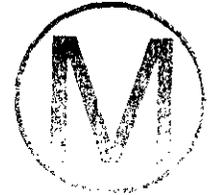
- 1 - Reduced-bandwidth direct solution with backward finite-difference approximation in time.

- 2 - Two-line successive-overrelaxation (L2SOR) solution with a backward finite-difference approximation in time.
- 1 - Reduced bandwidth direct solution with a centered finite-difference approximation in time.
- 2 - Two-line successive-overrelaxation solution (L2SOR) with a centered finite-difference approximation in time.

KOUTG Output control for the adjoint solver.

0 - All adjoint output is activated.

1 - No adjoint output is activated.



If KOUTG is equal to zero, binary files are written by SWIFT II that GRASP II will read. The names of these files are:

“SWGRSPTC” which contains the pressures, temperatures, and concentrations at each time step of the SWIFT simulation,

“SWGRSRCR” which contains a record of time-dependent input data,

“SWGRSXXX” which contains the last time step of the simulation, the time at which the restart record was written, the number of time-dependent input data sets,

“SWIFTRSO” which contains the entire blank common and the G, G2, G3, and IG arrays.

READ M-3-2 (815) Core Allocation and Control.

LIST: NTIME, KHEAT, NREP, KSLVD, NRTD, KOUTD, NTIMEMX, NBIOMX

NOTE: The following three parameters, NTIME, KHEAT, and NREP are leach model parameters.

NTIME Number of times for which concentrations of unleached radioactive components or heat-loading densities within the repository area are to be input.

0 - Repository submodels are not used.

- 1 - Only the waste-leaching submodel is invoked. Initial conditions are to be specified for the unleached concentrations and decay/production processes for such concentrations are to be calculated internally.
- >1 - Both waste-leaching and repository-heating may be considered, depending on the value KHEAT below, and interpolation tables of unleached concentrations versus time are to be used. Power-law interpolation is used in each case.

KHEAT Control parameter for heating loading in the repository blocks.

0 - No heat source.

1 - Heat source activated.

NREPB Number of repository blocks.

NOTE: The following three parameters, KSLVD, NRTD, and KOUTD pertain to the local subsystems, i.e., matrix.

KSLVD Local control parameter for solution of both primary and radionuclide equations for the matrix. See Table 2-2.

NRTD Number of local, i.e., matrix rock types.

KOUTD Output control for the local subsystems.

0 - All initialization output is activated.

1 - No initialization output is activated.

NTIMEMX The maximum number of time steps for the SWIFT II run. This parameter is needed only if the SWIFT II run is going to be used with GRASP II (i.e., KOUTG = 0 in READ M-3-1). If zero is input, then the default value is 400 time steps. If GRASP is not used (i.e., KOUTG = 1), then this variable is ignored. NTIMEMX may be > 400, but caution is required. The user must verify that their computer has sufficient memory to store the files generated by SWIFT II in the GRASP II option.



NBIOMX The maximum number of grid blocks used in the computation of nuclide discharge rates across biosphere (external) or internal regions. The code allows a default value of $(2 \cdot \text{NABLMX} + \text{NWMAX})$ where NABLMX is input in READ M-3-1 and NWMAX is presently hard dimensioned in the code at 100. If one enters zero, the default value will be used. If the specified number of grid blocks for nuclide discharge computations is in excess of the default, then the user will be required to enter NBIOMX.

Table 2-2

Local Solution Options for Both Primary
 and Radionuclide Equations*

<u>KSLVD</u>	<u>Primary Equations</u>	<u>Radionuclide Equations</u>
0		
1	T	
2		T
3	T	T



* Only the transient solution option T is available for the local subsystems.

NOTE: The mapping data consist of sets of input records, each of which contains READ's M-6, M-7, R2-14 - R2-15. If RSTRT = 0 (READ M-2) skip READ M-6 and M-7.

Enter as many of these sets as desired, following the last set with a blank card.

READ M-6 (15) Time-Step Number.

LIST: IMPT

IMPT The time-step number at which the maps (plots) are desired. A corresponding restart record must exist on the file SWIFTRSI, i.e.,

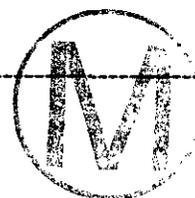
the control RSTWR = 1 (READ R2-13) must have been entered for a previous calculational run.

READ M-7 (I5) Mapping Control.

LIST: MAP

MAP The four-digit mapping-variable selector defined for READ R2-13.

Skip to Read R2-14.



2.2 The RO Cards

The RO cards are read by subroutine READ0. They input information pertaining to the radioactive components. This information defines each isotope in terms of its parents, branching ratios for each parent, isotopic mass, half-life, and distribution coefficient for each rock type.

NOTE: Data group RO should be entered only if RSTRT = 0 (READ M-2) and NCP > 0 (READ M-3-1). Otherwise, skip READ R0-1 and READ R0-2.

READ R0-1 (LIST 1: I3.2A4,4X,3I5.E10.0; LIST 2: 4(I5,5X,E10.0)).
Radioactive Component Information.

NOTE: Enter NCP (READ M-3-1, number of components) sets of R0-1 data.

LIST 1: MASS (I), (DI(J,I),J = 1,2), I, NP(I), LADJ(I), DEC(I)

- MASS Mass number of the isotope.
- DI Identification for radioactive component I.
- I Component number.

NP Number of parent components for I ($NP \leq NCP-1$).

NOTE: Lambda adjustment is used for relatively short half-lived radionuclides to permit the use of time steps $\Delta t > t$, the half-life. See Reeves et al. (1986b), Section 7.2.2, for the meaning and limitations of this procedure.

LADJ Lambda (rate-constant) adjustment index.

1 - Modify rate constant of the isotope I.

0 - Do not modify the rate constant.



DEC Half-life of component I in years. For stable components, enter zero.

NOTE: Skip the following list if $NP(I) = 0$ (LIST 1).

LIST 2: KP(J), AP(J), J = 1,NP

KP Parent component number.

AP Fraction of parent component KP that decays to the component I (LIST 1).

READ R0-2 (LIST 1: (7E10.0); LIST 2: (7E10.0); LIST 3: (7E10.0))
Rock-Dependent Parameters.

NOTE: Read one LIST-1 set for each rock type.

LIST 1: DIS1(I), I = 1,NCP

DIS1 Adsorption coefficient χ for a Freundlich isotherm, (ft³/lb) η or (m³/kg) η . Enter one value for each component for a total of NCP (READ M-3-1) values for each rock type. Start new rock-type values on a separate card.

NOTE: Read one LIST-2 set for each rock type.

LIST 2: DIS2(I), I = 1,NCP

DIS2 Adsorption exponent η for a Freundlich isotherm, dimensionless. Enter one value for each component for a total of NCP values for each rock type. Start new rock-type values on a separate card. The default value is $\eta = 1$.

NOTE: Read one LIST3 set for each rock type.

LIST 3: DMEFR(I), I = 1, NCP

DMEFR The molecular diffusion coefficient defined as a function of rock type (NRT) and nuclide (NCP). If zero is input as the diffusion coefficient, the code uses default values of 10^{-21} m²/s or 10^{-15} ft²/day depending upon the units used. Defined in units of m²/s or ft²/day. Start new rock type values on a separate card.

2.3 The ROD Cards

The ROD cards are read by subroutine READ0D. They provide both control and storage-allocation data for the local system.

NOTE: If KSLVD = 0 (READ M-3-2), skip all ROD input.

READ ROD-1 (15) Control of Convection/Dispersion.

LIST: KCNVD

KCNVD Convection/dispersion control for the local subsystems, i.e., matrix.

- 0 - No convection or dispersion for either primary equations or radionuclide equations. Also, for the latter, a constant fluid density and a constant porosity are assumed. For nuclide only molecular diffusion and decay processes are solved.
 - 1 - Convection and dispersion effects are included, and a variable fluid density and a variable porosity are assumed throughout.
-

READ ROD-2 (1415) Number of Local Grid Blocks.

LIST: NSD (IR), IR = 1, NRTD

NSD Number of local, i.e., matrix grid blocks as a function of local rock type.

READ ROD-3 (8I5) Matrix Rock Types.

LIST: I1A, I1B, J1A, J1B, K1A, K1B, IR, IFD

- | | |
|---------|---|
| I1A,I1B | Lower and upper limits, inclusive, on the I index of the region having rock type IR. |
| J1A,J1B | (Similar definition for J index). |
| K1A,K1B | (Similar definition for K index). |
| IR | Local matrix rock type. |
| IFD | Position and orientation control for the local subsystems. |
| 0 - | Local subsystems positioned interior to global block (dual-porosity option). |
| >0 - | Local subsystems positioned exterior to the global block on both sides (discrete fracture and extended boundary-condition options). |
| <0 - | Local subsystems positioned exterior to the global block but on only one side (extended boundary-condition option). |
| 1,-1 - | Local subsystems oriented parallel to the x axis. |
| 2,-2 - | Parallel to the y axis. |
| 3,-3 - | Parallel to the z axis. |

NOTE: Follow the last card of this data group with a blank card.



3. THE R1 CARDS

The information supplied by the R1 cards consists of time-independent data, all of which is read within subroutine READ1. This data specifies some of the physical properties of the global system including its geometry, boundary conditions, and initial conditions on pressure and temperature. The I data of Chapter 5 then refines the pressure initialization for the natural-flow field and provides initialization of the concentrations. The R1 cards also contain a partial statement of the wellbore source/sink parameters and a definition of the discretization of the global system. The general procedure for input of the spatially dependent parameters is to specify large homogeneous regions followed by modification cards to insert inhomogeneities.

3.1 Physical Properties

READ RI-1 (6E10.0) Physical Constants for Fluid and Rock.

LIST: CW, CR, CTW, CPW, CPR, GRAV

CW	Compressibility of the reservoir fluid, psi^{-1} (Pa^{-1}).
CR	Compressibility of the pore structure, psi^{-1} (Pa^{-1}).
CTW	Coefficient of thermal expansion of the reservoir fluid, $^{\circ}\text{F}^{-1}$ ($^{\circ}\text{C}^{-1}$).
CPW	Fluid heat capacity, $\text{Btu/lb-}^{\circ}\text{F}$ ($\text{J/kg-}^{\circ}\text{C}$).
CPR	Rock heat capacity per unit volume of solid, $\text{Btu/ft}^3\text{-}^{\circ}\text{F}$ ($\text{J/m}^3\text{-}^{\circ}\text{C}$).
GRAV	Gravitational acceleration constant, ft/s^2 (m/s^2). If this field is entered as 0.0 or left blank, a default value of 32.174 ft/s^2 (9.870 m/s^2) will be used.



READ R1-2 (7E10.0) Physical Constants for Fluid and Rock.

LIST: UKTX, UKTY, UKTZ, CONV, ALPHL, ALPHT, DMEFF

UKTX	Thermal conductivity of the fluid-saturated porous medium in the x direction, Btu/ft-d-°F (J/m-s-°C) (see CONV).
UKTY	Thermal conductivity of the porous medium in the y direction.
UKTZ	Thermal conductivity of the porous medium in the z direction.
CONV	Conversion factor for the thermal conductivities. The entered values of the thermal conductivities are multiplied by CONV to obtain units of Btu/ft-d-°F (J/m-s-°C). If entered as zero, thermal conductivities should be read in Btu/ft-d-°F (J/m-s-°C).
ALPHL	Longitudinal dispersivity factor, ft (m).
ALPHT	Transverse dispersivity factor, ft (m).
DMEFF	Global brine molecular diffusivity in the porous medium, includes porosity and tortuosity effects (porosity x fluid molecular diffusivity x tortuosity), ft ² /d (m ² /s). If zero is entered, the default value is 10 ⁻¹⁵ ft ² /day (10 ⁻²¹ m ² /s).

NOTE: Skip the following read if NRT = 1 (READ M-3-1) and proceed to READ R1-3. Otherwise enter sequentially one group (LIST1 and LIST2) for each rock type.

NOTE: If any of the values on the following LIST, or LIST2 are entered as zero, the default will be the corresponding value entered in READ R1-1 or READ R1-2 above.

READ R1-2.5 (LIST 1: 4E10.0; LIST 2: 4E10.0) Rock-Dependent Properties.

LIST 1: UTCX(I), UTCY(I), UTCZ(I), CONV

UTCX	Thermal conductivity of the fluid-saturated media in the x direction for rock type I, Btu/ft-d-°F (J/m-s-°C).
UTCY	Thermal conductivity in the y direction.
UTCZ	Thermal conductivity in the z direction.

CONV Conversion factor for thermal conductivities to obtain units of
Btu/ft-d-°F (J/m-s-°C).

LIST 2: ALPHAL(I), ALPHAT(I), RCMPB(I), DMEF(I)

ALPHAL Longitudinal dispersivity for rock type I, ft (m).

ALPHAT Transverse dispersivity for rock type I, ft (m).

RCMPB Rock compressibility for rock type I, psi^{-1} (Pa^{-1})

DMEF Global brine molecular diffusion coefficient defined as a function
of rock type I.

NOTE: The R1-2.5 cards are entered in NRT sets.

NOTE: The fluid densities are entered here for brine concentrations $\hat{C} = 0$ (natural aquifer fluid)
and concentration $\hat{C} = 1$ (contaminated fluid). Both densities must be entered at the same
reference temperature and pressure.

READ R1-3 (5E10.0) Reference Densities.

REFERENCE: Reeves et al. (1986b), Section 3.1.



LIST: BROCK, PBWR, TBWR, BWRN, BWRI

BROCK Rock density (solid particle), lb/ft^3 (kg/m^3).

PBWR Reference pressure at which the densities are to be entered, psi (Pa).

TBWR Reference temperature at which the densities are to be entered, °F (°C).

BWRN Density of the natural reservoir fluid ($C = 0$) at PBWR and TBWR, lb/ft^3
(kg/m^3).

BWRI Density of the contaminated fluid ($C = 1$) at PBWR and TBWR, lb/ft^3
(kg/m^3).

3.2 Wellbore Data

NOTE: If ISURF = 0 (READ M-2), omit READ R1-4 and READ R1-5 and proceed to READ R1-6.

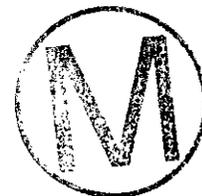
REFERENCE: Reeves et al. (1986b), Section 4.2.

READ R1-4 (I5) Output Control.

LIST: NOUT

NOUT Output control parameter for the wellbore calculations.

- 0 - No output is activated.
- 1 - An iteration summary, including the number of outer iterations, the flow rate and the bottom-hole pressure, is printed for each well.
- 2 - The well pressure and temperature, at the surface for an injection well and at the bottom-hole for a production well, and the flow rate are printed every time the wellbore subroutine, WELLB, is called.
- 3 - The pressure and temperature in the well are printed for each vertical increment (see DELPW in READ R1-5).



READ R1-5 (3E10.0) Wellbore Constants.

LIST: PBASE, DELPW, TDIS

PBASE Atmospheric or reference pressure at the wellhead psi (Pa). This is used to convert absolute pressure to gauge pressure.

DELPW Incremental value of pressure over which wellbore calculations are to be performed, psi (Pa).

NOTE: The pressure and temperature calculations in the wellbore proceed in increments. The length increments corresponding to DELPW are calculated, and the temperature change over each increment is simulated.

TDIS Thermal diffusivity of the rock surrounding the wellbore, ft²/d (m²/s).

3.3 Viscosity and Temperature Initialization

The input data described in this section define both the viscosity function and the initial-temperature definition. The latter is self evident since it consists of a simple interpolation table. The former, however, requires some explanation. Section 3.2 of Reeves et al. (1986b) provides a detailed description of the data necessary to generate the viscosity function. Thus, only a summary is given here. Figure 3-1 presents a useful visual aid. The minimum data necessary to specify the function shown there consists of the two points $VISRR = \mu(\hat{C} = 0, T = TRR)$ and $VISIR = \mu(\hat{C} = 1, T = TIR)$ (READ R1-7). The remainder of the function is then generated from the generalized curve of Lewis and Squires (for the dependence on temperature) and from interpolation (for the dependence on brine concentration). As discussed in the above reference, the generalized curves may introduce as much as an 18 percent error in the temperature dependence of the viscosity function. It is therefore desirable to supply additional data whenever possible. Temperature data for $\hat{C} = 0$ may be included by using arrays TR(I) and VISR(I) (READ R1-9) with control parameter NTVR. Temperature data for $\hat{C} = 1$ may be included by using arrays TI(I) and VISI(I) (READ R1-10) with control parameter NTVI. Concentration data for $T = TRR$ may be included by using arrays SC(I) and VCC(I) (READ R1-8) with control parameter NCV. In order to define a constant value of viscosity for $\hat{C} = 0$ (or $\hat{C} = 1$), it is necessary to specify the same value for two different temperatures. For example, a constant function $\mu(\hat{C} = 0, T) = 1$ cp is determined by specifying $NTVR = 1$ and $VISRR = VISR = 1.0$ with $TRR \neq TR$.

NOTE: The numbers called for immediately below (except for NDT) refer to the viscosity values to be entered in addition to the reference viscosities.

READ R1-6 (4I5) Control Parameters.

LIST: NCV, NTVR, NTVI, NDT

NCV Number of entries in the concentration-viscosity table. This table is for viscosities other than the reference values entered for $\hat{C} = 0$ and

$\hat{C} = 1$. This index refers to data points along curve c in Figure 3-1, exclusive of the end points. If only the two end-point, pure-fluid viscosities are available, enter zero and read in the viscosities of the pure fluids as reference viscosities.

NTVR Number of entries in the temperature-viscosity table for $C = 0$. This index refers to data points on curve r of Figure 3-1.

NTVI Number of entries in the temperature-viscosity table for $C = 1$. This index refers to data points on curve I of Figure 3-1.

NTD Number of entries in the depth-versus temperature table.

READ R1-7 (4E10.0) Reference Viscosity Values.

LIST: TRR, VISRR, TIR, VISIR



TRR Reference temperature for the resident-fluid viscosity, °F (°C).

VISRR Viscosity of the resident fluid at the reference temperature, TRR, cp (Pa-s).

TIR Reference temperature for the contaminated-fluid viscosity, °F (°C).

VISIR Viscosity of the contaminated fluid at TIR, cp (Pa-s).

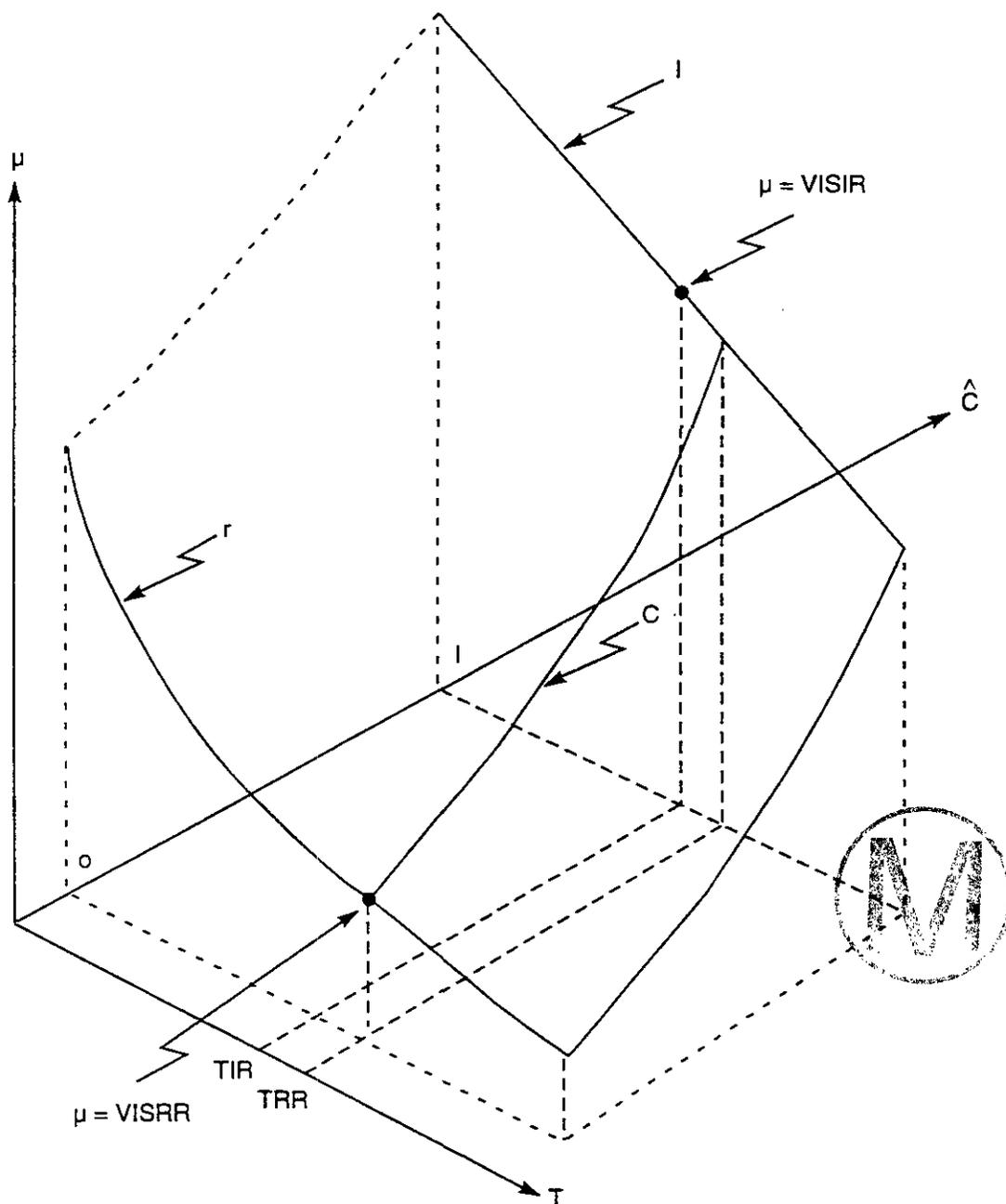
NOTE: If $NCV = 0$ (READ R1-6), omit READ R1-8.

READ R1-8 (7F10.0) Concentration-Dependent Viscosity Values.

LIST: SC(I), VCC(I), I=1..NCV

SC Concentration, mass fraction.

VCC Viscosity of fluid mixture at concentration SC and temperature TRR, cp (Pa-s).



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Figure 3-1. Fluid Viscosity as a Function of Temperature and Concentration.

NOTE: If NTVR = 0 (READ R1-6), skip READ R1-9 and proceed to READ R1-10.

READ R1-9 (7F10.0) Temperature-Dependent viscosity Values.

LIST: TR(I), VISR(I), I = 1, NTVR

TR Temperature, °F (°C).

VISR Viscosity of the resident fluid at the temperature TR, cp (Pa-s). Do not re-enter the reference viscosity at TRR (READ R1-7).

NOTE: If NTVI = 0 (READ R1-6), skip READ R1-10 and proceed to READ R1-11.

READ R1-10 (7F10.0) Temperature-Dependent Viscosity Values.

LIST: TI(I), VISI(I), I = 1, NTVI

TI Temperature, °F (°C).

VISI Viscosity of the contaminated fluid at the temperature TI, cp (Pa-s). Do not re-enter the reference viscosity at TIR (READ R1-7).

NOTE: Initial temperatures in the aquifer and the over/underburden blocks are to be entered here. The initial temperature is assumed to be a function of depth only.

REFERENCE: Reeves et al. (1986b), Section 5.1.2

READ R1-11 (2F10.0) Initial Temperatures.

LIST: ZT(I), TD(I), I = 1, NTD

ZT Depth relative to reference plane, ft (m).

TD Temperature, °F (°C).



3.4 Over/Underburden Parameters

NOTE: As described in Reeves et al. (1986b), Section 5.4, heat transport between the reservoir and the overburden and/or underburden is accounted for in the SWIFT code by means of a fully coupled, completely implicit heat-transport calculation within these neighboring regions. Boundary temperatures for the top of the overburden and the bottom of the underburden are obtained from the temperature versus depth table (READ R1-11). Initial conditions are also obtained from this table. Except for the assumptions of no lateral transport and no fluid flow within these external zones, the calculations there are completely general. The data defined in READ R1-12 through READ R1-15 gives the information necessary to discretize the over/underburden region and to define the heat-transport parameters therein.

REFERENCE: Reeves et al. (1986b), Section 5.4.

NOTE: If $NZ = 1$, the underburden heat loss is assumed to be equal to the overburden heat loss, and only the parameters of the overburden are utilized.

READ R1-12 (2I5) Number of Over/Underburden Grid Blocks.

LIST: NZOB, NZUB

- | | |
|------|---|
| NZOB | Number of overburden blocks. If $NZOB \leq 2$, overburden heat-loss calculations are <u>not</u> performed. |
| NZUB | Number of underburden blocks. If $NZUB \leq 2$, the underburden heat-loss calculations are <u>not</u> performed. |
-

NOTE: Skip this READ if both $NZOB = 0$ and $NZUB = 0$.

READ R1-13 (4E10.0) Physical Parameters.

LIST: KOB, CPOB, KUB, CPUB

- | | |
|------------|---|
| KOB, KUB | Vertical thermal conductivities of the overburden and the underburden blocks, respectively, $\text{Btu/ft-d-}^\circ\text{F}$ ($\text{J/m-s-}^\circ\text{C}$). |
| CPOB, CPUB | Heat capacities per unit volume of the overburden and underburden blocks, respectively, $\text{Btu/ft}^3\text{-d-}^\circ\text{F}$ ($\text{J/m}^3\text{-}^\circ\text{C}$). |

NOTE: Skip the following READ if NZOB = 0.

READ R1-14 (7E10.0) Discretization of the Overburden.

LIST: DZOB(K), K = 1,NZOB

DZOB Thickness of each overburden block, ft (m). The first overburden block is at the upper edge of the reservoir. The overburden block numbers increase moving away from the reservoir.

NOTE: Skip the following READ if NZUB = 0.

READ R1-15 (7E10.0) Discretization of the Underburden.

LIST: DZUB(K), K = 1,NZUB

DZUB Thickness of each underburden block, ft (m). The block numbers increase moving away from the reservoir.

3.5 Reference Data and Pressure Initialization

REFERENCE: Reeves et al. (1986b), Section 5.1.1.

READ R1-16 (4E10.0)

LIST: TO, PINIT, HINIT, HDATUM

TO Reference temperature for both hydraulic conductivities and densities, °F (°C).

PINIT Initial pressure at the depth HINIT, psi (Pa). Also used as the reference pressure PO = PINIT. See Figure 3-2.

NOTE: Permeabilities are determined assuming that the input conductivities are referenced to temperature TO. Densities are related internally to this temperature and to the pressure PINIT in that only changes from the density at TO and PO = PINIT (and C = 0) are calculated.

HINIT An arbitrary depth for setting up initial conditions measured relative to the reference plane, ft (m). HINIT can be any depth within the reservoir. HINIT is used only to set up initial pressures in the reservoir. See Figure 3-2.

NOTE: Quantities HINIT, HDATUM, DEPTH (READ R1-20) and UH (READ R1-21) are all measured from the reference plane shown in Figure 3-2.

HDATUM Datum depth measured relative to the reference plane, ft (m). See Figure 3-2.

NOTE: Quantity HDATUM is used only for the printing of the R1-16 dynamic pressures (p_{gh/g_c}) in that the depth h is measured from the datum HDATUM.

3.6 Discretization for a Cartesian Geometry

NOTE: If HTG = 3 (READ M-3-1), skip to READ R1-22.

READ R1-17 (List Directed)* **Grid-Block Definition.**

LIST: DELX(I), I = 1,NX

DELX Length of each row of blocks in the x direction, ft (m).

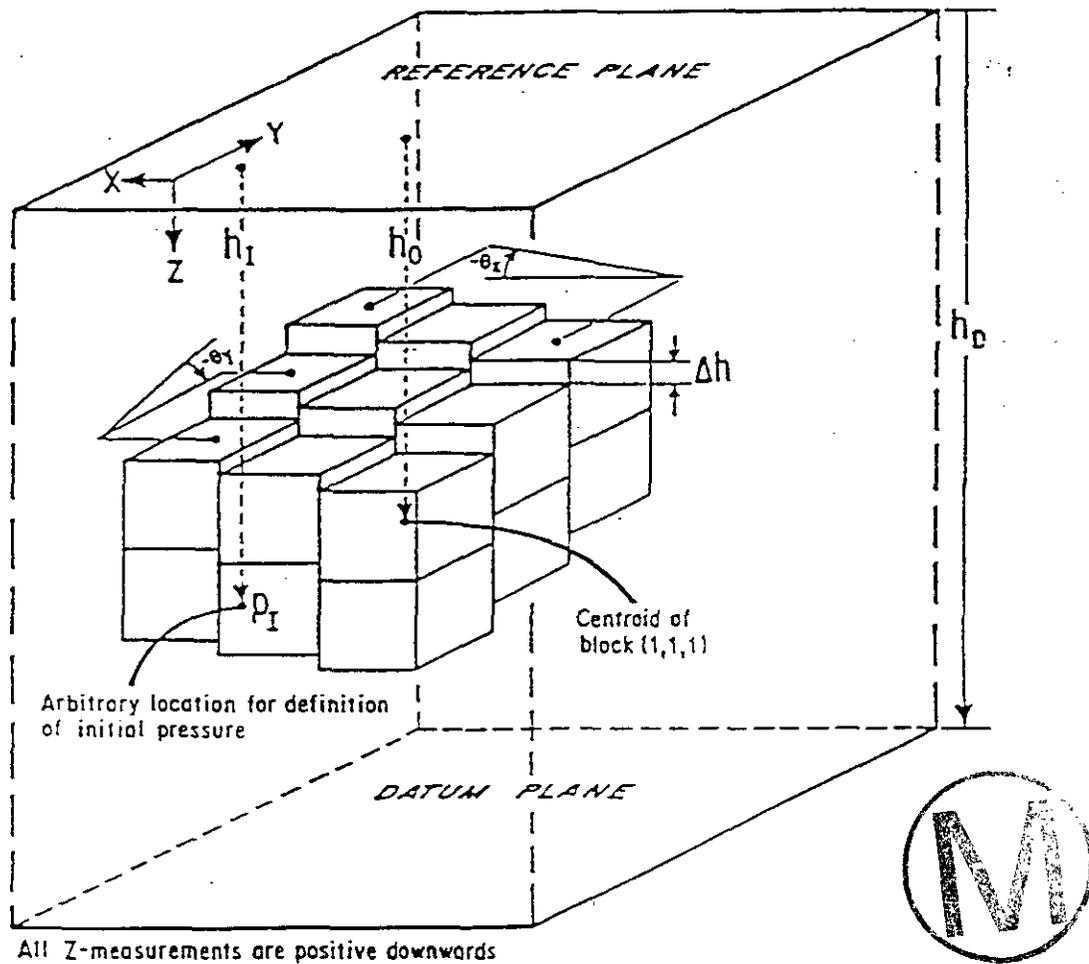
READ R1-18 (List Directed)* **Grid-Block Definition.**

LIST: DELY(J), J = 1,NY

DELY Length of each row of blocks in the y direction, ft (m).

READ R1-19 (List Directed)* **Grid-Block Definition.**

LIST: DELZ(K), K = 1,NZ



Here $p_I = \text{PINIT}$, $h_I = \text{HINIT}$, $h_D = \text{HDATUM}$, $\sin \theta_x = \text{SINX}$,
 $\sin \theta_y = \text{SINY}$, $h_0 = \text{DEPTH}$, and $\Delta h = \text{HADD}$.

Figure 3-2. Specification of Geometry and Initial Pressure in a Cartesian System.

DELZ Thickness of each vertical layer, starting with the top-most, ft (m).

***List Directed Read:**

Input data consists of a string of values separated by one or more blanks, a comma and terminated by a slash. To repeat a value, an integer constant is followed by an asterisk and the constant to be repeated. Example:

2*104.8, 3*96.3 is equivalent to 104.8 104.8 96.3 96.3 96.3

Marginal identifiers are illegal for records using a list directed format.

3.7 Reservoir Data for a Cartesian Geometry

NOTE: The following data are read only if HTG = 1 or 2 (READ M-3-1), and by themselves describe a homogeneous reservoir. Heterogeneity may be introduced by using READ R1-21 and/or regional modifications in READ R1-26, in addition to READ R1-20.

READ R1-20 (7E10.0) Homogeneous Reservoir Information.

LIST: KX, KY, KZ, PHI, SINX, SINY, DEPTH

- | | |
|------|---|
| KX | Hydraulic conductivity in x direction, ft/d (m/s). |
| KY | Hydraulic conductivity in y direction, ft/d (m/s). |
| KZ | Hydraulic conductivity in z direction, ft/d (m/s). |
| PHI | Porosity (fraction). |
| SINX | Sine of the reservoir dip angle along the x-axis (positive down). See Figure 3-2. |
| SINY | Sine of the reservoir dip angle along the y-axis (positive down). See Figure 3-2. |



DEPTH Depth to the center of grid block (1,1,1) measured from the reference plane. See Figure 3-2.

NOTE: The following data are read only if HTG = 2 (READ M-3-1). Enter as many sets of data as required.

READ R1-21 (List 1: 615, List 2: 7E10.0) **Heterogeneous Reservoir Information.**

LIST: 1: I1, I1, J1, J2, K1, K2

I1, I2 Lower and upper limits inclusive, on the I index of the region to be described.

J1, J2 (Similar definition for the J index).

K1, K2 (Similar definition for the K index).

LIST 2: KX, KY, KZ, PHI, UH, UTH, UCPR

KX x-direction hydraulic conductivity, ft/d (m/s).

KY y-direction hydraulic conductivity, ft/d (m/s).

KZ z-direction hydraulic conductivity, ft/d (m/s).

PHI Porosity, fraction.

UH Depth in ft (m) measured positive downward from reference plane to center of the cell. See Figure 3-2. If entered as zero, the depth is unaltered from the value calculated for a homogeneous aquifer.

UTH Grid-block thickness in the vertical direction, ft (m). If the layer thickness is equal to DELZ(K) (READ R1-19), UTH may be entered as zero.

UCPR Heat capacity of the rock, Btu/ft³-°F (J/m³-°C). If the rock heat capacity is equal to CPR (READ R1-1), UCPR may be entered as zero.

NOTE: Follow the last line of data of this group with a blank card.

3.8 Reservoir Data for a Cylindrical Geometry

The following three records are read for a radial geometry (HTG=3) with a well located at the center of the system. The user has the option of generating the grid block centers using an equal $\Delta \log(r)$ basis, (i.e., r_i / r_{i-1} is constant) or entering the radius of each grid-block center.

NOTE Skip to READ R1-26 if HTG \neq 3.

READ R1-22 (4E10.0) Geometrical Data.

REFERENCE: Reeves et al. (1986b), Section 7.1.2.

LIST: RWW, R1, RE, DEPTH

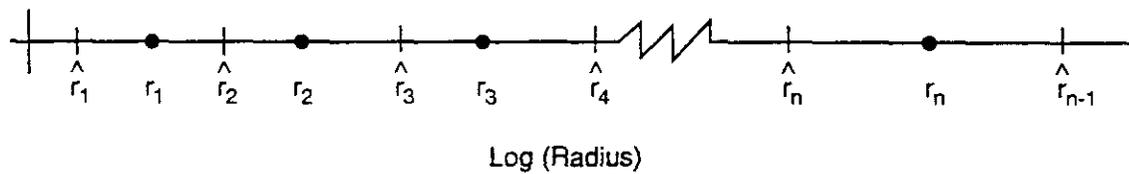
- 
- RWW Well radius, ft (m). See Figure 3-3.
- RI For mesh generation on an equal $\Delta \log(r)$ basis, $R1 > 0$ represents the center of the first grid block. See Figure 3-3. For direct specification, $R1 = 0$ should be used.
- RE External radius of the reservoir, ft (m). See Figure 3-3.
- DEPTH Depth from the reference plane to the center of the first layer of blocks, ft (m). See Figure 3-2.
-

READ R1-23 (5E10.0) Reservoir Parameters.

LIST: DELZ(K), KYY(K), KZZ(K), POROS(K), CPR1(K), K = 1,NZ

NOTE: One record should be entered for each vertical layer.

- DELZ Layer thickness in the vertical direction, ft (m).
- KYY Horizontal hydraulic conductivity, ft/d (m/s).



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Figure 3-3. Schematic of the Radial Mesh Including Grid-Block Centers, r_i , and Grid-Block Boundaries, \hat{r}_i .

KZZ	Vertical hydraulic conductivity, ft/d (m/s).
POROS	Porosity, fraction.
CPR1	Rock heat capacity, Btu/ft ³ -°F (J/m ³ -°C). If the rock heat capacity in the layer is equal to CPR (READ R1-1), CPRI may be entered as zero.

NOTE: Skip to READ R1-26 if R1 ≠ 0 (READ R1-22).

READ R1-24 (7E10.0) Radial Grid-Block Centers.

LIST: RR(1), I = 1,NX

RR	Radial grid-block centers, ft (m). See Figure 3-3.
----	--

3.9 Reservoir Description Modifications

NOTE: Read as many sets of these data as necessary to describe all the reservoir description modifications that are desired. Follow the last set with a blank card, which the program recognizes as the end of this data set. Even if no regional modifications are desired, the blank card must be included.

READ R1-26 (LIST 1: 615; LIST 2: 7E10.0; LIST 3: 3E10.0)

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2	Lower and upper limits, inclusive, on the I index of the region to be modified.
J1, J2	(Similar definition for J index).
K1, K2	(Similar definition for K index).

NOTE: The x transmissibility indexed as (I, J, K) refers to the transmissibility at the boundary separating grid blocks (I-1, J, K) and (I, J, K). Similarly the y transmissibility indexed as (I, J, K)

refers to the transmissibility at the boundary separating grid blocks (I,J-1,K) and (I,J,K).

LIST 2: FTX, FTY, FTZ, FPV, FPHI, HADD, THADD

FTX If positive or zero, this is the factor by which the x-direction transmissibilities within the defined region are to be multiplied. If negative, the absolute value of FTX will be used for the x-direction transmissibilities within the region to be modified.

FTY This has the same function of FTX, but applies to the y-direction transmissibilities.

FTZ This has the same function of FTX, but applies to the vertical transmissibilities.

FPV This has the same function of FTX, but applies to pore volumes.

FPHI If positive, this is the factor by which the values of porosity used in the heat storage calculation within the defined region are to be multiplied. If negative, the absolute value of FPHI will be used. A zero or unit value has no effect.

HADD This is an increment that will be added to the depths within the defined region, ft (m). A positive value moves the designated cells deeper, and a negative value brings them closer to the surface. See Figure 3-2.

THADD This is an increment that will be added to the thickness values within the defined region, ft (m). A positive value makes the cell thicker, and a negative value makes it thinner. Pore volumes are implicitly modified with thickness changes.

LIST 3: FTUX, FTUY, FTUZ

FTUX If positive, this is the factor by which the x direction Darcy velocities within the region defined are to be multiplied. The modified velocities are used in the heat and solute dispersion coefficients. A zero or unit value has no effect.

FTUY This has the same function of FTUX, but applies to the y-direction Darcy velocities.

FTUZ This has the same function of FTUX, but applies to the z-direction Darcy velocities.

NOTE: Follow the last set of data by a blank card.

NOTE: In regions in which more than one modification has been made to a parameter, the order of the modifications has no effect, and the final net adjustment is simply the algebraic sum of all the additive factors or the product of all the multiplicative factors that apply to the region. The program will accept a zero modifier as a valid parameter. Therefore, if no changes are desired to data that are affected by multiplicative factors FTX, FTY, FTZ, or FPV, read the corresponding factors as 1.0, not zero. If no changes are desired for FPHI, FTUX, FTUY, or FTUZ, read the factor as 1.0 or zero. Zero additive factors (HADD and THADD) result in no changes to the depth and thickness values.

3.10 Aquifer-Influence Functions and Boundary Conditions

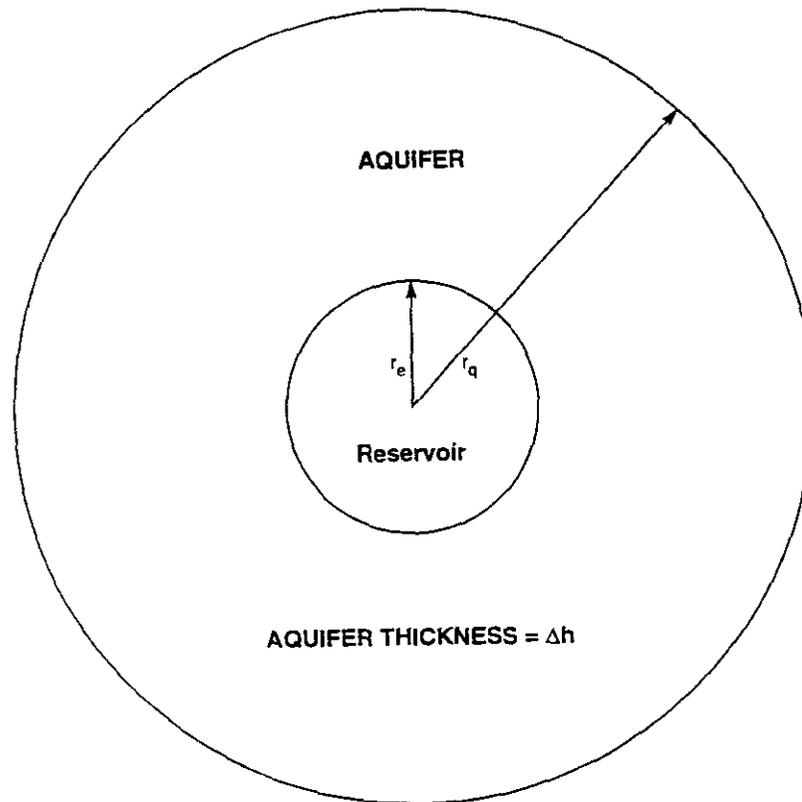


Aquifer-influence functions specify the effects of an aquifer upon the reservoir via an analytic submodel of the aquifer. Conceptually reservoir and aquifer are related as shown by Figure 3-4. For the SWIFT model three different aquifer submodels are available. These submodels are implicitly coupled to the reservoir via the influence functions. In general, both pressure and flow vary as a function of time. The application of such functions means that the aquifer itself need not be modeled as a part of the grid system. Boundary conditions, however, are more simple. They derive from specified constants for pressure, temperature, and concentration. Hence, they do not implicitly vary with the internal condition of the reservoir as do the aquifer influence functions.

REFERENCE: Reeves et al. (1986b), Sections 5.2 and 5.3.

NOTE: If no aquifer-influence functions or boundary conditions are to be specified (no flow across aquifer boundaries), insert a blank card and proceed to READ R1D-1.

SWIFT II has the capability of applying multiple types of boundary conditions to a single finite-difference grid. This is made possible by looping over the cards that specify boundary conditions (Cards R1-27 through R1-33). The last set of R1-27 through R1-33 cards must be followed by a blank card.



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Figure 3-4. Geometrical Characterization of the Aquifer.

READ R1-27 (2I5) Control Parameters.



LIST: IAQ, PRTAB

- IAQ** Control parameter for selecting the type of boundary control.
- 0 - No aquifer-influence or boundary-condition blocks are to be used. Skip to READ RID-1.
 - 1 - A pot-aquifer representation will be used. The aquifer is assumed to be at steady-state with a no-flow outer boundary.
 - 2 - A steady-state aquifer representation will be used. The aquifer is assumed to be at steady-state with a constant pressure at the outer aquifer boundary.
 - 3 - An unsteady-state aquifer representation will be implemented using the Carter-Tracy approximation.
 - 4 - Constant pressure and brine-component boundary conditions will be used. Boundary conditions for heat transport may be either constant-temperature or radiative.
- PRTAB** Print control key for the aquifer-influx coefficient.
- 0 - No printing of aquifer-influence coefficients will be activated.
 - 1 - The locations and values of the aquifer influence coefficients will be printed.

3.10.1 Steady-State Aquifer-Influence Functions and Boundary Conditions

This data group consists of two cards or any number of sets of two cards, each set defining a rectangular region and the value of VAB to be assigned that region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set read being assigned to the overlapping subregion. In addition, SWIFT II can compute nuclide discharge rates and total nuclides released at a specified boundary. The integration is performed both spatially and temporally. For definition of the boundary, there are two available options.

- (a) The user may consider the aquifer influence blocks or the pumping wells as regions for the computation of nuclide discharge rates and cumulative release. The boundaries are referred to as biosphere discharge regions. Biosphere discharge regions are specified in Card R1-28 and are discussed below.
- (b) The user can define internal discharge regions. These are specified in Card N-2 and are discussed there.

NOTE: If IAQ = 3 (READ R1-27), skip the following READ and proceed to READ R1-29.

READ R1-28 (LIST 1: 8I5; List 2: 6E10.0) **Region Specification.**

LIST 1: I1, I2, J1, J2, K1, K2, KAQ, IREG

- | | |
|-------|---|
| I1,I2 | Lower and upper limits, inclusive, on the I index of the aquifer-influx region. |
| J1,J2 | (Similar definition for J index). |
| K1,K2 | (Similar definition for K index). |
| KAQ | Control variable for the heat-transport equation used only for IAQ = 4. <ul style="list-style-type: none">1 - Type 3 radiation condition only. In List 2, T1 is not used. T2 and T3 are used.0 - Type 1 temperature condition only. In List 2, T1 is used. T2 and T3 are not used.1 - Type 1 temperature condition and Type 3 radiation condition. In List 2, T1, T2 and T3 are all used. |



NOTE: The code is designed so that a maximum of four internal (Card N-2) and four biosphere (external) discharge regions (Card R1-28) can be specified in a given simulation.

NOTE: IREG is only operative for IAQ = 4 (READ R1-27) boundary conditions.

IREG Variable that specifies whether the user wants to consider the model boundary block edges as nuclide biosphere discharge points.

0 - No action.

For IREG - 1, 2, 3, or 4 means that some grid blocks are to be considered for nuclide biosphere discharge blocks. The number of IREG defines the index of that region. There can be a maximum of 4 biosphere discharge regions specified.

NOTE: If NCP = 0 (READ M-3-1), this option is not operational. Further, if there is no water efflux from the aquifer-influence function blocks, the nuclide discharge will be equal to zero. The nuclide discharge will be integrated spatially along each region indicated in these cards. The discharge rates will be in units of kg/s and Curies/year and the time-integrated mass released will be in kg and Curies. At present, this option is available only when using SI units.

The unit to which the discharge rates and accumulated masses will be written for each nuclide are given below:

<u>(External) Biosphere Region</u>	<u>Unit</u>	<u>Filename</u>
1	41	SWIFTER1
2	42	SWIFTER2
3	43	SWIFTER3
4	44	SWIFTER4

LIST 2: VAB, P1, T1, C1, T2, T3

For IAQ = 1 or 2, the LIST 2: VAB, P1, T1, C1, T2, T3

For IAQ = 1 or 2, the Pot-Aquifer or Steady-State Options,



VAB Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The units of VAB are ft³/psi (m³/Pa) for a pot-aquifer representation and ft³/psi-d (m³/Pa-s) for a steady-state representation.

P1, T1, C1, T2, and T3 are not used.

For IAQ = 4, the Boundary-Condition Option,

VAB Face-type indicator used to assign transmissibility.

1.0 - Block is located on an I = 1 edge.

- 2.0 - Block is located on an I = NX edge.
 - 3.0 - J = 1 edge.
 - 4.0 - J = NY edge.
 - 5.0 - K = 1 edge.
 - 6.0 - K = NZ edge.
- P1, T1, C1 Constant values of pressure at block-centroid elevation in psi (Pa), temperature in °F (°C) and concentration (fraction at the block boundary specified according to VAB and KAQ. See Figure 3-5.
- T2 Temperature of surrounding media, °F (°C).
- T3 Coefficient of surface-heat transfer, Btu/d-ft²-°F (J/s-m²-°C).

NOTE: Follow the last card of this data group with a blank card.

3.10.2 Unsteady-State Aquifer-Influence Function

NOTE: If IAQ ≠ 3, omit these data and proceed to READ R1-33. This section is used to enter data for the Carter-Tracy method of calculating aquifer-influence functions. In general, the Carter-Tracy Boundary Condition option is a transient boundary condition which allows the user to attach an infinite aquifer to the modeled region through the method of Carter and Tracy (1960). The advantage to this method is that one can model an infinite reservoir without boundary influences with a significant decrease in model blocks. One can also attach an external reservoir to an internal finite-difference grid block. This is referred to as an internal Carter-Tracy boundary condition.

READ R1-29 (6I5) Control Parameters.

LIST: NCALC, NPT, PRTIF, KPAQ, KSWAQ

- NCALC Control parameter for selecting how the Carter Tracy aquifer coefficients are to be assigned.
- 0 - The Carter-Tracy aquifer coefficients (VAB) will be read as input data.

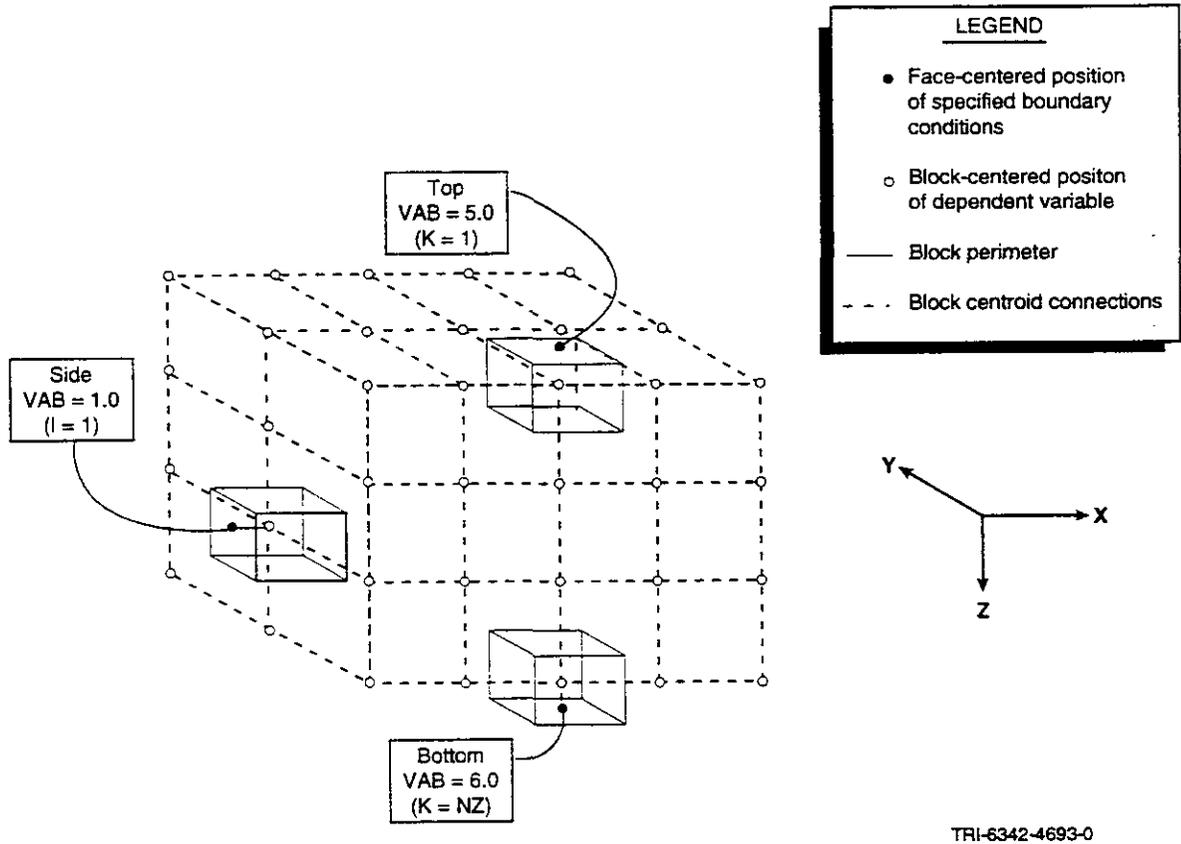


Figure 3-5. Positions for the Boundary Conditions.

- 1 - The VAB will be calculated by the program and assigned to each edge (perimeter) block in each areal plane, $K = 1, 2, \dots, NZ$.
- NPT Number of points in the table of influence function versus dimensionless time ($P(t_D)$ versus t_D). If $NPT = 0$, the program selects the infinite-aquifer solution from the appropriate table.
- PRTIF Print control key for the influence-function table.
- 0 - Suppress printing.
- 1 - Print the table of $P(t_D)$ versus t_D .

The following three variables that these control integers refer to will be defined in the discussion of the R1-31-2 card. The control integers are defined as:

- KPAQ Control parameter governing whether the variable PAQ will be read in Card R1-31-2.
- KTPAQ Control parameter governing whether the variable TPAQ will be read in Card R1-31-2.
- KSWAQ Control parameter governing whether the variable SWAQ will be read in Card R1-31-2.

For all three control integers:

- 0 - The parameter will be read
- 1 - The parameter will not be read



NOTE: Enter the following data only if $NCALC = 0$. Otherwise, skip to READ R1-31.

NOTE: This READ group consists of two cards, or any number of sets of two cards, with each set defining a rectangular region and the value of VAB to be assigned within that region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set being assigned to the overlapped subregion.

READ R1-30 (LIST 1: 6I5; LIST 2: E10.0) Boundary Specification.

LIST 1: I1, I2, J1, J2, K1, K2

- | | |
|--------|--|
| I1, I2 | Lower and upper limits, inclusive, on the I index of the aquifer-influence region. |
| J1, J2 | (Similar definition for J index). |
| K1, K2 | (Similar definition for K index). |



LIST 2: VAB

- | | |
|-----|--|
| VAB | Geometrical coefficient for each block within the defined region. The coefficient VAB, for the Carter-Tracy method, is actually the fraction of the total reservoir-aquifer boundary that the block surface comprises. For this reason it is possible to calculate the VAB from input data previously read, and the VAB does not have to be calculated externally. |
|-----|--|

NOTE: Follow the last VAB card of the above data group by a blank card.

READ R1-31-1 (4E10.0) Carter-Tracy Aquifer Properties.

SWIFT II permits the assignment of multiple Carter Tracy Boundary Conditions to a finite difference grid. The CT/BC's can be attached both externally and internally to the finite difference grid. Each CT/BC is entered through the input of 1 set of cards R1-27 through R1-33.

LIST: KH, PHIH, RAW, THETAQ

- | | |
|------|---|
| KH | Aquifer transmissivity, ft^2/d (m^2/s). An average value of transmissibility along the edges should be used. |
| PHIH | Porosity-thickness for aquifer, ft (m). |
| RAQ | Equivalent aquifer radius, ft (m). The approximate method of Carter and Tracy is valid for circular aquifers. However, it may be used, nevertheless, to approximate the effects of an infinite aquifer upon a rectangular system. |

THETAQ Angle of influence, degrees. This angle should indicate the portion of the aquifer covered by the aquifer-influence boundary. If mass flow is permitted across all the boundaries, enter 360°.

READ R1-31-2 (7E10.0) Carter-Tracy Aquifer Parameters.

LIST: BWAQ, VISCAQ, CTAQ, TAQ, PAQ, TPAQ, SWAQ

These parameters further define the physical character of the attached Carter-Tracy boundary condition and also the connection between the external aquifer (Carter-Tracy BC) and the finite-difference grid. Parameters PAQ, TPAQ, and SWAQ are read only if the control integers read in R1-29 (KPAQ, KTPAQ, and KSWAQ) specify that they are to be read. The parameters BWAQ, VISCAQ, CTAQ, and TAQ are used if a value greater than zero is entered, otherwise default values taken from the modeled global system are used.

- BWAQ External aquifer fluid density, lb/ft³ (kg/m²).
- VISCAQ External aquifer fluid viscosity, cp (Pa-s).
- CTAQ Total compressibility of the external aquifer, psi⁻¹ (Pa⁻¹).
- TAQ Conductance between the external aquifer and the finite-difference grid, ft²/day (m²/sec).
- PAQ Pressure differential between the external aquifer and the finite-difference grid, psi (Pa).
- TPAQ External aquifer fluid temperature.
- SWAQ External aquifer brine fraction.

The parameters KH, PHIH, and THETAQ of card R1-31-1 and parameters BWAQ, VISCAQ, and CTAQ are all used to calculate the appropriate time constant and pressure constant for dimensionalization of the dimensionless time vs dimensionless pressure table. This allows for the attachment of an external aquifer with different properties than the finite-difference region it is attached to.

NOTE: The following data are entered if $NPT \neq 0$ (READ R1-29). If $NPT = 0$, the program will select the aquifer-influence fractions for an infinite aquifer and the influence-function data need not be entered. If $NPT = 0$, omit this READ and proceed to READ R1-33.

READ R1-32 (2F10.0) Terminal-Rate Function.

LIST: TD(I), PTD(I), I = 1,NPT

TD	Dimensionless time, $kt/\mu\phi(c_w + c_r)r_e^2$.
PTD	Terminal-rate function.

3.10.3 Geometrical-Coefficient Modification

These data allow the user to modify the coefficient VAB by the relation $VAB(I,J,K) = VAB(I,J,K) \times FAB$. This is useful when a reservoir may experience no or limited water influx across one boundary. In this case, in the region where influx is limited, the FAB may be used to reduce the VAB along that boundary. For the case when $IAQ = 4$, i.e., Dirichlet boundary conditions and prescribed pressures, the value of FAB is interpreted as a multiplicative modifier of the transmissivity between the block center and the block edge.

READ R1-33 (LIST 1: 6I5; LIST 2: E10.0)

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2	Lower and upper limits, inclusive, on the I index of the VAB to be modified.
J1, J2	(Similar definition for the J index).
K1, K2	(Similar definition for the K index).

LIST 2: FAB

FAB	Factor by which the VAB will be modified in the defined region.
-----	---



NOTE: Follow these data with one blank card. If no modifications are desired, one blank card is still required.

Because it is possible to assign multiple types of boundary conditions by looping through cards R1-27 to R1-33, a blank card is required when boundary condition specification is completed.



4. THE R1D CARDS

The R1D input defines the physical properties and discretization of the local subsystems. These are one-dimensional units that may be attached to any global block within the system. They may be used to simulate the second porosity of a fractured media or they may be used to broaden the boundaries of the global system at minimal expense. This particular capability of the SWIFT II code is described by Reeves et al. (1986b), Sections 2.3, 5.6, and 7.1.3.

NOTE: If KSLVD = 0 (READ M-3-2), then all R1D input should be skipped.

4.1 Physical and Discretization Parameters

READ R1D-1 (E10.0) Rock Compressibility

List: CRD

CRD Compressibility of the rock within the local subsystems, psi^{-1} (Pa^{-1}).

READ R1D-2 (LIST 1: 7E10.0; LIST 2: 2I5, 3D10.0; LIST 3: 7E10.0) Properties Dependent upon Local Rock Type.

NOTE: A set of three cards is read for each local rock type assuming a natural ordering of the rock types, i.e., IR 1,2,..., NRTD (READ M-3-2).

LIST 1: DMEFD, DMFD1, PHID, AKSD, ALPD, UKTD, CPRKD

DMEFD	Value of molecular diffusivity for brine and default value for radionuclides, ft^2/d (m^2/s).
DMFD1	Coefficient of thermal increase in diffusivity, $^{\circ}\text{F}^{-1}$ ($^{\circ}\text{C}^{-1}$).
PHID	Porosity.
AKSD	Permeability, ft/d (m/s).



ALPD	Dispersivity, ft (m).
UKTD	Thermal conductivity, Btu/ft-d-°F (J/m-s-°C).
CPRKD	Heat capacity, Btu/ft ³ -°F (J/m ³ -°C).

LIST 2: KGDP, KGRD, SAD, DSD, DSDO

KGDP	Geometry control. 0 - Spherical structural units. 1 - Prismatic structural units.
KGRD	Local grid control. 0 - Node-to-node increment values are input. 1 - Single-mesh generation. 2 - Double-mesh generation.
SAD	Length of prismatic units or radius of spherical units.
DSD	Increment specification at interface of local subsystem with global system, ft (m).
DSDO	Increment specification at the outer extremity of local subsystem, ft (m).

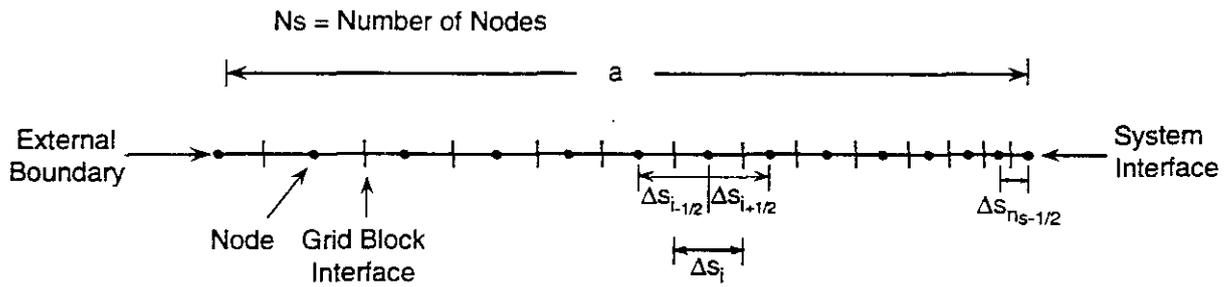
NOTE: For single-mesh generation, the three parameters NSD (READ ROD-2), SAD and DSD are used to generate nodal positions for the local subsystem (see Figure 4-1). For double-mesh generation, the four parameters, NSD, SAD, DSD and DSDO are used to generate nodal positions (see Figure 4-1).

REFERENCE: Reeves et al. (1986b), Section 7.1.3.

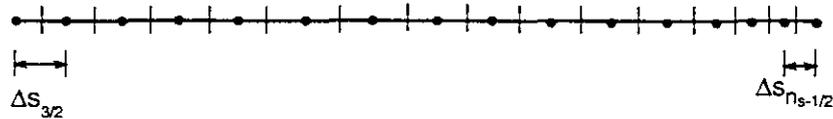
NOTE: If KGRD ≠ 0 skip this list.

LIST 3: DS(I), I=1, NSD-1

DS	Node-to-node increment values where I = 1 denotes the outermost increment and I = NSD-1 denotes the increment at the system interface, ft (m).
----	--



(A) Single Mesh Generation



(B) Double Mesh Generation

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For single-mesh generation $\Delta_{n_s - \frac{1}{2}} = \text{DSD}$ specified together with $a = \text{SAD}$ and $n_s = \text{NSD}$. The mesh is then graded to the external boundary. For double-mesh generation $\Delta_{3/2} = \text{DSDO}$ is also specified. The mesh is then graded to the interior of the local subsystem.

Figure 4-1. Mesh Generation for the Local Subsystems

4.2 Initial and Outer Boundary Conditions for the Primary Variables

In this section boundary conditions for the outer extremity of the local subsystem and initial conditions for the local subsystem are prescribed for the primary variables as a function of local rock type. The boundary condition at the local/global interface is not under user control since it is always matched implicitly to the value of the corresponding global variable.

NOTE: Enter as many cards as necessary to define all initial and boundary conditions.

READ R1D-3 (LIST 1: 5I5; LIST 2: E310.0) **Boundary Conditions.**

LIST 1: IR, KBC, KPB, KTPB, KSWB



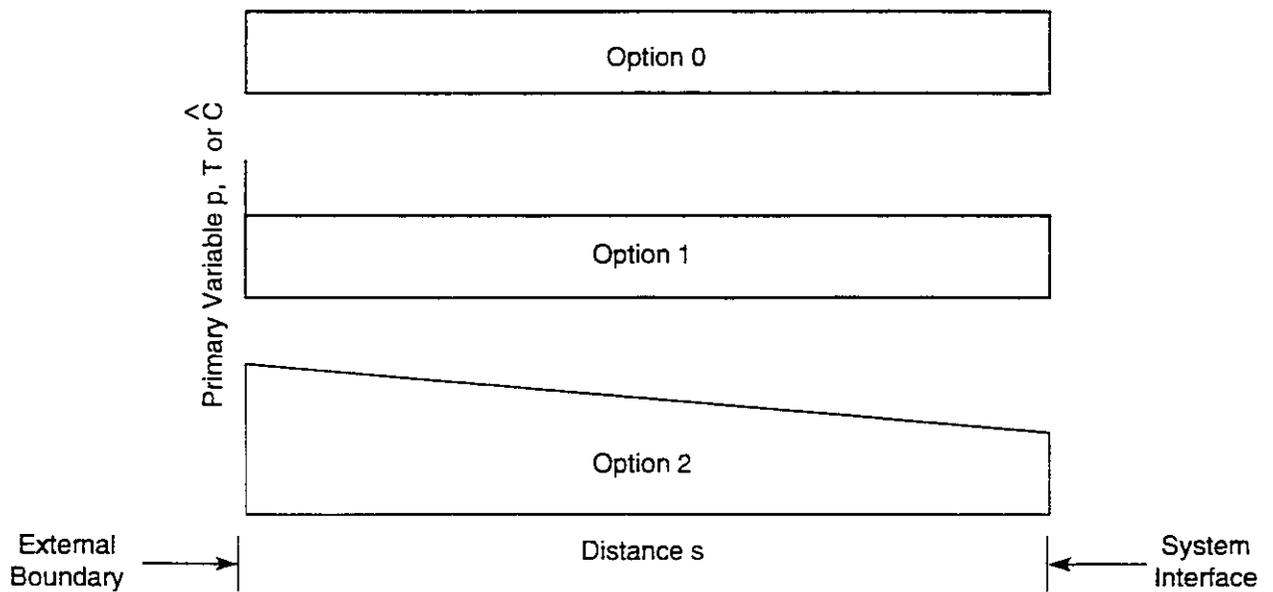
IR Local rock type

KBC Boundary-condition control

- 0 - No-flow (no-flux) conditions are invoked for all primary variables, p' , T' , and C' .
- 1 - Dirichlet conditions are taken for all primary variables.
- 2 - Dirichlet conditions are used for the variables T' and a no-flux conditions is used for p' and C' .
- 3 - Dirichlet conditions are used for the variables C' and a no-flux condition is used for T' . Note: A fluid flux is calculated due to density changes.

KPB Conditional pressure control. Operative only for $KBC > 0$. See Figure 4-2 for a pictorial definition of the available options.

- 0 - Both boundary and initial conditions are fixed at the global-block value.
- 1 - The boundary condition is set at the value prescribed in List 2, and the initial condition is fixed at the global-block value.



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Figure 4-2. Initial/Boundary Conditions for the Primary Variables Within the Local Sybsystems.

-
- 2 - The boundary condition is set at the value prescribed in List 2, and the initial condition is fixed at the boundary-condition value.
 - 3 - The boundary condition is set at the value prescribed in List 2, and the initial condition varies directly from the Dirichlet condition at the outer extremity to the global-block value at the system interface.

KTPB Temperature control. Operative for KBC = 1 and KBC = 2 only. The options here are the same as that of KPB (see Figure 4-2).

KSWB Brine control. Operative for KBC = 1 and KBC = 3 only. The options here are the same as that of KPB (see Figure 4-2).

LIST 2: PBD, TPBD, SWBD

PBD Specified boundary value for pressure, psi (Pa).

TPBD Specified boundary value for temperature, °F (°C).

SWBD Specified boundary value for brine concentration, mass fraction.

NOTE: Terminate the input here with a blank card. Even if no boundary specifications are desired, a blank card must still be used.

4.3 Nuclide Distribution Coefficients and Diffusion Coefficients

NOTE: If there are no radioactive components, i.e., NCP = 0 (READ M-3-1), skip this input set. Otherwise read one data set for each rock type.

READ R1D-4-1 (7E10.0) Distribution Coefficients.

LIST: DISD(IC), IC = 1,NCP

DISD Distribution coefficient in ft³/lb (m³/kg) for local rock-type IR and component IC.

READ R1D-4-2 (7E10.0) **Nuclide Dependent Diffusion Coefficients**

LIST: DMEFRD(IC), IC = 1, NCP

DMEFRD Molecular radionuclide diffusion coefficient for the local system. This is specified according to nuclide and rock type. The units it may be specified in are m^2/s and ft^2/day . If zero values are input, then the diffusion coefficient will be $10^{-21} m^2/s$ to $10^{-15} ft^2/day$ depending upon the unit system used.

NOTE: The input is constructed such that first NRTD R1D-4-1 cards are entered then followed by NRTD R1D-4-2 cards. No blank card is required.

4.4 Radionuclide Boundary Conditions

Radionuclide boundary conditions are not under the direct control of the analyst. They are set internally to be consistent with the condition used for the flow. Thus, for a constant pressure condition, a convective flux condition is set on the radionuclide transport. For a no-flow condition, of course, a no-flux condition is used for the radionuclide equation.

4.5 Dual Porosity Block Modifications

READ R1D-5 (LIST 1: 615; LIST 2: E10.0) **Block Modifiers.**

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2	Lower and upper limits, inclusive on the I index of the global blocks to be modified.
J1, J2	Similar definition for the J index.
K1, K2	Similar definition for the K index.

LIST 2: FAMD



FAMD If positive, this is a factor by which the cross sectional area within the defined region is to be multiplied. If negative, the absolute value of FAMD will be used within the region to be modified.

NOTE: Follow these data with one blank card. If no modifications, one blank card is still required.



5. THE I CARDS

The I data group is devoted basically to a definition of initial conditions for the global system. It supplements similar data read by subroutine READ1. Pressures are initialized within READ1 by assuming hydrostatic equilibrium with pressure PINIT at depth HINIT (READ R1-16). Temperatures are also initialized within that routine by linear interpolation from the table (ZT(I), TD(I)) (READ R1-11). The I cards are read by subroutine INIT. The data obtained thereby may then be used to modify the initial pressure distribution to that appropriate for a natural flow within the reservoir. In this case, global boundary conditions prescribed in READ R1-28 for the up-and down-gradient faces of the system are respecified to their natural-flow values. In addition, both brine and radionuclide concentrations may be modified as desired from their default value of zero.

REFERENCE: Reeves et al. (1986b), Section 5.1.



5.1 Control Parameters

NOTE: If the initial concentrations are zero everywhere for both brine and radionuclides, and there is no natural flow, insert a blank card for READ I-1 and proceed to READ R1A-1.

READ I-1 (4I5) Control Parameters for Initial Conditions.

LIST: ICOMP, INAT, IRD, IPINIT

- | | |
|-------|---|
| ICOMP | Control parameter for initializing brine concentrations. |
| 0 - | Initial concentrations in all the grid blocks are zero. |
| 1 - | The initial brine concentrations are not zero everywhere. Nonzero concentrations will be entered in READ I-2. |

- INAT Control parameter for entering initial fluid velocity.
- 0 - The reservoir fluid is static initially.
 - 1 - The resident fluid velocity will be entered in READ I-3.
- IRD Control parameter for initializing radioactive/trace component concentrations.
- 0 - Initial concentrations in all the grid blocks are zero.
 - 1 - Nonzero concentrations for each component will be entered in READ I-4.
- IPINIT Control parameter that specifies whether the initial pressure for the model initial conditions are to be read as input from UNIT19 (file SWIFTINT) or are to be calculated internally.
- 0 - Pressures are not to be input externally.
 - 1 - Pressures are to be read.

5.2 Initial Brine Concentrations

NOTE: Skip this READ if ICOMP = 0 (READ I-1). If ICOMP ≠ 0, read as many cards as necessary, following the last card with a blank card.

READ I-2 (6I5, F10.0) Initial Brine Conditions.

LIST: I1, I2, J1, J2, K1, K2, CINIT

- I1, I2 Lower the upper limits, inclusive, on the I index of the region having a nonzero initial brine concentration.
- J1, J2 Similar definition for the J index.
- K1, K2 Similar definition for the K index.
- CINIT Initial brine concentration in each of the blocks of the defined region, mass fraction.

NOTE: Follow the last data card with a blank card.

5.3 Initial Velocity Condition

REFERENCE: Reeves et al. (1986b), Section 5.1.1.

NOTE: If INAT = 0 (READ I-1), skip this record.



READ I-3 (F10.0) Initial Velocity.

LIST: VEL

VEL Initial velocity of the resident reservoir fluid in the x direction, ft/d (m/s).
Initial velocities in the y and z directions are assumed to be zero.

NOTE: Under this option, boundary pressures corresponding to the initial velocity are calculated and fixed at their natural-flow values. This option is not intended to replace the steady-state pressure solution, but rather, initial conditions for transient simulation.

5.4 Initial Radionuclide Concentrations

NOTE: If IRD = 0 (READ I-1), skip this READ. If IRD \neq 0, read as many cards as necessary, following the last card with a blank card. A total of NCP (READ M-3-1) such sets of data are required. in the order of increasing component number. with a blank card terminating each set.

READ I-4 (6I5, F10.0) Initial Radionuclide Concentrations.

LIST: I1, I2, J1, J2, K1, K2, CINIT

I1, I2 Lower and upper limits, inclusive, on the I index of the region having z nonzero initial radionuclide concentration.

J1, J2 Similar definition for the J index.

K1, K2 Similar definition for the K index.

CINIT Initial radionuclide concentration for the component being entered, mass fraction.

6. THE R1A CARDS

Four different physical properties are taken to be functions of global rock type, namely thermal conductivities, dispersivities, distribution coefficients and salt-dissolution rates. Thermal conductivities and dispersivities are read by READ1 and distribution coefficients by READ0. Here, as part of the input to READ1A, the rock-type specification and the salt dissolution rates are prescribed. In addition, all of the parameters defining the waste-leaching process within the repository are specified by the R1A input data set.

6.1 Prescription of Rock Types and Salt-Dissolution Constants

NOTE: If NRT = 1 (READ M-3-1), skip this and proceed to READ R1A-2 since all blocks are assumed by default to be of Type 1. Otherwise, enter the desired number of changes (one set per rock type).

READ R1A-1 (7I5) Modification of rock Types.

LIST: I1A, I1B, J1A, J1B, K1A, K1B, IRT

I1A, I1B	Upper and lower limits, inclusive, on the I index of region of modified rock type.
J1A, J1B	(Similar definition for the J index).
K1A, K1B	(Similar definition for the K index).
IRT	Rock type.



NOTE: Follow the last data card by a blank card.

REFERENCE: Reeves et al. (1986b), Section 3.3.

READ R1A-2 (7F10.0) Salt-Dissolution Coefficients.

LIST: (ACS(I), I = 1,NRT)

ACS Product of the rate of salt dissolution and the mass fractions of solubles to total dry mass, d^{-1} (s^{-1}).

6.2 Definition of the Repository Parameters

REFERENCE: Reeves et al. (1986b), Section 3.4.

NOTE: The analyst should skip to READ R2-1 if NREP B = 0 (READ M-3-2). If NCP = 0 (READ M-3-1) and NREP B \neq 0, skip to READ R1A-5.

READ R1A-3 (15) Waste Type.

LIST: ILEVEL

ILEVEL Waste-type identifier.

0 - The waste-volume density to be input directly.

1 - Canistered-storage data is to be input and used internally to calculate the waste-volume density.



READ R1A-4 (4F10.0) Storage Specifications.

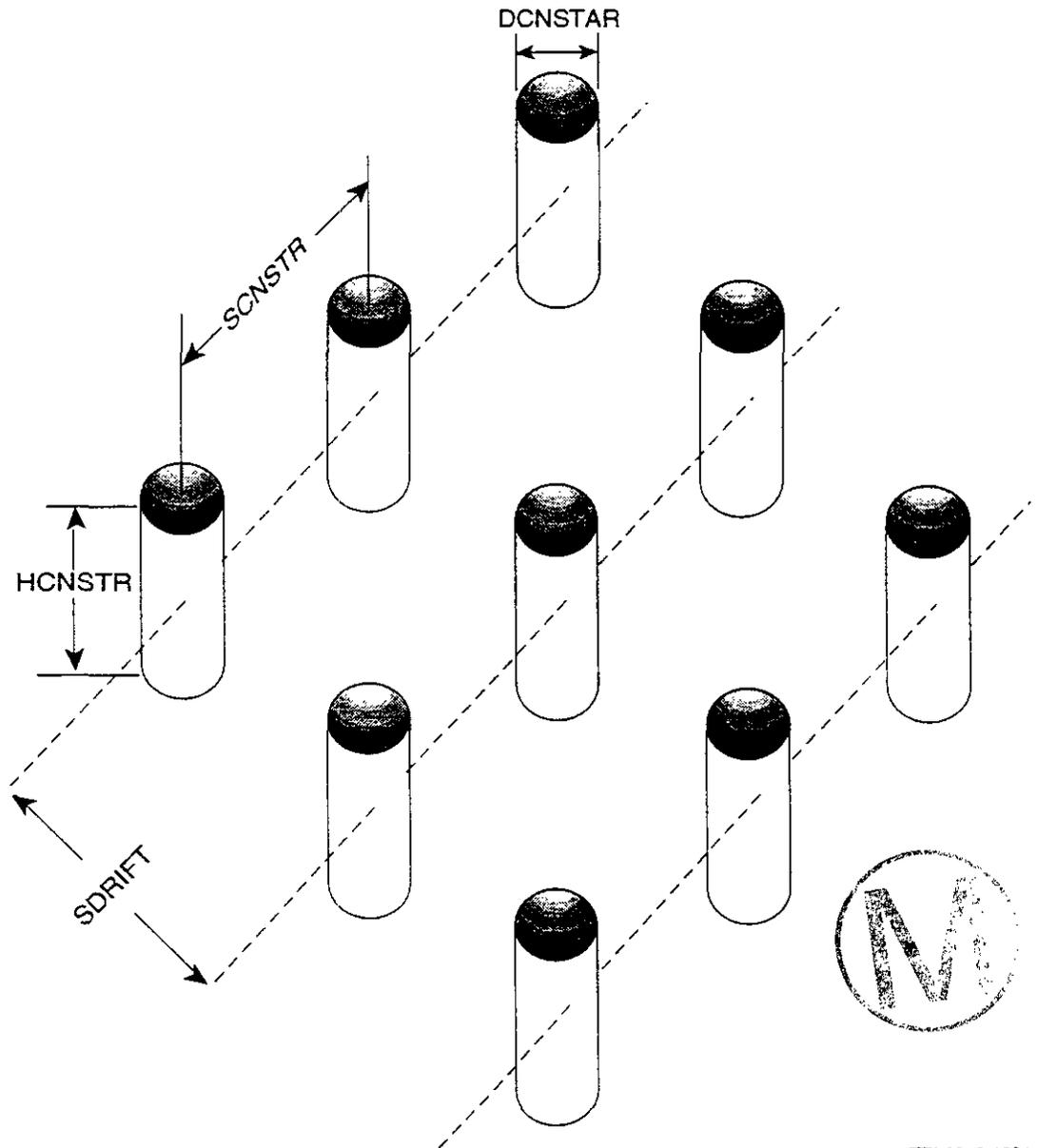
LIST: SDRIFT, SCNSTR, DCNSTR, HCNSTR

NOTE: See Figure 6-1 for a pictorial definition of the following parameters for canistered waste (ILEVEL = 1).

SDRIFT Separation of rows of canisters, ft (m). Used only for storage of canistered wastes.

SCNSTR Center-to-center canister separation within each row, ft (m). Used only for storage of canistered wastes.

DCNSTR For canistered wastes (ILEVEL = 1) DCNSTR is the diameter of each canister, ft (m). For uncanistered wastes (ILEVEL = 0) DCNSTR is the volumetric waste density (volume of wastes per bulk volume of repository blocks).



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Figure 6-1. Specification of the Canistered Waste.

HCNSTR Canister height, ft (m). Used only for storage of canistered wastes.

NOTE: Arbitrary units may be used above and then converted to the English Engineering System (SI System) via R1A-5.



READ R1A-5 (4F10.0) Unit Conversions.

LIST: CONVL, CONV C, CONVT, CONVH

- CONVL For canistered wastes (ILEVEL = 1) CON L multiplies SDRIFT, SCNSTR, DCNSTR, and HCNSTR to convert to ft (m). For uncanistered wastes (ILEVEL = 0) CNVL multiplies only DCNSTR to convert to ft³ (m³) of wastes per bulk ft³ (m³).
- CONV C This parameter multiplies the waste concentrations (R1A-8) to convert to lb/ft³ (kg/m³).
- CONVT This parameter multiplies the given interpolation times (R1A-7) to convert to days (seconds).
- CONVH This parameter multiplies the repository heat loadings (R1A-8.5) to convert to Btu/ ft²-d (J/m²-s).

NOTE: The default value for CONVL, CONV C, CONVT and CONVH is one. Thus, a blank or zero input value is reset to unity.

READ R1A-6 (6I5) Repository Location.

LIST: I1A, I1B, J1A, J1B, K1A, K1B

- I1A, I1B Upper and lower limits, inclusive, on the I index of the repository region.
- J1A, J1B Similar definition for the J index.
- K1A, K1B Similar definition for the K index.

NOTE: The repository blocks are assumed to be contiguous. Thus, only one input card R1A-6 is permitted, and no terminating blank card is necessary.

NOTE: An error condition exists if the specified repository region contains more than NREPB blocks.

READ R1A-7 (7F10.0) Interpolation Times.

NOTE: Waste concentrations may be obtained either by interpolation from a table of values or by integration of the radionuclide-transformation equations. If the integration option has been specified (NTIME = 1 (READ M-3-2)), then insert a blank card here and proceed to READ R1A-8.

LIST: CTIME(I), I = 1,NTIME

CTIME Interpolation times, d (s).



NOTE: Arbitrary units may be used here and then converted via CONVY (READ R1A-5) if desired.

NOTE: If NCP = 0 (READ M-3-1), skip to READ R1A-8.5.

NOTE: The analyst must enter NCP groups of cards below. However, the information will be used only for those components being tracked within the entire global system, i.e., the information will be used only if CNAME below matches one of the DI identifiers (READ R0-1).

READ R1A-8 (2A4,2X,6F10.0/(7F10.0)) Interpolation of Unleached Concentrations.

LIST: (CNAME(1), I=1,2), (CNDUM(I), I = 1,NTIME)

CNAME Identification of radioactive component.

CNDUM If interpolation is to be used, then CNDUM represents the concentrations at the interpolation times expressed as mass per unit volume of waste. If interpolation is not used, then CNDUM(1) is the initial condition for the chain decay.

NOTE: If KHEAT = 0 (READ M-3-2), skip to READ R1A-9.

READ R1A-8.5 (7F10.0) Repository Heat Loadings.

LIST: (ARHLD(I), I = 1,NTIME)

ARHLD Repository heat loading expressed as energy input per unit time per unit area in the x-y plane.

NOTE: If NCP = 0 (READ M-3-1), skip to READ R2-1.

READ R1A-9 (7F10.0) Solubility Limits.

LIST: CS(I), I = 1,NCP

CS Solubility limits expressed as mass fractions.

NOTE: The code applies the solubility constraint $C(I) \leq CS(I)$ for component I only within the repository region specified in READ R1A-6.



7. THE N CARDS

The nuclide monitor blocks are identified to facilitate postprocessing of radionuclide simulations. Nuclide concentrations are written to UNIT 9 (file SWIFTNMD) at each time step for each block as identified. The file is formatted beginning with the value of time, followed by a set of concentration values. In each record the nuclide component is identified, followed by a sequential list of concentrations, one for each monitor block. Subsequent components follow sequentially.

Postprocessing may consist of time series plots or tables. Because of device dependence of graphics software, postprocessing must be provided by the user.

7.1 Nuclide Monitor Block

NOTE: Skip to N-2 if LBIO = 0 (READ M-2).

READ N-1 (3I5) Monitor Block Location.

LIST: IDSC, JDSC, KDSC

IDSC I index for block location.

JDSC J index for block location.

KDSC K index for block location.

NOTE: Read as many cards as necessary, terminating with a blank card.



NOTE: Skip to CARD R2-1 if LBIOR = 0 (READ M-2)

READ N-2 (815) Internal Nuclide Discharge Region Specification.

The user can define an internal region and an appropriate direction to the coordinate axes for the calculation of nuclide discharge rates and cumulative release. This is referred to as an internal discharge region. The addition of internal nuclide discharge regions to SWIFT II was necessitated by the desire to calculate cumulative release of nuclides at some fixed boundary within the modeled grid. The internal discharge region is simply defined as a grid block(s) face in the x, y, or z plane of a finite-difference grid across which nuclide mass is integrated as a function of time. The code is designed so that a maximum of four internal (READ N-2) and four biosphere (external) (READ R1-28) discharge regions can be specified in a given simulation.

LIST: I1, I2, J1, J2, K1, K2, IREG, IDIR

NOTE: Follow internal regional specification(s) with a blank card.

I1, I2	Lower and upper limits, inclusive on the I index of the global blocks to be considered an internal discharge.
J1, J2	Similar definition for the J index.
K1, K2	Similar definition for the K index.
IREG	The region index for internal nuclide discharge areas. (IREG may equal 1, 2, 3, or 4). There are a maximum of four possible internal discharge areas that can be specified.
IDIR	The boundary face over which integrated release is to be considered for the region IREG. 1 - Nuclide discharge in the positive direction of the x-axis only will be computed. 2 - Nuclide discharge in the positive direction of the y-axis only will be computed. 3 - Nuclide discharge in the positive direction of the z-axis only will be computed. -1 Nuclide discharge in the negative direction of the x-axis only will be computed.



- 2 Nuclide discharge in the negative direction of the y-axis only will be computed.
- 3 Nuclide discharge in the negative direction of the z-axis only will be computed.

NOTE: A N-2 card must be specified for each separate internal discharge region with a possible maximum specified set at 4. The discharge rate and accumulated mass across the region(s) defined above are written to tape at every time step and to the general SWIFT II output with the frequency specified by parameter I06 (READ R2-13-1). The nuclide discharge will be integrated spatially along the region indicated in this card. The discharge rates will be in units of kg/s and Curies/year and the time-integrated mass released will be in kg and Curies. At present, this option is available only when using SI units.

The unit to which the discharge rates and accumulated masses will be written for each nuclide are given below.

<u>Internal Region</u>	<u>Unit</u>	<u>Filename</u>
1	45	SWIFTIR1
2	46	SWIFTIR2
3	47	SWIFTIR3
4	48	SWIFTIR4



8. THE R2 CARDS

In contrast to previous sections, the R2 data are time-dependent. Two different time regimes are used by the code. The first regime is a set of relatively coarse recurrent time steps. The time-dependent parameters are changed at the beginning of each such step by input from subroutine READ2. The second regime is a relatively finer time grid within each recurrent time step used for numerical integration of the transport equations. The recurrent data consists of control integers, source information, numerical-solution control and output control.

8.1 Control Integers

READ R2-1 (10I5) Control Parameters.

LIST: INDQ, IWELL, IMETH, ITHRU, IRSS, IPROD, IOPT, INDT, ICLL, IRCH

- | | |
|-------|---|
| INDQ | Control parameter for reading well rates. |
| 0 - | Do not read well rates. |
| 1 - | Read seven well rates per card in READ R2-5. |
| 2 - | Read one card per well rate in READ R2-6. |
| IWELL | Control parameter for reading well definition data. |
| 0 - | Do not read well data. |
| 1 - | Read new or altered well data. |
| IMETH | Control parameter for reading method of solution. |
| 0 - | Do not read method of solution. |
| 1 - | Read new nor altered method of solution. |



-
- ITHRU** Run termination
- 0 - Run is to continue.
 - 1 - Run is to terminate at this point. No more recurrent data will be read after this card. If no plots are desired, i.e., if NPLP, NPLT and NPLC are all zero, this should be the last card in your data deck.
- IRSS** Control parameter for reading radionuclide source data.
- 0 - Do not read source data for the trace components.
 - 1 - Read new or altered source-rate or waste-leach data, as defined by block number.
- IPROD** Control parameter for reading wellbore data.
- 0 - Do not read well-head data.
 - 1 - Read new or altered well-head data.
- IOPT** Control parameter for reading iteration data for the wellbore calculations.
- 1 - Read new or altered wellbore iteration data.
- INDT** Control parameter for reading iteration data for the reservoir solution.
- 0 - Do not read iteration data. If no such data has been read for previous recurrent data sets, then default values are used.
 - 1 - Read new or altered iteration data.
 - 2 - Read new or altered iteration data and L2SOR data.
- ICLL** Equation-solution control.
- 0 - Do not read change in equation solution control, NCALL.
 - 1 - Read new equation solution control, NCALL.

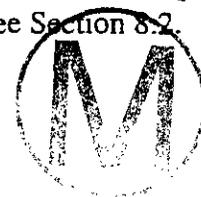
- IRCH Control parameter for reading recharge data.
- 0 - Do not read recharge data.
 - 1 - Read new or altered recharge data.

8.2 Differencing and Matrix Solution Control

NOTE: These data are entered if IMETH \neq 0 (READ R2-1). If this is a new run and IMETH = 0, the program selects METHOD = 1 and WTFAC = 1.0 (direct solution with backward space and time approximations).

REFERENCE: For a description of time and space differencing, see Reeves et al. [1986b], Sections 6.1.4 and 6.1.5. For a description of the matrix-solution options see Section 8.2.

READ R2-2 (I5,F10.0) Solution Control.



LIST: METHOD, WTFAC

- METHOD Method of solution. Direct solution may be entered only if direct solution is specified in READ M-3-1.
- 1 - Reduced-bandwidth direct solution with backward finite-difference approximation in time.
 - 2 Tow-line successive-overrelaxation (L2SOR) solution with a backward finite-difference approximation in time.
 - 1 Reduced bandwidth direct solution with a centered finite-difference approximation in time.
 - 2 - Tow-line successive-overrelaxation solution (L2SOR) with a centered finite difference approximation in time.
- WTFAC Weight factor for the finite-difference approximation in space.
- 1.0 - Backward differencing.
 - 0.5 - Central differencing.

NOTE: If WTFAC < 0 is entered, the program selects WTFAC = 1.0.

8.3 Surface Recharge Specification

NOTE: These data are entered if IRCH \neq 0 (READ R2-1). Read as many cards as necessary.

READ R2-2.5 (415,E10.0) **Surface Recharge.**

LIST: I1, I2, J1, J2, RCHG

I1,I2	Lower and upper limits, inclusive, for the I index of the region having recharge rate, RCHG.
J1,J2	Similar definition for the J index.
RCHG	Recharge rate, ft/d (m/s).

NOTE: Follow the last data card with a blank card.



8.4 Well Data

NOTE: These data are entered if IOPT > 0 (READ R2-1). If default values are desired, insert a blank card and proceed to READ R2-4. The default values of the parameters are discussed below.

**THIS FEATURE DOES NOT CONFORM TO QUALITY ASSURANCE STANDARDS.
ITS USE IS NOT RECOMMENDED.**

READ R2-3 (I5,4F10.0) **Wellbore Data.**

REFERENCE: Reeves et al. (1986b), Section 4.2

LIST: NITQ, TOLX, TOLDP, DAMPX, EPS

NITQ	Maximum number of outer iterations in the wellbore calculations. For example, if the injection rate for a well is specified, the well-head
------	--

pressure is calculated iteratively to obtain the bottom-hole pressure necessary to inject the specified rate. If $NITQ \leq 0$, the program selects the default value of 20.

- TOLX The tolerance on the fractional change in pressure over an iteration. If $TOLX \leq 0$, the default value of 0.001 is selected.
- TOLDP The tolerance on pressure, psi (Pa). The default value is 7000 psi (4.8×10^7 Pa).
- DAMPX Damping factor in estimating the next value of the pressure (at the surface for an injection well and at the bottom-hole for a production well). If the frictional pressure drop in the well is high, a linear extrapolation may lead to oscillations around the right value. The default value is 2.0.
- EPS The tolerance on calculating temperature from given values of enthalpy and pressure. The fluid temperatures in the wellbore are calculated over each pressure increment as specified in READ R1-3. The default value is 0.001.

NOTE: If $INDQ = 0$ (READ R2-1), skip READ R2-4 through READ R2-6 and proceed to R2-7.

R2-4 (I5) Rate Specifications.

LIST: NWT

NWT Total number of wells.



NOTE: Enter these data only if $INDQ = 1$ (READ R2-1).

READ R2-5 (7E10.0) Rate Specifications.

LIST: Q(I), 1 =1,NWT

Q Production rate, ft^3/d (m^3/s). For an injection well, enter the value as a negative production rate. All the well rates must be entered even if none of them have changed from the previous recurrent time step.

NOTE: Enter the following data only if $\text{INDQ} = 2$ (READ R2-1). Read as many cards as necessary to describe all the modified injection and production well rates.

READ R2-6 (15, E10.0) Rate Specifications.

LIST: I, QWELL

I Well number.

QWELL Production rate, ft^3/d (m^3/s). Enter negative values for injection rates. Enter only the well rates that are to be changed from an earlier recurrent data set.

NOTE: Follow the last data card with a blank card.

NOTE: The following data are entered for $\text{IWELL} = 1$ (READ R2-1). Read one set of data for each well.

READ R2-7 (LIST 1: (8I5); LIST 2: (4E10.0); LIST 3: (8E10.0); LIST 4: (7E10.0))
Well Location/Option Definition.

LIST 1: I, IW, JW, IC1, IC2, IINDW1, KCPINJ(I), IREG

I Well number.

IW I index of the grid cell containing the well.

JW J index of the grid cell containing the well.

IC1 Uppermost layer in which the well is completed.

IC2 Lowermost layer in which the well is completed.



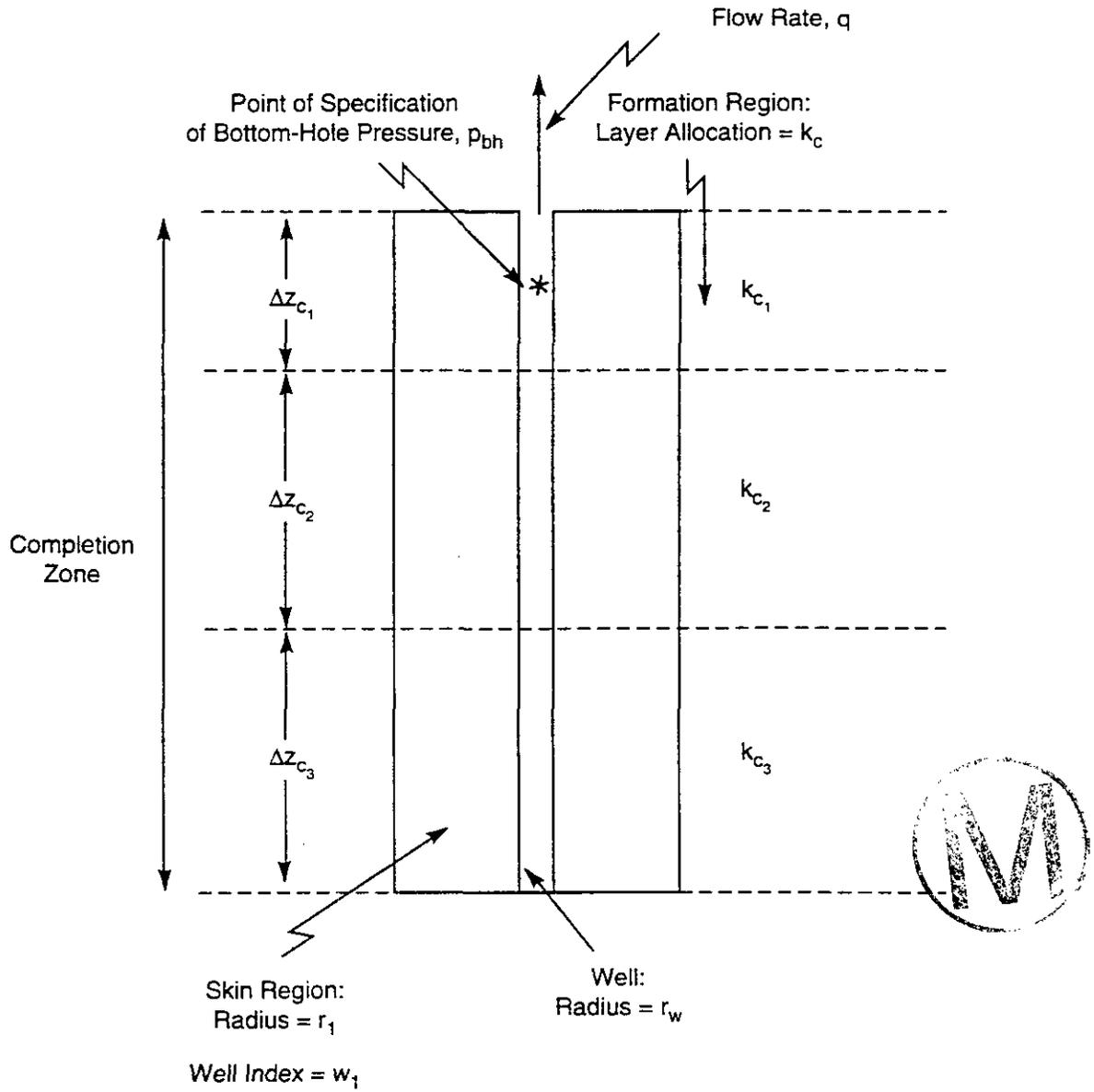
- IINDW1 Well specification option.
- 1 - Layer allocation via mobilities alone. Rate control only.
 - +2 - Layer allocation via mobility and pressure drop between wellbore and grid block. Rate control only.
 - 3 - Layer allocation via mobility and pressure drop between wellbore and grid block. Variable rate-pressure control.
 - 2, 3 - Explicit implementation.
 - 2,-3 Semi-implicit implementation.
 - 4 Steady-state pressure-limited.



NOTE: Reeves et al. (1986b), Section 4.1, discusses the four topics, pressure/rate control, explicit/implicit rate terms, layer allocation and transient/steady-state implementation, all of which are crucial to a proper implementation of the well submodels. There is another point, however, that should be reiterated here related to pressure control. Specifically, the point of application of the bottom-hole pressure. Figure 8-1 shows a well completed into three layers. As indicated there, the enforcement position for the specified bottom-hole pressure is the block center of the top layer of the completion zone. Usually this is also the position of the physical pressure measurement.

KCPINJ(I) If the integer is specified as 1, and transport of a radionuclide is taking place, SWIFT II will implicitly correct the concentration of that radionuclide in the specified block according to the fluid flux in or out of that block as specified in cards R2-5 or R2-6. A zero means to not correct concentrations, and a 1 means do correct the grid-block concentrations for fluid flux into each grid block. This option is very task specific and was introduced to prevent concentration dilution or growth due to injected or produced fluids in a grid block.

IREG It allows the user to define a well as an external biosphere discharge point. IREG is the index of the biosphere discharge region and can be specified from 1 to 4. A value of 0 makes the option non-operative. Both nuclide discharge rates and cumulative release are computed for each nuclide simulated at a biosphere discharge region.



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Figure 8-1. Characterization of a Well.

NOTE: All the notes that are given in association with external biosphere discharge regions in READ R1-28-1 are equally applicable here. The user is referred to READ R1-28-1 for details on operation.

LIST 2: WI, BHP, TINJ, CINJ

- WI Well index, ft^2/d (m^2/s).
- BHP Bottom-hole pressure, psi (Pa). This must be specified only if $|IINDW1| \geq 3$.
- TINJ Temperature of the injected fluid, °F (°C). If surface conditions are being specified, TINJ is the temperature at the surface.
- CINJ Brine concentration of the injection fluid, dimensionless.

NOTE: Skip LIST 3 if ISURF = 0 (READ M-2).

REFERENCE: Reeves et al. (1986b), Section 4.2.

LIST 3: X, DW, ED, OD, TTOPW, TBOTW, UCOEF, THETA

- X Wellbore length from surface to top of perforations, ft (m).
- DW Inside diameter of the tubing, ft (m).
- ED Roughness of the inner surface of the tubing for a smooth pipe, ft (m).
- OD Outside diameter of the casing, ft (m).
- TTOPW Initial rock temperature at the top-hole, °F (°C).
- TBOTW Initial rock temperature at the bottom-hole, °F (°C).
- UCOEF Overall heat transfer coefficient between the inner surface of the tubing and the outer surface of the casing, $\text{Btu}/\text{ft}^2\text{-}^\circ\text{F}\text{-d}$ ($\text{J}/\text{m}^2\text{C}\text{-s}$).
- THETA Angle of deviation of the well bore from the vertical direction, degrees.

NOTE: Skip LIST 4 if the well is completed in only one layer, i.e., if IIC1 = IIC2.

LIST 4: KHL(K), K = IIC1 IIC2

KHL(K) Layer allocation factors for well I, layer K, dimensionless.

NOTE: Follow the last data card with a blank card.

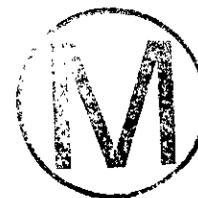
NOTE: Layer-allocation factors should be proportional to the total productivity of the individual layers, taking into account layer values of $k\Delta z$ (permeability x thickness). Only relative values are important since these factors are renormalized to a unit sum. The productivity (injectivity) of layer K is computed as $WI \times KHL(K)$.

NOTE: Skip this READ if $IPROD = 0$ (READ R2-1). However, it is used only for those wells having specification option $IINDW1 = \pm 3$ (READ R2-7).

READ R2-8 (7E10.0) Wellbore Data.

LIST: THP(I), I = 1,NWT

THP Surface pressure for each well, psi (Pa).



8.5 Sink/Source Information

NOTE: If $IRSS = 0$ (READ R2-1), skip this section of input and proceed to READ R2-11.

NOTE: If $NREPB > 0$ (READ M-3-2), skip to READ R2-10-5.

READ R2-9 (I5) Specified-rate Data.

LIST: NSS

NSS Number of sink/source blocks.

NOTE: Enter one set of data for each source.

REFERENCE: Reeves et al. (1986b), Section 4.3.

READ R2-10 (LIST 1: 415; LIST 2: 7E10.0) Specified-Rate Data.

LIST 1: I, IIS, IJS, IKS

I	Source Number.
IIS	I index of the source block.
IJS	J index of the source block.
IKS	K index of the source block.



LIST 2: QWW(I), QHH(I), (QCC(I,J)J = 1,NCP)

QWW	Fluid discharge rate, lb/d (kg/s). A negative rate denotes a source, and a positive rate denotes a sink.
QHH	Heat discharge rate, Btu/d (J/s).
QCC	Discharge rates of radioactive components, lb/d (kg/s). Omit this parameter is NCP = 0.

NOTE: Follow the last data card with a blank card.

NOTE: If NREPB = 0 (READ M-3-1), skip the following READ.

REFERENCE: Reeves et al. (1986b), Section 3.4.

READ R2-10.5 (2E10.0) Waste-Leach Data.

LIST: ALCH, BLCH

ALCH	Leach time for radioactive waste within the repository boundaries, d (s).
BLCH	Lag time from start of simulation to initiation of waste leaching or heat loading of the repository.

8.6 Iteration and L2SOR Directional Control

NOTE: These data are entered if $INDT \neq 0$ (READ R2-1). If default values are desired, enter $INDT = 0$ and skip to READ R2-11.5

READ R2-11 (4I5) Iteration and L2SOR Directional Control.

LIST: MINITN, MAXITN, IMPG, ICRSS

- 
- MINITN** Maximum number of outer (nonlinear-property) iterations in the subroutine ITER. The default value is one.
- MAXITN** Minimum number of outer (nonlinear-property) iterations in subroutine ITER. The default value is 5.

REFERENCE: Reeves et al. (1986b), Section 8.2.

- IMPG** Number of time steps after which the optimum parameters for the inner iterations are recalculated for the two-line successive over-relaxation method. These data need be entered only if $METHOD = \pm 2$. The default value for IMPG is 5.
- ICRSS** Determines how the cross-derivative terms in the dispersivity tensor are treated.
- 0 Cross-derivative terms (off-diagonal) are added to the diagonal terms. This is the default.
 - 1 Cross-derivative terms are neglected.
 - +n Cross-derivative terms are included semi-implicitly with n iterations. A value of ICRSS greater than zero will provide a more accurate solution to the transport equations when flow is not parallel to one of the principle axis directions; however, run times will significantly increase. A value of $ICRSS = 2$ should provide adequate convergence and higher values are not recommended.

NOTE: If $INDT = 1$ (READ R2-1), skip to R2-11.5.

READ R2-11.1 (2I5, E10.0) L2SOR Solution Data.

LIST: IXYZ, IBUD, TBUD

- | | | |
|------|-----|---|
| IXYZ | 0 - | Code automatically chooses optimal direction for solution sweep based on minimum over-relaxation parameter. |
| | 1 - | Override to force sweep in x-direction. |
| | 2 - | Override to force sweep in y-direction. |
| | 3 - | Override to force sweep in z-direction. |
| IBUD | | Maximum number of L2SOR sweeps. The default value is 100. |
| TBUD | | Convergence (not normalized) criteria for iterations. The default value is 1×10^{-5} units. |

NOTE: One card is required for each equation being solved. The order of equations is pressure, temperature, brine, and radionuclides. Only one set of parameters is used for all radionuclide components.

8.7 Equation Control



This section of input is frequently used for computational efficiency in the transient coupled solution of the primary and radionuclide equations. In such a solution, the primary transport processes frequently reach steady-state. The radionuclide processes, however, due to the usual time dependence of the decay/production processes and of the source strength, frequently never reach steady-state. The ICLL option (READ R2-1) allows one to "turn off" the primary solution after steady-state has been reached so that the major computational effort may then be devoted to the radionuclide solution.

NOTE: Skip this READ if ICLL = 0 (READ R2-1).

READ R2-11.5 (I5) Equation Control.

LIST: NCALL

- | | | |
|-------|--|----------------------------------|
| NCALL | | Same definition as for READ M-2. |
|-------|--|----------------------------------|

8.8 Recurrent Time and Time-Step Specification



READ R2-12 (8E10.0) Recurrent Time and Time-Step Specification.

LIST: TCHG, DT, DCMX, DSMX, DPMX, DTPMX, DTMAX, DTMIN

TCHG Time at which next set of recurrent data will be read, d (s).

NOTE: The restart records can be written at TCHG only. Also, the mapping subroutine can be activated at TCHG only.

DT Time step specifications, d (s). If DT is positive it will be the time step used from the current time to TCHG. If DT is zero, the program will select the time step automatically.

>0 - Time step to be used from the current time to TCHG.

0 - Automatic time stepping to be used.

NOTE: DT must not be zero for the first time step of the simulation time, unless a steady-state option NCALL = 4 or 5 (READ R2-11.5) is used.

NOTE: The following six parameters are used only if the automatic time-step feature is selected, i.e., if DT = 0. If this feature is selected, the program will automatically vary the time-step as it seeks a value such that the maximum changes in the concentration, pressure, and temperature are less than or equal to the specified values.

DCMX Maximum change desired per time step for the trace-component concentration. The default value is 0.95.

DSMX Maximum change desired per time step for the brine concentration. The default value is 0.25.

DPMX Maximum change desired per time step for the pressure, psi (Pa). The default value is 50 psi (350,000 Pa).

DTPMX Maximum change desired per time step for the temperature, °F (°C). The default value is 9°F (5°C).

- DTMAX Maximum time step allowed, d (s). The default value is 30 d (2.6×10^6 s).
- DTMIN Minimum time step required, d (s). The default value is 1.0 d (8.64×10^4 s).

8.9 Output Control



READ R2-13-1 (14I5) Output Control.

LIST: IO1, IO2, IO3, IO4, IO5, IO6, IO8, RSTWR, MAP, MDAT, IIPRT, IO5D, IO8D, IIPRTD

- IO1 Control parameter for the frequency of time-step summary. The time-step summary gives mass-balance information for both the global system and the local subsystems. It also characterizes the state of the global system via the average reservoir pressure, and the maximum pressure, concentration and temperature changes in any block during the time step.
- IO2 Control parameter for the frequency of the well summary. For each well this summary gives production and injection rates of fluid, heat and brine, cumulative production and injection, well-head and bottom-hole pressures, well-head and bottom-hole temperatures, and the grid-block pressure in which the bottom-hole of the well is located. This summary also gives the total production and injection rates and the total cumulative production and injection.
- IO3 Frequency control for listing the grid-block values of concentration, temperature, and pressure for the global system and the local subsystems.
- IO4 Control parameter for printing the injection/production rates in each layer for each well.
- IO5 Control parameter for listing the grid-block values of radionuclide concentrations for the global system.
- IO6 Control parameter for listing of aquifer-influence and boundary rates.

NOTE: The following values apply to all six of the above parameters:

- 1 Omit printing for all time steps from the current time through TCHG, inclusive.
- 0 - Print at the end of each time step.

1 - Print only at time TCHG.

n(>1) Print at the end of every nth time step and at the time TCHG.

I08 Control parameter for selectively listing the grid-block values of the primary variables for the global system. The listings are printed according to the frequency specified by I03. This parameter gives one the option for not printing selected tables, as desired. This parameter requires a three-digit specification. The first (left-most) digit refers to pressure, the second to temperature, and the third to brine concentration.

0 - The grid-block values will be printed.

1 - The grid-block values (pressure at datum or temperature or brine concentration) will not be printed.

2 - Refers to the first digit only. Neither the pressure nor the pressure at datum will be printed.

For example, if only grid block values of temperature are desired, then enter I08 = 201.

RSTWR Restart-record control parameter.

0 - No restart record will be written.

1 - Restart record will be written on Unit 8 at time TCHG.



MAP Parameter for printing contour maps at time TCHG. Only two-dimensional maps are printed. The maps are printed for r-z coordinates in a cylindrical system and for x-y coordinates (areal maps) in a Cartesian system. If NY = 1 then maps may also be obtained for x-z coordinates (vertical cross sections) in a Cartesian system. This parameter requires a four digit specification, the first digit referring to parent radionuclide concentrations, the second to pressures, the third to temperatures and the fourth to brine concentrations.

0 - The variable will not be mapped.

1 - Areal map (x-y) at TCHG.

2 - Vertical cross sectional maps (x-z or r-z).

- 3 - Both areal and vertical maps.
For example, if contour maps are desired for areal pressure at datum and vertical temperature only enter $MAP = 0120$.

MDAT Control parameter for entering the mapping specifications.

- 0 - The mapping specifications are not to be changed.
- 1 - Read new mapping specifications. If activating the printing of contour maps for the first time during the current run, MDAT must be entered as one and MAP must be greater than zero.

IIPRT Intermediate print control for the global system. This parameter requires two or more digits for its specification of the form $10n + i$. Here n is the frequency control with the same options as those used for I01 through I06 (see note following I06).

Parameter i is the function control with the following options.

- 0 - None of the output listed below will be activated.
- 1 - Darcy velocities will be printed.
- 2 - Transmissibilities will be printed in addition to the velocities.
- 3 - Fluid densities, viscosities, enthalpies and dispersivities will be printed, in addition to the quantities listed above.



For example, if transmissibilities and Darcy velocities are desired for every 5th time step, $IIPRT = 52$.

I05D Control parameter for listing the grid-block values of the radionuclide concentrations for the local subsystems, i.e., matrix.

I08D Control parameter for selectively listing the grid-block values of the primary variables for the local subsystems. The listings are printed according to the frequency specified by I03.

IIPRTD Intermediate print control for the local subsystems. This parameter is analogous to the global control IIPRT. It also has the form $10n + I$ where n carries the frequency options used for I01 through I06 (see note following I06) and where n carries the function control given under IIPRT.

NOTE: Based on the input on Card R2-13-2, R2-16 cards may have to be input. R2-16 cards when used, will follow the R2-15 cards.

R2-13-2 (6I5) Output Control.

NOTE: This output is exclusively in relation to the SWIFT capability to generate auxiliary disc files, for subsequent processing, on personal computers, to generate computer plots, vector plots, etc. using advanced graphic software, such as SURFER, GRAPHER, etc. A user not interested in this capability may use -1 (columns 4&5) and ignore the rest of the fields on this card. Also, the R2-16 cards are not required.

LIST: I03P, (MAPP(I), I = 1,4), MDATP

I03P Frequency control parameter (similar to parameters I01 through I06 of R2-13-1 (governing the frequency at which the disc files will be written to by SWIFT II. (The details of the files is defined by further input variables on this READ R2-13-2.)

MAPP(1) through MAPP(4) are four digit specifiers that determine which variables get written to file. If MAPP(1) through MAPP(4) indicate that a variable is to be printed, a R2-16 card is required to specify over what part of the model region did the user want the dependent variable written to file. SWIFT II allows one to enter multiple mapping specifications for one variable. If one wants to specify two regions where pressure is printed to file, then one puts a 2 in the correct control integer location. Up to 16 different mapping specifications can be specified in one simulation. The number of R2-16 cards required is equal to the sum of all control integers listed in MAPP(1) to MAPP(4). As mentioned, this must not exceed 16. The R2-16 printing region specification cards should be entered in the same order that the variables are called in R2-13-2 from left to right.

MAPP(1) This parameter governs the variables of the Pressure Equation.

0 - None of the variables of the pressure equation will be written to a disc file (logical unit).

>0 - Some of the variables of the pressure equation will be written to a disc file (logical unit) in as many regions as specified by this number.

NOTE: A maximum of 16 regions is allowed per simulation (e.g., the sum of all the regions from MAPP(1) to MAPP(4) ≤ 16.



The following I/O units are assigned:

<u>Unit</u>	<u>Variable</u>	<u>Filename</u>
21	Pressure at elevation	SWIFTPAE
22	Freshwater Heads	SWIFTFWH
23	Velocities in the x-y plane	SWIFTVEC
24	Not used	

When MAPP(1) >0, a four digit specification is used, with the first digit (left most digit) being not currently used.

First digit : not used.
(left most)
Second digit : x-y Darcy velocities.
Third digit : freshwater heads.
Fourth digit : pressures at elevation.
(right most)



0 - The variable will not be written to a disc file.

>0 - The variable will be written to a file in as many regions as specified.

An example will be used to clarify the input.

1 0002 0000 0000 0112 1

The card above is a R2-13-2 card that calls for pressure at elevation to be written to file for two different region specifications, and for daughter 2 and daughter 1 radionuclides (MAPP(4)) to be written to file for one region each, and the parent nuclide to be written to file for two different region specifications. Therefore, four R2-16 cards would be required to specify the regions where the variables will be written. The first two R2-16 cards would specify the regions where pressure at elevation would be printed and the last two would specify the regions where the parent radionuclide would be printed.

MAPP(2) This parameter governs the variables of the Temperature Equation.

0 - None of the variables of the temperature equation will be written to a disc file.

>0 - Some of the variables of the temperature equation will be written to logical units in as many regions as specified by this number. (See NOTE after MAPP(1)).

MAPP(2) >0, requires a four digit specification. The first three digits are currently not used. The fourth digit is used for temperature.

First digit : not used.
(left most)
Second digit : not used
Third digit : not used
Fourth digit : temperature
(right most)



0 - The variable will not be written to a logical unit.

>0 - The variable will be written to a logical unit in as many regions as specified by this number (see NOTE after MAPP(1)).

The following logical units (disc files) are used:

<u>Unit</u>	<u>Variable</u>	<u>Filename</u>
25	Temperature	SWIFTTEM
26	Not used	
27	Not used	
28	Not used	

MAPP(3) This parameter governs the variables of the Brine Transport Equation.

0 - None of the variables of this equation will be written to a disc file.

>0 - Some of the variables of this equation will be written to a disc file in as many regions as specified by this number. (See NOTE after MAPP(1)).

MAPP(3) > 0 requires a four digit specification, with the first two digits being not currently used.

First digit : not used
(left most)
Second digit : not used
Third digit : fluid density
Fourth digit : brine concentration (salinity).
(right most)

- 0 - The relevant variable will not be written to a disc file.
- >0 - The relevant variable will be written to a disc file in as many regions as specified. (See NOTE after MAPP(1)).

Thus MAPP(3) = 0020 implies fluid density will be written to the disc file in two specified regions. The following logical units are used:

<u>Unit</u>	<u>Variable</u>	<u>Filename</u>
29	Brine concentration	SWIFTBRN
30	Fluid density	SWIFTDEN
31	Not used	
32	Not used	



MAPP(4) This governs the variables of the radionuclide transport.

- 0 - None of the variables of the radionuclide equation will be written to disc files.
- >0 - Some of the variables of the radionuclide equation will be written to disc files in as many regions as specified by this number. (See NOTE after MAPP(1)).

MAPP(4) > 0 requires a four digit specification. The first (left most) digit is currently not used.

First digit : not used. (Should be blank or zero.)
(left most)
Second digit : Concentration of radionuclide component 3.
Third digit : Concentration of radionuclide component 2.
Fourth digit : Concentration of the parent radionuclide.
(right most)

- 0 - The variable will not be written to a disc file.
- >0 - The variable will be written to a disc file in as many regions as specified.

The following logical units (disc files) are assigned to the variables:

<u>Unit</u>	<u>Variable</u>	<u>Filename</u>
	Concentration of:	
33	Parent radionuclide	SWIFTPR1
34	Radionuclide - Component 2	SWIFTPR2
35	Radionuclide - Component 3	SWIFTPR3
36	Not used	

MDATP Control parameter for entering the region specification in the R2-16 cards.

- 0 - The region specifications are not to be changed.
- 1 - Read new region specifications. If writing to the disc files for the first time during the current run, MDATP must be entered as one and at least one of the MAPP(I) variables must be greater than zero.

8.10 Mapping Control

NOTE: Enter the following data in READ R2-14, R2-14.5, R2-15 only if contour maps are desired, i.e., if MAP \neq 0000 (READ R2-13-1) and if MDAT = 1 (READ R2-13-1).

READ R2-14 (2I5)

LIST: NORNX Y, NORNX Z

- NORNX Y Map orientation factors for vertical and areal
- NORNX Z maps, respectively.

- 0 - The map is printed with x-coordinate (r for radial geometry) increasing from left to right and y (or z) increasing up the computer page, i.e., the $x=0, y/z=0$ point is the bottom left hand corner.
- 1 - x increases from left to right and y (or z) increases down the computer page. The origin is the upper left hand corner. Use this for cross sections as depth is positive downward.

READ R2-14.5 (4E10.0)

LIST: XYXL, XYYL, XZXL, XZZL

- | | |
|------------|--|
| XYXL, XYYL | The x and y map lengths in inches, respectively for all the areal maps. |
| XZXL, XZZL | The x/r and z map lengths in inches, respectively for all the vertical maps. |

NOTE: Assume output device is 10 characters per inch, 6 lines per inch.

READ R2-15 (6I5, 2E10.0)

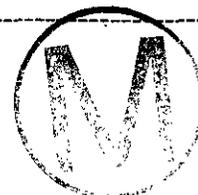
NOTE: Enter one card for each map requested on R2-13-1 card. For example, if MAP = 0103, areal pressures, areal concentration and vertical concentration maps will be generated. Therefore, three data cards should be entered here for this example.

LIST: I1(I), I2(I), J1(I), J2(I), K1(I), K2(I), AMIN(I), AMAX(I), I = 1, Number of MAPS requested.

- | | |
|------------|--|
| I1, I2 | Lower and upper limits, inclusive, on the I-coordinate of the region to be mapped. |
| J1, J2 | Lower and upper limits, inclusive, on the J-coordinate of the region to be mapped. |
| K1, K2 | Lower and upper limits, inclusive, on the K-coordinate of the region to be mapped. |
| AMIN, AMAX | The minimum and maximum values of the variable used to derive the 20 contour intervals. If the variable in any grid block is higher than |

AMAX, it will be indicated as AMAX. If AMAX is entered as zero, the program will search for the maximum among all the grid block values and use it as AMAX. Similarly, a large negative number for AMIN (≤ -99) will cause the program to search for the minimum and use it as AMIN.

READ R2-16 (6I5, RE10.0)



NOTE: Read only if MDATP (READ R2-13-2) > 0.

Enter one card for each of the disc files requested, in the variables: MAPP(1), MAPP(2), MAPP(3) and MAPP(4) on the R2-13-2 card. Thus, out of the 16 digits (including blanks) entered in these (MAPP(I), I = 1,4) variables, if there are six "ones" and two "twos" entered, ten cards should be input here. Then the first card relates to the variable governing the left most non zero entry in the (MAPP(I), I = 1,4) variables. The last card relates to the right most non-zero entry in the MAPP variables.

LIST: (I1(I), I2(I), J2(I), K1(I), K2(I), AMIN(I), AMAX(I), VSCALE(I), TSCALE(I)), I = 1, Number of disc files requested.

NOTE: Number of disc files requested must be ≤ 16 .

- | | |
|-----------|--|
| I1, I2 | Lower and upper limits, inclusive, on the I-coordinate of the region. |
| J1, J2 | Lower and upper limits, inclusive, on the J-coordinate of the region. |
| K1, K2 | Lower and upper limits, inclusive, on the K-coordinate of the region to be mapped. |
| AMIN,AMAX | The minimum and maximum values of the variable used to derive the plots on the PC. Currently, these values are not used. |
| VSCALE | If positive, this is the factor by which the dependent variable within the defined region will be divided before being written to disc. This factor is not used with velocities. |
| TSCALE | If positive, this is the factor by which the time at which the dependent variable is written to disc is divided. |

If VSCALE or TSCALE or 0, the default value of 1.0 is used by SWIFT II. These two scalars allow the user to simulate in one set of units yet print out results to files in another set which might be more

desirable for plotting. The user may also de-dimensionalize and quickly view results in terms of dimensionless pressure, dimensionless time, dimensionless concentration, etc.

Output to the Disc Files:

The variable written to the Disc files and their format is given below. There is one record (line) for every grid block. The output and the format remains the same for all the disc files, except for the velocity file (Disc File 23).

For all files except the velocity file:

<u>Entry</u>	<u>Variable</u>
1	X coordinate of the grid block center
2	Y coordinate of the grid block center
3	Plot variable (pressure or head or density, etc).
4	Time (sec)
5	I (grid block index: x-direction)
6	J (grid block index: y-direction)
7	K (grid block index: z-direction)
8	Height of the grid block center above the datum

Format (5x, 4(2x, G16.8), 3I5, G16.8)

However for the velocity file, the entries are as below:

<u>Entry</u>	<u>Variable</u>
1	X coordinate of the grid block center
2	Y coordinate of the grid block center
3	Darcy velocity: x-direction
4	Darcy velocity: y-direction
5	Resultant (Darcy) velocity
6	Angle of the resultant velocity with positive direction of the x-axis (0° - 360°)
7	Porosity
8	Time (sec)
9	I (grid block index: x-direction)
10	J (grid block index: y-direction)
11	K (grid block index: z-direction)
12	Height of the grid block center above the datum

Format (5x, 8(2x, G10.4), 3I5, G10.4)



Variables Written as Specified in The R2-13-2 and R-2-16 Cards

<u>Variable Name</u>	<u>Disc File Unit Number</u>	<u>Filename</u>
Pressure	21	SWIFTPAE
Freshwater Heads	22	SWIFTFWH
X,Y Darcy Velocities	23	SWIFTVEC
Temperature	25	SWIFTTEM
Brine Concentration	29	SWIFTBRN
Fluid Density	30	SWIFTDEN
Concentration Parent Radionuclide	33	SWIFTPR1
Concentration Radionuclide - Comp 2	34	SWIFTPR2
Concentration Radionuclide - Comp 3	35	SWIFTPR3



General I/O Unit Numbers and File Names

<u>Unit</u>	<u>Purpose</u>	<u>Form</u>	<u>Filename</u>
15	Data Input	(Formatted)	SWIFTINP
16	Printed Output	(Formatted)	SWIFTOUT
4	Restart Record Input	(Unformatted)	SWIFTRSI
7	Velocity Output	(Unformatted)	SWIFTVEL
8	Restart Record Output	(Unformatted)	SWIFTRSO
9	Nuclide Monitoring Data Output	(Formatted)	SWIFTNMD
11	Data for Use by GRASP Code	(Unformatted)	SWIFTGRS
12	Well Plotting Data Output	(Formatted)	SWIFTWEL
21	Pressure at Elevation	(Formatted)	SWIFTPAE
22	Freshwater Heads	(Formatted)	SWIFTFWH
23	Velocity Vectors in x-y Plane	(Formatted)	SWIFTVEC
24	Not Used	---	---
25	Temperature	(Formatted)	SWIFTTEM
26	Not Used	---	---
27	Not Used	---	---
28	Not Used	---	---
29	Brine Connection	(Formatted)	SWIFTBRN
30	Fluid Density	(Formatted)	SWIFTDEN
31	Not Used	---	---
32	Not Used	---	---
33	Parent Radionuclide Concentration	(Formatted)	SWIFTPR1
34	Radionuclide Comp. 2	(Formatted)	SWIFTPR2
35	Radionuclide Comp. 3	(Formatted)	SWIFTPR3
36	Not Used	---	---
41	External Discharge Region 1	(Formatted)	SWIFTER1
42	External Discharge Region 2	(Formatted)	SWIFTER2
43	External Discharge Region 3	(Formatted)	SWIFTER3
44	External Discharge Region 4	(Formatted)	SWIFTER4
45	Internal Discharge Region 1	(Formatted)	SWIFTIR1
46	Internal Discharge Region 2	(Formatted)	SWIFTIR2
47	Internal Discharge Region 3	(Formatted)	SWIFTIR3
48	Internal Discharge Region 4	(Formatted)	SWIFTIR4



NOTE: The data entered up to this point are sufficient for simulation of the system through time TCHG. To continue, another recurrent data set is read. However, to terminate the simulation phase of the run, one should enter ITHRU = 1 in a single READ R2-1 termination card. If any plots are desired, i.e., if NPLP or NPLT or NPLC equals one, then the plotting data (READ P-2 through P-4) should follow. If no plots are desired, then ITHRU = 1 will terminate the execution.

9. THE P CARDS



The P cards, like the M cards, are read by the main routine. Here, however, the input is identified by its function (plotting) rather than by the routine from which it is read. Plotting, within the SWIFT model, is identified with well data in that pressure, temperature, and brine concentrations, both at the surface and at the bottom-hole, may be plotted as functions of time. Table 9-1 exhibits the various dependent variables which may be plotted as functions of the well characteristics. Plots for an observation well are particularly useful since they simply indicate the behavior of the grid-block variables as functions of time.

In order to facilitate model calibrations, printer plots are used. The time axis is always directed down the page with range and resolution determined by the input parameters. The dependent-variable axes, on the other hand, are always directed across the page. Here the range is determined externally by the input parameters, but the resolution is fixed internally in that the specified range is divided into 100 columns in each case. The plotting symbols which are used are given in Table 9-2. If there are several values of the dependent variables within the prescribed resolution on the time scale, then the average value is plotted. If there are no such values, no values are plotted.

NOTE: Calculated plot data is stored by the code on file SWIFTWEL. If plots are desired for a previous run, then this file must exist.

NOTE: If $NPLP = 0$, $NPLT = 0$, and $NPLC = 0$ (READ M-2) (i.e., no plots are desired), skip all P cards.

NOTE: The plotting data for one well consist of the data from READ P-2 through READ P-4. Enter as many sets of these data as there are wells for which plots are desired. If plots are desired for all the wells, enter NWT (READ R2-4) sets of these data. If less than NWT sets are entered, then follow the last set with a blank card to end the input of plotting data.

READ P-2 (I5, 5X, 10A4) Well Identity.

Table 9-1

Dependent Plotting Variables Versus Well Characteristics

<u>Well Type</u>	<u>Point of Specification¹</u>	<u>Plotting Variables^{2,3}</u>	
		Bottom-Hole	Surface
Observation ⁴	-	p, T, C	
Injection	Bottom-Hole	p	
Injection	Surface	p, T	p
Production	Bottom-Hole	p, T, C	
Production	Surface	p, T, C	p, T

¹ The point of specification is controlled by integer ISURF (READ M-2), i.e., ISURF = 0 for bottom-hole conditions and ISURF = 1 for surface conditions.

² Notation here is consistent with that of Reeves et al. (1986b), i.e.,

p - pressure
 T - temperature
 C - brine concentrations

³ The list of plotting variables given here assumes that NCALL = 0 (READ M-2).

⁴ An observation well is defined by the flow rate, Q = 0.

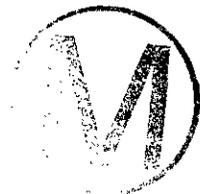


Table 9-2

Plotting Symbols

<u>Symbol</u>	<u>Data Type</u>
X	Calculated
0	Observed
*	Coincident Calculated and Observed

LIST: KW, ID

KW The well number.
ID A title to the plots for well number KW.

READ P-3 (7F10.0) Variable Ranges and Resolutions.

LIST: TMN, TMX, D1, PWMN, PWMX, PSMN, PSMX, TWMN, TWMX, TSMN, TSMX, CMN, CMX

TMN Lower limit on time, d (s).
TMX Upper limit on time, d (s).
D1 time step for each row, d (s).



NOTE: The three parameters immediately above determine the number of rows, NROWS, to be used, i.e., $NROWS = (TMX - TMN) / D1$. Current fixed dimensions restrict this quantity to $NROWS \leq 400$.

NOTE: If D1 is set to zero, then, a default value is calculated assuming 50 rows, i.e., $D1 = (TMX - TMN) / 50$.

PWMN,PSMN,
TWMN,TSMN Lower limits on bottom-hole pressure, psi
(Pa): face pressure, psi (Pa): bottom-hole temperature, surface
temperature, °F (°C): and brine concentration, dimensionless,
respectively.

PWMX,PSMX,
TWMX,TSMX Upper limits on bottom-hole pressure, psi
(Pa): surface pressure, psi (Pa): bottom-hole temperature, °F (°C):
surface temperature, °F (°C): and brine concentration,
dimensionless, respectively.

NOTE: If there are no observed data, then enter any negative number in the first field of the following record. Fixed P-4 dimensions limit the number of values for any one variable to 300 or less. If there are such data, then enter up to 300 (inclusive) of these records in the read set below, and terminate the read with any negative number in the first field.

READ P-4 (6F10.0) Observed Data.

NOTE: Read as many cards (up to 300) as there are observed data points (one card for each value of time at which the observed values are available). Follow the last card with a negative number in the first field specification (F10.0).

LIST: TOX, POW, POS, TOW, TOS, COC

TOX	Observation time, d (s).
POW	Bottom-hole pressure, psi (Pa).
POS	Surface pressure, psi (Pa).
TOW	Bottom-hole temperature, °F (°C).
TOS	Surface temperature, °F (°C).
COC	Brine concentration, dimensionless.



10. USE OF AUXILIARY DISC FILES



Auxiliary disc files are used by the SWIFT model to perform the six different functions given in Table 10-1. Two of these functions are standard input and standard output, which require no discussion. The others consist of calculational restarts, mapping restarts, plots of well data, and streamline postprocessing. These functions are discussed below.

10.1 Calculational Restarts

Figure 10-1 shows the basic sequence of events for restarting a calculation. As illustrated there, unit 8 is written during the execution of the direct run. This information is then read from unit 4 and the first restart run commences. Although it is not illustrated by the figure, another restart record may be written (on unit 8) during the second execution and the restarting process may be continued indefinitely.

Aside from the temporary-storage variables, which are defined locally within each subroutine, all scalars and arrays are partitioned within the four common-block arrays shown in Table 10-2. A restart procedure is initiated by simply setting the control

$$\text{RSTWR} = 1 \qquad (\text{READ R2-13-1}) \qquad (10-1)$$

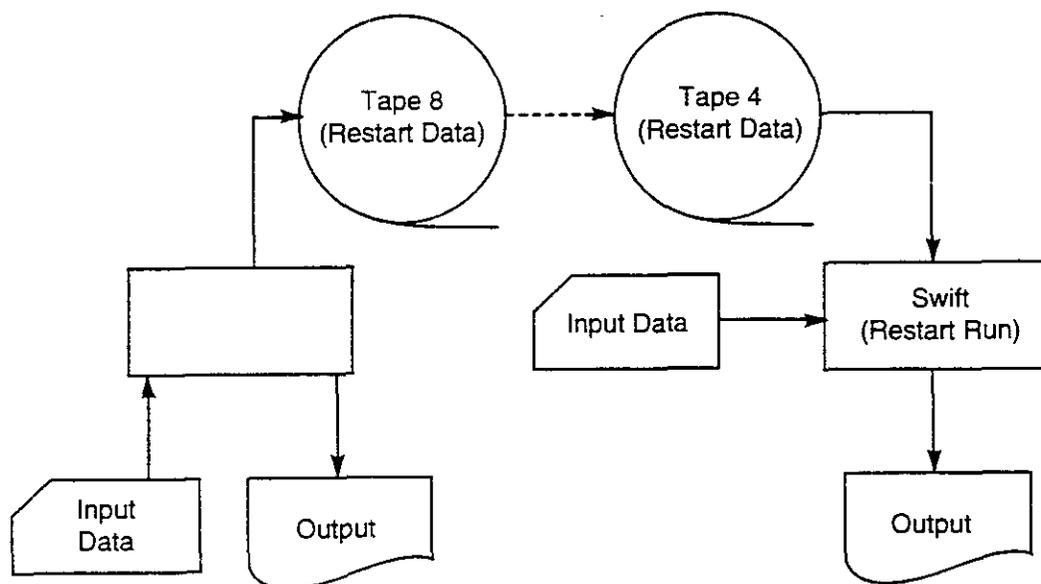
If this is done, say, by the direct run of Figure 10-1, then the common-block arrays are written on auxiliary storage using the following unformatted write commands:

$$\begin{array}{ll} \text{WRITE}(8) & (\text{TWRITE}(I), I = 1, \text{LTWRT}) \\ \text{WRITE}(8) & (\text{G3}(I), I = 1, \text{IG3LST}) \\ \text{WRITE}(8) & (\text{G2}(I), I = 1, \text{IG2LST}) \\ \text{WRITE}(8) & (\text{G}(I), I = 1, \text{IGLSTR}) \\ \text{WRITE}(8) & (\text{IG}(I), I = 1, \text{IGLSTI}) \end{array} \qquad (10-2)$$

For protection against an abnormal termination, it is a good practice to write restart records at several different times during a relatively long run. The calculation may be restarted with the control

$$\text{RSTRT} = \text{ITIME} \qquad (\text{READ M-2}) \qquad (10-3)$$

where *ITIME* indicates the time step of the particular restart record which is to be used to initialize the follow-up calculation. The code then simply reads the list of restart records written during the previous run(s) until the appropriate one is found, loads the common block arrays and continues the calculation. A list of the appropriate data input is given in Table 10-3.



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Figure 10-1. Schematic of a Restart Calculation.

Table 10-1

Auxiliary Disc files Used by SWIFT II

<u>Unit</u>	<u>Function</u>	<u>Filename</u>
4	Input for restart calculation	SWIFTRSI
5	Standard input	SWIFTINP
6	Standard output	SWIFTOUT
7	Output for streamline postprocessing	SWIFTVEL
8	Output for subsequent restart calculation	SWIFTRSO
9	Output for nuclide monitor post-processing	SWIFTNMD
12	Input and output for plotting via SWIFT	SWIFTWEL

Table 10-2

Memory Utilization by SWIFT II

<u>Array</u>	<u>Dimension</u>
TWRITE	LTWRT
G3	IG3LST
G2	IG2LST
G	IGLSTR
1G	IGLST1



Table 10-3

Data Input for a Computational Restart

<u>Card Identifier</u>	<u>Function</u>
M-1	Title
M-2	Option Parameters (RSRT >0)
R2Group(s)	Recurrent-Data Input
P Group*	Plotting of Well Data

* Optional depending upon values of NPLP, NPLT and NPLC.

10.2 Mapping Restarts

Assume that an auxiliary disc file has been loaded with several restart records, as described in the preceding section, and that it is desired to map the results present in some of those records. There are options in SWIFT that permit this to be done. The configuration is similar to that shown on the right-hand side of Figure 10-1. Thus, unit 4 contains the restart data that is read by the code, along with data from cards, and maps are obtained in the output. The necessary card input is presented in Table 10-4. Basically, the function of this entire set of input data is to search the auxiliary unit for the appropriate restart record(s), as indicated by the time-step number(s), and then to map the primary variables as contour plots over the specified spatial domain. Mapping specifications may be changed from that originally given (at the time the restart record was made) as desired.

10.3 Plots of Well Data

As in the case of mapping, plots may be obtained either at the time of a calculational run or from a separate plotting run. The purpose of this section is to elaborate on the latter. Figure 10-2 configures the case to be considered. As illustrated there, all plotting variables are written on Unit 12 by SWIFT. Providing, then, that this auxiliary file has been properly preserved, it may be attached for a plotting run.

To write unit 12, a formatted output statement is used, specifically,

```
WRITE(12,1670) KW, I2, TCX(IPT), PCW(IPT), PCS(IPT), TCW(IPT),  
TCS(IPT), CCC(IPT), QW(IPT)
```

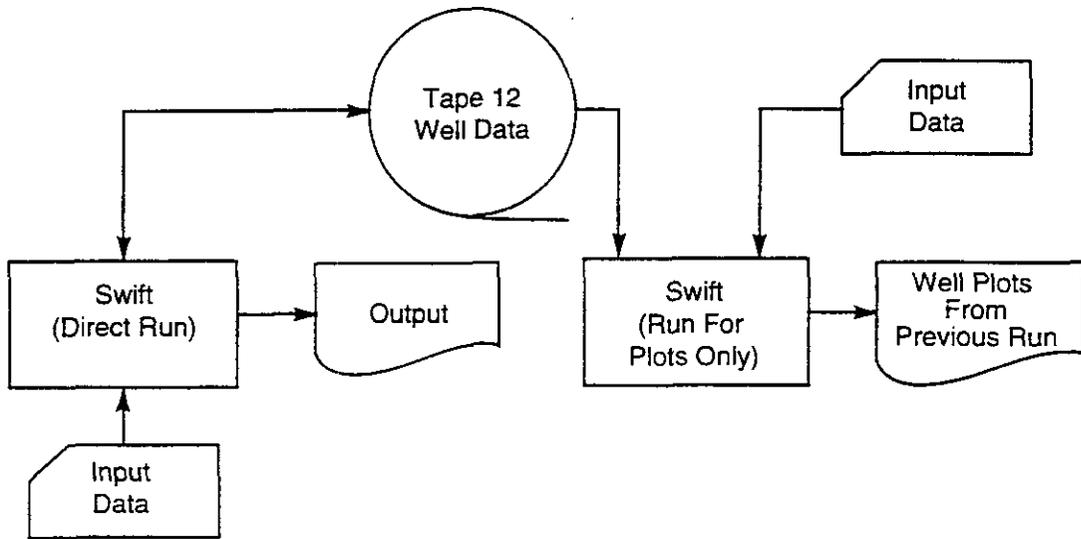
```
1670 FORMAT (2I5,7E10.3)
```

The variables are defined as follows:

KW	Well number
I2	Control parameter
TCX	Time
PCW	Pressure at bottom-hole
PCS	Pressure at surface
TCW	Temperature at bottom-hole
TCS	Temperature at surface
CCC	Brine concentration
QW	Well flow rate



A record of the above form is written for each time step during the calculation.



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Figure 10-2. Schematic of Plotting from a Previous Run.

Table 10-4

Data Input for a Mapping Restart

<u>Card Identifier</u>	<u>Function</u>
M-1	Title
M-2	Option Parameters (RSTRT = -1)

---First Map From Restart Record---

M-6	Time-Step Number (IMPT > 0)
M-7	Mapping Control
R2-14 - R2-15*	Map Specifications

---Additional Maps From Restart Records+

M-6 - R2-15	
-	
-	
M-6	Blank



* Optional depending on MDAT and MAP (READ M-7)
 + Enter as many sets of these data as desired.

In contrast to the writing of a restart record, the writing of Unit 12 is not controlled by an integer such as RSTWR (READ R2-13). It is controlled only by the requirement that there must be wells in the system, i.e., NWT > 0 (READ R2-4). The control parameter I2 specifies the plots that are to be made. As discussed in Chapter 9 (see especially Table 9-1) the specification of plotting variables depends upon the well characteristics. Thus, only a selected number of the dependent variables of the above output list will be plotted depending upon whether the well is an injection, production or observation well and upon whether surface or bottom-hole conditions are specified. Parameter I2 takes into account these factors.

The additional information necessary for plotting is entered on the standard input unit. Table 10-5 characterizes this data. As illustrated, negative values of the plot controls NPLP, NPLT and NPLC (READ M-2) are necessary to trigger the plotting from a previous run in that control is transferred immediately to the plotting routines. As many wells as desired may be used for plotting.

Table 10-5

Data Input for Plots from a Previous Run

<u>Card Identifier</u>	<u>Function</u>
M-1	Title
M-2	Option Parameters (NPLP<0, NPLT <0)
P-2 - P-4	Data for One Well
P-2 - P-4	Data for Another Well*

* Enter data for each well for which plots are desired.

10.4 Streamline Postprocessing

It is frequently helpful to present flow results in terms of streamlines. For this reason the appropriate information is written to the auxiliary file so that it may be processed by a streamline postprocessor. Figure 10-3 gives the configuration of such an operation. As shown there, Unit 7 is prepared during the SWIFT run and is subsequently read by a streamline utility. The latter is denoted there by the acronym "STLINE".

The first six records of information on unit 7 comes from the unformatted output statements:

```
WRITE(7) TITLE  
WRITE(7) LBDAT, LBTIM  
WRITE(7) NX, NY, NZ  
WRITE(7) (DELX(I), I=1, NX)  
WRITE(7) (DELY(I), J=1, NY)  
WRITE(7) (DELZ(I), Z=1, NZ)
```

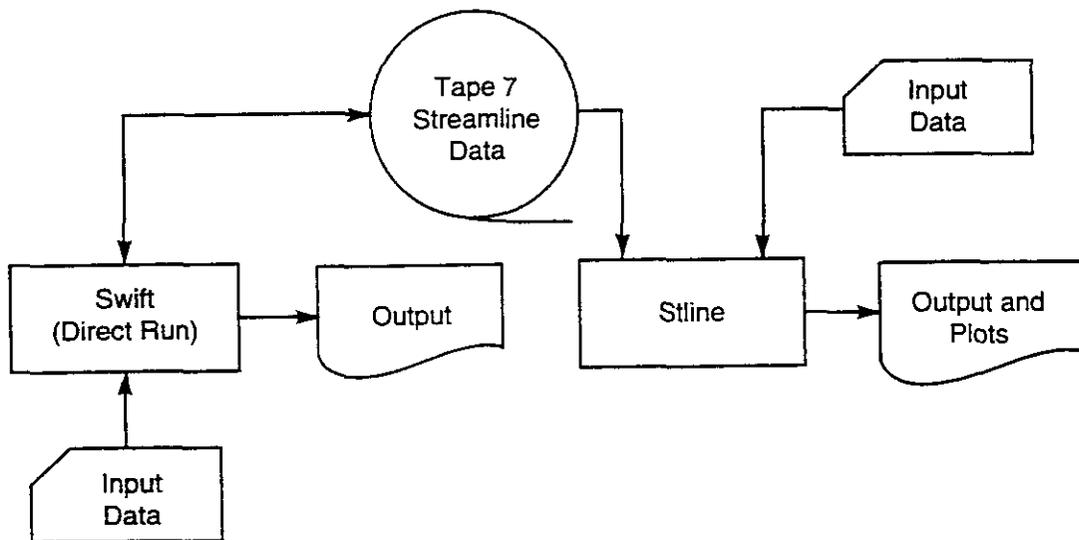


They contain the title, date and time of run, incrementation integers, NX, NY and NZ and the increments, DELX, DELY, and DELZ. The five records on Unit 7 are created from the following unformatted writes:

WRITE(7)	TIME
WRITE(7)	(PV(M),M = 1,NB)
WRITE(7)	(UXX(M),M = 1,NB)
WRITE(7)	(UYX(M),M = 1,NB)
WRITE(7)	(UZZ(M),M = 1,NB)

They contain time, pore volumes, PV, and Darcy velocities, UXX, UYY and UZZ. The writing of unit 7 is controlled by the integer IIPRT (see READ R2-13).





TRI-6342-4686-2



Figure 10-3. Schematic of Streamline Postprocessing.

11. REFERENCES



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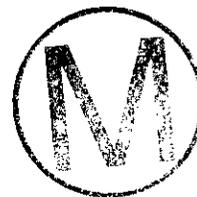
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APPENDIX A



DEFINITION OF INPUT VARIABLES

ACS(NRT)	Product of the rate of salt dissolution and the mass fractions of solubles to total dry mass, d^{-1} (s^{-1}).
AKSD(NRTD)	Permeability of the local subsystems, ft/d (m/s).
ALCH	Leach time for radioactive waste within the repository boundaries, d (s).
ALPD(NRTD)	Dispersivity within the local subsystem, ft (m).
ALPHAL(NRT)	Longitudinal dispersivity within the global system, ft (m).
ALPHAT(NRT)	Transverse dispersivity within the global system, ft (m).
ALPHL	Longitudinal dispersivity within the global system, ft (m).
ALPHT	Transverse dispersivity within the global system, ft (m).
AMAX	Maximum contour value in plotting submodel.
AMIN	Minimum contour value in plotting submodel.
AP	Fraction of parent component KP that decays to the component I.
ARHLD(NTIME)	Areal density of the repository heat source, Btu/ft ² -d (J/m^2 -s).
BHP	Bottom-hole pressure for a well, psi (Pa).
BLCH	Lag time for initiation of leaching of waste from repository, d (s).
BROCK	Rock density of the solid particle, lb/ft ³ (kg/m^3).
BWAQ	External aquifer fluid density (Carter-Tracy aquifer parameter), lb/ft ³ (kg/m^3).

BWRI	Density of the contaminated fluid ($C = 1$) at PBWR and TBWR, lb/ft^3 (kg/m^3).
BWRN	Density of the natural reservoir fluid ($C = 0$) at PBWR and TBWR, lb/ft^3 (kg/m^3).
CINT	Initial concentration (brine and radionuclide) of each of the blocks within a defined region, mass fraction.
CINJ	Brine concentration in the injection fluid, mass fraction.
CMN	Lower limit on the brine concentrations to be plotted, mass fraction.
CMX	Upper limit on the brine concentrations to be plotted, mass fraction.
CNAME(2)	Identification of the radioactive component.
CNDUM(NTIME)	Radionuclide concentrations within the unleached repository wastes, expressed as mass per unit volume of wastes (see CTIME), lb/ft^3 (kg/m^3).
COC	Observed concentrations to be plotted, mass fraction.
CON	Conversion factor for the thermal conductivities to obtain units of $\text{Btu/ft-d-}^\circ\text{F}$ ($\text{J/m-s-}^\circ\text{C}$).
CONVC	Conversion factor for the waste concentrations to obtain units of lb/ft^3 (kg/m^3).
CONVH	Conversion factor for the repository heat densities to obtain units of $\text{Btu/ft}^2\text{-d-}$ ($\text{J/m}^2\text{-s}$).
CONVL	For canistered wastes, CONVL multiples SDRIFT, SCNSTR, DCNSTR, and HCNSTR to convert them to ft^3 (m^3). For uncanistered wastes CONVL multiplies only DCNSTR to convert it to ft^3 (m^3) of wastes per bulk ft^3 (m^3).
CONVT	Conversion factor for the interpolation times to obtain units of d (s).
CPOB	Heat capacity of the overburden, $\text{Btu/ft}^3\text{-}^\circ\text{F}$ ($\text{J/m}^3\text{-}^\circ\text{C}$).
CPR	Heat capacity of the fluid-saturated global medium, $\text{Btu/ft}^3\text{-}^\circ\text{F}$ ($\text{J/m}^3\text{-}^\circ\text{C}$).

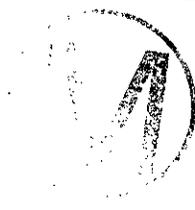


CPRKD(NRTD)	Heat capacity of the fluid saturated local medium, Btu/ft ³ -°F (J/m ³ -°C).
CPRI(NZ)	Heat capacity of the fluid-saturated global medium with cylindrical geometry, Btu/ft ³ -°F (J/m ³ -°C).
CPUB	Heat capacity of the underburden, Btu/ft ³ -°F (J/m ³ -°C).
CPW	Heat capacity of the reservoir fluid, Btu/lb-°F (J/kg-°C).
CR	Compressibility of pore structure within the global system, psi ⁻¹ , (Pa ⁻¹).
CRD	Compressibility of the pore structure within the local subsystems, psi ⁻¹ , (Pa ⁻¹).
CRTDST	Time-dependent values of pore structure compressibility, psi ⁻¹ , (Pa ⁻¹).
CS(NCP)	Solubility limit, mass fraction.
CTAQ	Total compressibility of the external aquifer (Carter-Tracy aquifer parameters) psi ⁻¹ , (Pa ⁻¹).
CTIME(NTIME)	Interpolation time for concentrations within the unleached waste and/or heat density in the repository (see CNDUM and ARHLD), d (s).
CTW	Coefficient of thermal expansion of the reservoir fluid, °F ⁻¹ (°C ⁻¹).
CW	Compressibility of the reservoir fluid, psi ⁻¹ , (Pa ⁻¹).
C1	Boundary brine concentration of the global system, mass fraction.
DAMPX	Damping factor used in the wellbore calculations, dimensionless.
DCMX	Maximum change desired per time step in the trace-component concentration, mass fraction.
DCNSTR	For canistered wastes, the diameter of each canister in ft (m). For uncanistered wastes, the volumetric waste density, volume of waste/bulk volume.
DEC(NCP)	Component half-life in years.



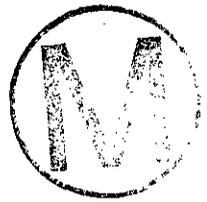
DELPW	For the wellbore submodel, the incremental value of pressure used in wellbore integrations, psi (Pa).
DELX(NX)	Length of each column of blocks in the x direction, ft (m).
DELY(NY)	Length of each column of blocks in the y direction, ft (m).
DELZ(NZ)	Thickness of each vertical layer, ft (m).
DEPTH	Depth to top of grid-block (1,1,1) from the reference plane, ft (m).
DI(2,NCP)	Identification of the radioactive component I.
DIS(NCP)	Adsorption coefficient χ for a Freundlich isotherm in the global system, $(\text{ft}^3/\text{lb})\eta$ or $(\text{m}^3/\text{kg})\eta$.
DIS(2*NCP)	Adsorption coefficient η for a Freundlich isotherm in the global system, dimensionless.
DISD(NCP)	Adsorption distribution coefficient for the local system, $(\text{ft}^3/\text{lb}) (\text{m}^3/\text{kg})$.
DMEFD(NRTD)	Molecular diffusivity for the local medium, $\text{ft}^2/\text{d} (\text{m}^2/\text{s})$.
DMEFF	Molecular diffusivity in the global medium, $\text{ft}^2/\text{d} (\text{m}^2/\text{s})$.
DMEF(I)	Global brine molecular diffusion coefficient defined as a function of rock type, $\text{ft}^2/\text{day} (\text{m}^2/\text{s})$.
DMEFR(I)	Molecular diffusion coefficient defined as a function of rock type (NRT) and nuclide (NCP), $\text{ft}^2/\text{day} (\text{m}^2/\text{s})$.
DMFDI(NRTD)	Coefficient of thermal increase in diffusivity for the local medium, $^{\circ}\text{F}^{-1} (^{\circ}\text{C}^{-1})$.
DMEFRD(IC)	Molecular radionuclide diffusion coefficient for the local system, specified according to nuclide and rock type, $\text{ft}^2/\text{day} (\text{m}^2/\text{s})$.
DPMX	For automatic time stepping, the maximum pressure change (over the grid) desired per time step, psi (Pa).
DS(NSD)	Separation of nodes I and I+1 in the local subsystems, a function of rock type, ft (m).
DSD(NRTD)	Local increment at the system interface, ft (m).

DSDO(NRTD)	Local increment at the outer extremity of the subsystem, ft (m).
DSMX	For automatic time stepping, the maximum change in brine concentration (over the grid) desired per time step, mass fraction.
DT	Time-step specification, d (s).
DTMAX	For automatic time stepping, the maximum time step allowed, d (s).
DTMIN	For automatic time stepping, the minimum time step allowed, d (s).
DTPMX	For automatic time stepping, the maximum temperature change desired per time step, °F (°C).
DW	Inside wellbore diameter, ft (m).
DZOB	Thickness of each overburden block, ft (m).
DZUB	Thickness of each underburden block, ft (m).
ED	Inside tubing roughness, ft (m).
EPS	Tolerance on the calculation of temperature within the wellbore, °F (°C).
FAB	Factor by which the aquifer-influence coefficient VAB will be modified, dimensionless.
FAMD	Modification for cross-sectional area of dual porosity block.
FPHI	Factor by which porosity (as used in heat storage calculation) will be modified.
FPV	Modification factor for the pore volume, dimensionless.
FTUX	Modification factor for x-direction Darcy velocity, heat and solute dispersion coefficients.
FTUY	Same as FTUX, but for y direction.
FTUZ	Same as FTUX, but for z direction.
FTX	Modification factor for the x-direction transmissibility, dimensionless.



FTY	Same as FTX, but for y direction.
FTZ	Same as FTX, but for z direction.
GRAV	Gravitational acceleration constant, $\text{ft/s}^2(\text{m/ s}^2)$.
HADD	Depth modification factor, ft (m).
HCNSTR	Canister height for the waste-leach model, ft (m).
HDATUM	Datum depth measured relative to the reference plane, ft (m).
HINIT	Depth used for setting up initial pressure condition (see PINIT), ft (m).
HTG	Geometry/heterogeneity control parameter.
I	Dummy index.
IAQ	Control parameter for aquifer-influence functions and boundary conditions.
IBUD	Number of L2SOR iteration sweeps.
ICRSS	Control parameter for determining how the cross-derivative terms in the dispersivity tensor are treated.
IICL	Control parameter for changing the mode of solution of the primary equations.
ICOMP	Control parameter for initializing the brine concentrations.
ID	Title of the plots for a specific well.
IDIR	The boundary face over which integrated release is to be considered for the region IREG (internal nuclide discharge region specification).
IDSC	Position and orientation control for the local subsystems.
IFD	Position and orientation control for the local subsystems.
IFREE	Control parameter for free-water surface.
IIC1	Uppermost layer in which the well is completed.

IIC2	Lowermost layer in which the well is completed.
IINDWI	Well specification option.
IIPRT	Printing control for intermediate variables in the global system.
IIPRTD	Printing control for intermediate variables in local subsystems.
IIS	I-index location of a source block for fluid, heat, or radionuclides.
IIW	I-index location of a grid cell containing a well.
IJS	J-index location of a source block for fluid, heat, or radionuclides.
IJW	J-index location of a grid cell containing a well.
IKS	K-index location of a source block for fluid, heat, or radionuclides.
ILEVEL	Indicator for specifying either canistered waste storage or uncanistered waste storage.
IMETH	Control parameter for reading the method of solution.
IMPG	Number of time steps after which the optimum parameters for the inner iterations are recalculated for the two-line successive overrelaxation method.
IMPT	Time-step number at which maps are desired.
INAT	Control parameter for entering the initial fluid velocity.
INDQ	Control parameter for reading well rates.
INDT	Control parameter for iteration data for the reservoir solution.
IOPT	Control parameter for reading iteration data for the wellbore solution.
IPINT	Control integer specifying whether the initial pressure for the model initial conditions are to be used as input from file SWIFTINT or are to be calculated internally.
IREG	Control parameter governing whether the user wants to consider the model boundary block edges as nuclide biosphere discharge points. A maximum of 4 internal discharge areas may be specified.



I01	Frequency control parameter for output of the time-step summaries.
I02	Frequency control parameter for output of the well summaries.
I03	Control parameter for entering printing specifications of the grid-block values for the primary variables.
I03P	Frequency control parameter (similar to parameters I01 through I06) governing the frequency at which output files will be written to SWIFT.
I04	Control parameter for listing layer allocations of the injection/production rate.
I05	Control parameter for listing the grid-block values of radionuclide concentrations for the global systems.
I05D	Control parameter for listing the grid-block values of the radionuclide concentrations for the local subsystems.
I06	Control parameter for listing the aquifer influence rates.
I08	Control parameter for selectively listing the grid-block values of the primary variables for the global system.
I08D	Control parameter for selectively listing the grid-block values of the primary variables for the local subsystems.
IPROD	Control parameter for reading wellbore data.
IRCH	Control parameter for reading recharge data.
IRD	Control parameter for initializing the concentrations of the radioactive trace components.
IRSS	Control parameter for reading source data for fluid, heat, and radioactive components.
IRT,IR	Rock-type indicators for the global system and for the local subsystems.
ISURF	Control parameter for the wellbore calculations.
ITHRU	Run termination control and pressure-at-datum option parameter.



IUNIT	Units control parameter specifying either the English Engineering system or the SI system.
IWELL	Control parameter for reading well-definition data.
IXYZ	Control parameter for directional sweep of L2SOR.
I1	Parameter used several times to specify the lower limit on the I index of a region.
I1A	Same as I1.
I1B	Same as I2.
I2	Parameter used several times to specify the upper limit on the I index of a region.
JDSC	Nuclide monitor block, J index.
J1	Parameter used several times to specify the lower limit on the J index of a region.
J1A	Same as J1.
J1B	Same as J2.
J2	Parameter used several times to specify the upper limit on the J index of a region.
KAQ	Control parameter for setting boundary conditions on the heat-flow equation.
KBC(NRTD)	Local boundary-condition control.
KCNVD	Convection/dispersion control for the local subsystems.
KCPINJ(I)	If transport of radionuclide is taking place, variable which causes SWIFT II to implicitly correct the concentration of that radionuclide in the specified block (according to the fluid flux in or out of the block).
KDSC	Nuclide monitor block, K index.
KGDP(NRTD)	Local geometry control.



KGRD(NRTD)	Local grid control.
KH	The conductivity-thickness of the aquifer, ft^2/d (m^2/s).
KHEAT	Control parameter for the areal repository heat source.
KHL	Layer-allocation factor for the well, dimensionless.
KOB	Vertical thermal conductivities of the overburden, $\text{Btu}/\text{ft-d-}^\circ\text{F}$ ($\text{J}/\text{m-s-}^\circ\text{C}$).
KOUT	Output control parameter for the global system.
KOUTD	Output control for the local subsystems.
KOUTG	Output control for adjoint solver that specifies whether to write GRASP output files.
KP(NP)	Parent component number.
KPAQ	Control parameter solving whether the variable PAQ will be read in card R1-31-2 (see PAQ).
KPB(NRTD)	Pressure-boundary control for the local subsystems.
KSLVD	Local control parameter for solution of both primary and radionuclide equations.
KSWAQ	Control parameter solving whether the variable SWAQ will be read in card R1-31-2 (see SWAQ).
KSWB(NRTD)	Brine boundary control for the local subsystems.
KTPAQ	Control parameter governing whether the variable TPAQ will be read in card R1-31-2 (see TPAQ).
KTPB(NRTD)	Temperature boundary control for the local subsystems.
KUB	Vertical thermal conductivities of the underburden, $\text{Btu}/\text{ft-d-}^\circ\text{F}$ ($\text{J}/\text{m-s-}^\circ\text{C}$).
KW	Well number identifying a well for plots.
KR(NB)	Hydraulic conductivity in the x direction for the global system, ft/d (m/s).
KY(NB)	Same as KX, but in the y direction.

KYY(NZ)	Hydraulic conductivity in the radial direction for cylindrical coordinates, ft/d (m/s).
KZ(NB)	Same as KX, but in the z direction.
KZZ(NZ)	Same as KYY, but in the z direction.
K1	Parameter used several times to specify the lower limit on the K index of a region.
K1A	Same as K1.
K1B	Same as K2.
K2	Parameter used several times to specify the upper limit on the K index of a region.
LADJ(NCP)	Lambda index for adjustment of the rate constant of a radioactive component.
LBIO	Control option for nuclide monitor blocks.
LIBOR	Control option for indicating the use of an internal nuclide discharge region.
MAP	Control parameter for selectively printing contour maps for the dependent variables.
MAPP(1)	Parameter which governs which variables of the Pressure Equation are written to file.
MAPP(2)	Parameter which governs which variables of the Temperature Equation are written to file.
MAPP(3)	Parameter which governs which variables of the Brine Transport Equation are written to file.
MAPP(4)	Parameter which governs which variables of the Radionuclide Transport Equation are written to file.
MASS(NCP)	Mass number of a radioactive component.





MAXITN	Maximum number of outer nonlinear iterations in the solutions of the primary equations.
MDAT	Control parameter for entering the mapping specifications.
MDATP	Control parameter for entering the region specification in the R2-16 cards.
METHOD	The method-of-solution indicator.
MINITN	Minimum number of outer nonlinear iterations in the solution of the primary equations.
NABLMX	Storage allocation for the number of boundary condition blocks and aquifer-influence function blocks.
NAQMAX	Control parameter specifying the number of times that the data input must loop over cards R1-27 through R1-33 (boundary condition cards).
NCALC	Control parameter for the Carter-Tracy aquifer coefficients.
NCALL	Control parameter for selecting the primary partial differential equations to be solved.
NCP	Number of radioactive/trace components in the system.
NCV	Number of entries in the table of viscosity versus concentrations.
NDT	Number of entries in the table of depth versus temperature.
NITQ	Maximum number of outer iterations in the wellbore calculations.
NORNXY,NORNXXZ	Control parameters for map orientation.
NOUT	Output control parameter for wellbore results.
NP(NCP)	Number of parent components for a radionuclide.
NPLC	Control parameter for plotting concentrations for the wells.
NPLP	Control parameter for plotting pressures for the wells.
NPLT	Control parameter for plotting temperatures for the wells.

NPT	Number of points in the table of influence function versus dimensionless time.
NPTDST	Number of points in the table of time versus pore structure compressibility.
NRCHMX	Storage allocation for the number of recharge blocks.
NREPB	Number of repository blocks.
NRT	Number of global rock types.
NRTD	Number of local rock types.
NSD(NRTD)	Number of local grid blocks.
NSMAX	Storage allocation for the number of radioactive trace components that will be used during the run.
NSS	Number of source blocks for fluid, heat, and radionuclides.
NTIME	Number of entries in the table of concentration (CNDUM) versus time (CTIME) for the unleached radioactive components and/or heat density (ARHLD) versus time (CTIME) for the repository blocks.
NTIMEMX	Control parameter specifying the maximum number of time steps for the SWIFT II run (only needed if the SWIFT II run will be used with GRASP II).
NTVI	Number of entries in the table of viscosity (VISI) versus temperature (TI) for the contaminated fluid.
NTVR	Number of entries in the table of viscosity (VISR) versus temperature (TR) for the resident reservoir fluid.
NWT	Total number of wells.
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.
NZOB	Number of overburden blocks.



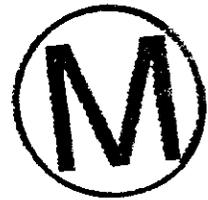
NZUB	Number of overburden blocks.
OD	For the wellbore model, the outside diameter of the casing, ft (m).
PAQ	Pressure differential between the external aquifer and the finite-difference grid (Carter-Tracy aquifer parameters), psi? (Pa).
PBASE	Atmospheric or reference pressure at the well head, psi (Pa).
PBD	Pressure boundary condition for the local subsystem, psi (Pa).
PBWR	Reference pressure for the input fluid densities, BWRN and BWRI, psi (Pa).
PHI(NB)	Porosity of the global system, volume fraction.
PHID(NRTD)	Porosity of the local subsystems, volume fraction.
PHIH	Porosity-thickness product for the aquifer, ft (m).
PINIT	Initial pressure at the depth HINIT and at the standard pressure $P_0 = P_{INIT}$ for the density calculations, psi (Pa).
POROS(NZ)	Porosity for cylindrical coordinates, volume fraction.
POS	Observed surface pressure used for plotting, psi (Pa).
POW	Observed bottom-hole pressure used for plotting, psi (Pa).
PRT	Orientation control for the output arrays.
PRTAB	Print control key for the aquifer-influence coefficients.
PRTIF	Print control key for the influence-function table.
PSMN	Lower limit on the well-head pressures to be plotted, psi (Pa).
PSMX	Upper limit on the well-head pressures to be plotted, psi (Pa).
PTD(NPT)	Terminal-rate influence function, dimensionless.
PWMN	Lower limit on the bottom-hole pressures to be plotted, psi (Pa).
PWMX	Upper limit on the bottom-hole pressures to be plotted, psi (Pa).

P1	Boundary pressure of the global system, psi (Pa).
Q(NWT)	Well production rate, ft ³ /d (m ³ /s).
QCC(NSS,NCP)	Radioactive-component discharge rate, lb/d (kg/s).
QHH(NSS)	Heat discharge rate, Btu/d (J/s).
QRCH	Recharge rate, ft/d (m/s).
QWELL	Well production rate, ft ³ /d (m ³ /s).
QWW(NSS)	Fluid discharge rate, lb/d (kg/s).
RAQ	Internal radius of the aquifer, ft (m).
RCHG	Recharge rate, ft/d (m/s).
RCMPB	Rock compressibility for rock type I, psi ⁻¹ (Pa ⁻¹).
RE	External radius of the aquifer, ft (m).
RR(NX)	Radius of the grid-block centers, ft (m).
RSTRT	Control parameter for restarting a calculation.
RSTWR	Control parameter for writing a restart record.
RWW	Well radius, ft (m).
R1	For radial coordinates, the center of the first grid-block, ft (m).
SAD(NRTD)	Length of the prismatic local units or radius of the spherical local units, ft (m).
SC(NCV)	Concentrations for the table of viscosity (VCC) versus concentration, mass fraction.
SCNSTR	Center-to-center waste-canister separation within each row for the waste-leach model, ft (m).
SDRIFT	Separation of rows of waste canisters for the waste-leach mode, ft (m).

SINX	Sine of the reservoir dip angle along the x-axis, dimensionless.
SINY	Sine of the reservoir dip angle along the y-axis, dimensionless.
SWAQ	External aquifer brine fraction.
SWBD(NRTD)	Brine boundary condition for the local subsystems, ft (m).
TAQ	Conductance between the external aquifer and the finite-difference grid (Carter-Tracy aquifer parameters), ft^2/day (m^2/s).
TBWR	Reference temperature for the input densities BWRN and BWRI, °F (°C).
TBOTW	For the wellbore model, the initial rock temperature at the bottom-hole depth, °F (°C).
TBUD	Convergence for L2SOR (units depend on equation solved.)
TCHG	Time at which the next set of recurrent data will be read, d (s).
TD(NDT)	Temperature in the table of temperature versus depth (see PTD), °F (°C).
TD(NPT)	Time in the table of influence function versus time (see ZT), dimensionless.
TDIS	Thermal diffusivity of the rock surrounding the wellbore, ft^2/hr (m^2/s).
THADD	Additive thickness modifier for a grid-block, ft (m).
THETA	Angle of deviation of the wellbore from the vertical direction, degrees.
THETAQ	Angle of influence of the aquifer-influence functions, degrees.
THP(NWT)	For the wellbore model, the tubing-hole or surface pressure, psi (Pa).
TI(NTVI)	Temperatures for the table of viscosity (VISI) versus temperature for the contaminated fluid, °F (°C).
TIMTDST	Interpolation time for pore structure compressibility, d (s).
TINJ	Temperature of the injected fluid, °F (°C).
TIR	Reference temperature for the viscosity (VISIR) of the contaminated fluid, °F (°C).



TITLE(40)	Title for the run.
TMN	Lower limit on the times to be plotted, d (s).
TMX	Upper limit on the times to be plotted, d (s).
TO	Standard temperature for calculating fluid density, °F (°C).
TOLDP	Tolerance on the pressure used in the wellbore calculations, psi (Pa).
TOLX	Tolerance on the fractional change in pressure used in the wellbore calculations, dimensionless.
TOS	Observed surface temperatures to be plotted, °F (°C).
TOW	Observed bottom-hole temperature to be plotted, °F (°C).
TOX	Observed times for data to be plotted, d (s).
TPAQ	External aquifer fluid temperature, °F (°C).
TPBD(NRTD)	Temperature boundary condition for the local subsystems, °F (°C).
TR(NTVR)	Temperatures for the table of viscosity (VISR) versus temperature for the resident fluid, °F (°C).
TRR	Reference temperature for the viscosity (VISRR) of the resident fluid, °F (°C).
TSCALE(I)	If positive, factor by which the time at which the dependent variable is written to file is divided.
TSMN	Lower limit on the surface temperatures to be plotted, °F (°C).
TSMX	Upper limit on the surface temperatures to be plotted, °F (°C).
TTOPW	For the wellbore model, the initial rock temperature at well-head level, °F (°C).
TWMN	Lower limit on the bottom-hole temperatures to be plotted, °F (°C).
TWMX	Upper limit on the bottom-hole temperatures to be plotted, °F (°C).
T1	Boundary temperature of the global system, °F (°C).



T2	For a radiation boundary condition, the temperature of the surrounding media, °F (°C).
T3	For a radiation boundary condition, the coefficient of surface heat transfer, Btu/d-ft-°F (J/s-m-°C).
UCOEF	For the wellbore model, the heat-transfer coefficient between the inner surface of the tubing and the outer surface of the casing, Btu/d-ft ² -°F-hr (J/m ² -°C-s).
UCRP	Modified heat capacity of the rock, Btu/ft ³ °F (J/m ³ -°C).
UH	Modified depth of the top of the grid-block relative to the top of the reference plane, ft (m).
UKTX	Thermal conductivity of the fluid-saturated global medium in the x direction, Btu/ft-°F-d (J/m-°C-s).
UKTY	Same as UKTX, but for the y direction.
UKTZ	Same as UKTX, but for the z direction.
UTCX(NRT)	Thermal capacity of the fluid-saturated global media in the x direction, Btu/ft-°F-d (J/m-°C-s).
UTCY(NRT)	Same as UTCX, but for the y direction.
UTCZ(NRT)	Same as UTCX, but for the z direction.
UTH	Modified grid-block thickness, ft (m).
VAB	Parameter used to specify both boundary conditions and aquifer-influence functions. The dimensions depend on the option chosen.
VCC(NCV)	Viscosities in the table for viscosity versus concentration (SC), cp (Pa-s).
VEL	Initial velocity of the resident reservoir fluid in the x direction, ft/d (m/s).
VISCAQ	External aquifer fluid viscosity (Carter-Tracy aquifer parameter) cp (Pa-s).
VISI(NTVI)	Viscosities in the table of viscosity versus temperature (TI) for the contaminated fluid, cp (Pa-s).



VISIR	Reference viscosity of the contaminated fluid at the reference temperature (TIR), cp (Pa-s).
VSCALE(I)	If positive, factor by which the dependent variable within the defined region (R2-16 card) will be divided before being written to file. Not used with velocities.
WI	Well index, ft^2/d , (m^2/s).
WTFAC	Weight factor for finite differencing in space.
X	For the wellbore model, the length of the tubing from the surface to the top of the perforations.
XYXL,XYYL	Length of the areal computer-output maps in the x and y directions, inches.
YZXL,XZZL	Length of the vertical computer-output map in the x/r and z direction, inches.
ZT(NDT)	Depths in the table of temperature (TD) versus depth, ft (m).

APPENDIX B

VARIABLE INDEX

<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
ACS(NRT)	R1A-2	7E10.0	1-70	$d^{-1}(s^{-1})$
AKSD(IR)	R1D-2	E10.0	31-40	ft/d(m/s)
ALCH	R2-10.5	E10.0	1-10	d(s)
ALPD(IR)	R1D-2(List 1)	E10.0	41-50	ft(m)
ALPHAL(NRT)	R1-2.5(List 2)	E10.0	1-10	ft(m)
ALPHAT(NRT)	R1-2.5(List 2)	E10.0	11-20	ft(m)
ALPHL	R1-2	E10.0	41-50	ft(m)
ALPHT	R1-2	E10.0	51-60	ft(m)
AMAX	R2-15	E10.0	41-50	+
AMIN	R2-15	E10.0	31-40	+
AP(NP)	R0-1(Card 2)	E10.0	11-20, 31-40...	*
ARHLD(NTIME)	R1A-8.5	7F10.0	1-70	Btu/ft ² -d(J/s-m ²)
BHP	R2-7 (List 2)	E10.0	11-20	psi(Pa)
BLCH	R2-10.5	E10.0	11-20	d(s)
BROCK	R1-3	E10.0	1-10	lb/ft ³ (kg/m ³)
BWAQ	R1-31(List 2)	E10.0	1-10	lb/ft ³ (kg/m ³)
BWRI	R1-3	E10.0	41-50	lb/ft ³ (kg/m ³)
BWRN	R1-3	E10.0	31-40	lb/ft ³ (kg/m ³)
CINIT	I-2	E10.0	31-40	*
	I-4	E-10	31-40	*
CINJ	R2-7(List 2)	E10.0	31-40	*
CMN	P-3(Card 2)	E10.0	41-50	*
CMX	P-3(Card 2)	E10.0	51-60	*
CNAME(2)	R1A-8	2A4	1-8	**

+ Depends on Input
 * Dimensionless
 ** Alphanumeric



<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
CNDUM(NTIME)	R1A-8	6E10.0	11-70	*
COC	P-4	E10.0	51-60	*
CONV	R1-2	E10.0	31-40	+
	R1-2.5	E10.0	31-40	+
CONVC	R1A-5	E10.0	11-20	+
CONVH	R1A-5	E10.0	31-40	+
CONVL	R1A-5	E10.0	1-10	+
CONVT	R1A-5	E10.0	21-30	+
CPOB	R1A-5	E10.0	11-20	Btu/ft ³ -°F(J/m ³ -°C)
CPR	R1-1	E10.0	41-50	Btu/ft ³ -°F(J/m ³ -°C)
CPRKD(NRTD)	R1D-2(List 1)	E10.0	61-70	Btu/ft ³ -°F(J/m ³ -°C)
CPR1(NZ)	R1-23	E10.0	41-50	Btu/ft ³ -°F(J/m ³ -°C)
CPUB	R1-13	E10.0	31-40	Btu/ft ³ -°F(J/m ³ -°C)
CPW	R1-1	E10.0	31-40	Btu/ft ³ -°F(J/m ³ -°C)
CR	R1-1	E10.0	11-20	psi ⁻¹ (Pa ⁻¹)
CRD	R1D-1	E10.0	1-20	psi ⁻¹ (Pa ⁻¹)
CRTDST	R1-1.5	E10.0	11-20	psi ⁻¹ (Pa ⁻¹)
CS(NCP)	R1A-9	7F10.0	1-70	*
CTAQ	R1-31(List 2)	E10.0	21-30	psi ⁻¹ (Pa ⁻¹)
CTIME(NTIME)	R1A-7	7F10.0	1-70	d(s)
CTW	R1-1	E10.0	21-30	°F ⁻¹ (°C ⁻¹)
CW	R1-1	E10.0	1-10	psi ⁻¹ (Pa ⁻¹)
C1	R1-28(List 2)	E10.0	31-40	*
DAMPX	R2-3	E10.0	26-35	*
DCMX	R2-12	E10.0	21-30	*
DCNSTR	R1A-4	E10.0	21-30	ft(m)
DEC(NCP)	R0-1(List 1)	E10.0	31-40	yr
DELPW	R1-5	E10.0	11-20	psi(Pa)



* Dimensionless
 + Depends on Input

<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
DELX(NX)	R1-17	***		ft(m)
DELY(NY)	R1-18	***		ft(m)
DELZ(NZ)	R1-19	***		ft(m)
	R1-23	E10.0	1-10	ft(m)
DEPTH	R1-20	E10.0	61-70	ft(m)
	R1-22	E10.0	31-40	ft(m)
DI(2,NCP)	R0-1(List 1)	2A4	4-11	**
DIS1(NCP)	R0-2(List 1)	7E10.0	1-70	ft ³ /lbη or (m ³ /kg) η
DIS2*(NCP)	R0-2(List 2)	7E10.0	1-70	*
DISD(NCP)	R1D-4	7E10.0	1-70	ft ³ /lb(m ³ /kg)
DMEF	R1-2.5	E10.0	31-40	ft ² /day(m ² /s)
DMEFD(NRTD)	R1D-2(List 1)	E10.0	1-11	ft ² /d(m ² /s)
DMEFF	R1-2	E10.0	61-70	ft ² /d(m ² /s)
DMEFR(1)	R0-2(List 3)	E10.0	1-70	ft ² /day(m ² /s)
DMEFRD(NCF)	R1D-4(List 2)	E10.0	1-70	ft ² /day(m ² /s)
DMFD1(NRTD)	R1D-2 (List 1)	E10.0	11-20	°F ⁻¹ (°C ⁻¹)
DPMX	R1-12	E10.0	41-50	psi(Pa)
DS(NSD)	R1D-2(List 3)	7E10.0	1-70	ft(m)
DSD	R1D-2(List 2)	E10.0	21-30	ft(m)
DSDO	R1A-2(List 2)	E10.0	31-40	ft(m)
DSMX	R2-12	E10.0	31-40	*
DT	R2-12	E10.0	11-20	d(s)
DTMAX	R2-12	E10.0	61-70	d(s)
DTMIN	R2-12	E10.0	71-80	d(s)
DTPMX	R2-12	E10.0	51-60	°F (°C)
DW	R2-7(List 3)	E10.0	11-20	ft(m)
DZOB(NZOB)	R1-14	7E10.0	1-70	ft(m)
DZUB(NZUB)	R1-15	7E10.0	1-70	ft(m)

* Dimensionless
 ** Alphanumeric
 *** List-directed



<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
D1	P-3 (Card 1)	E10.0	21-30	d(s)
ED	R2-7 (List 3)	E10.0	21-30	ft(m)
EPS	R2-3	E10.0	36-45	*
FAB	R1-33(List 2)	E10.0	1-10	*
FAMD	R1D-5(List 2)	E10.0	1-10	*
FPHI	R1-26(List 2)	E10.0	41-50	*
FPV	R1-26(List 2)	E10.0	31-40	*
FTUX	R1-26(List 3)	E10.0	1-10	*
FTUY	R1-26(List 3)	E10.0	11-20	*
FTUZ	R1-26(List 3)	E10.0	21-30	*
FTX	R1-26(List 2)	E10.0	1-10	*
FTY	R1-26(List 2)	E10.0	11-20	*
FTZ	R1-26(List 2)	E10.0	21-30	
GRAV	R1-1	E10.0	51-60	ft/s ² (m/s ²)
HADD	R1-26(List 2)	E10.0	51-60	ft(m)
HCNSTR	R1A-4	F10.0	31-40	ft(m)
HDATUM	R1-16	E10.0	31-40	ft(m)
HINIT	R1-16	E10.0	21-30	ft(m)
HTG	M-3(Card 1)	I5	16-20	++
I	R0-1(Card 1)	I5	16-20	++
	R2-6	I5	1-5	++
	R2-7(List 1)	I5	1-5	++
	R2-10(List 1)	I5	1-5	++
IAQ	R1-27	I5	1-5	++
IBUD	R2-11.1	I5	6-10	++
ICLL	R2-1	I5	41-45	++
ICOMP	I-1	I5	1-5	++
ICRSS	R2-11	I5	16-20	++

* Dimensionless

** Alphanumeric

++ Indicates a program flag, switch, option indicator, or other indicator for which dimensions do not apply.

<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
ID	P-2	10A4	11-50	**
IDIR	N-2	I5	36-40	++
IDSC	N-1	I5	1-5	++
IFD	ROD-3	I5	36-40	++
IFREE	M-2	I5	16-20	++
IIC1	R2-7(List 1)	I5	16-20	++
IIC2	R2-7(List 1)	I5	21-25	++
IINDW1	R2-7(List 1)	I5	26-30	++
IIPRT	R2-13	I5	51-55	++
IIPRTD	R2-13	I5	66-70	++
IIS	R2-10(List 1)	I5	6-10	++
IIW	R2-7(List 1)	I5	6-10	++
IJS	R2-10(List 1)	I5	11-15	++
IJW	R2-10(List 1)	I5	11-15	++
IKS	R2-10(List 1)	I5	16-20	++
ILEVEL	R1A-3	I5	1-5	++
IMETH	R2-1	I5	11-15	++
IMPG	R2-11	Is	11-15	++
IMPT	M-6	I5	1-5	++
INAT	I-1	I5	6-10	++
INDQ	R2-1	I5	1-5	++
INDT	R2-1	I5	36-40	++
IOPT	R2-1	I5	31-35	++
I01	R2-13	I5	1-5	++
I02	R2-13	I5	6-10	++
I03	R2-13	I5	11-15	++
I03P	R2-13(List 2)	I5	1-5	++
I04	R2-13	I5	16-20	++
I05	R2-13	I5	21-25	++

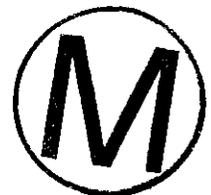


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<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
I05D	R2-13	I5	55-60	++
I06	R2-13	I5	26-30	++
I08	R2-13	I5	31-35	++
I08D	R2-13	I5	61-65	++
IPINIT	I-1	I5	16-20	++
IPROD	R2-1	I5	26-30	++
IR	R0D-3	I5	31-35	++
	R1D-3(List 1)	I5	1-5	++
IRCH	R2-1	I5	46-50	++
IREG	R1-28(List 1)	I5	36-40	++
	N-2	I5	31-35	++
	R2-7(List 1)	I5	36-40	++
IRD	I-1	I5	11-15	++
IRSS	R2-1	I5	21-25	++
IRT	R1R-1	I5	31-35	++
ISURP	M-2	I5	11-15	++
ITHRU	R2-1	I5	16-20	++
IUNIT	M-2	I5	36-40	++
IWELL	R2-1	I5	6-10	++
IXYZ	R2-11.1	I5	1-5	++
II	R1-21(List 1)	I5	1-5	++
	R1-28(List 1)	I5	1-5	++
	R1-30(List 1)	I5	1-5	++
	R1-33(List 1)	I5	1-5	++
	R1D-5(List 1)	I5	1-5	++
	I-2	I5	1-5	++
	R2-15	I5	1-5	++
	R2-21(List 1)	I5	1-5	++
IIA	R0D-3	I5	1-5	++
	R1A-1	I5	1-5	++
	R1A-6	I5	1-5	++

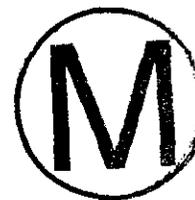
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<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
I1B	R0D-3	I5	6-10	++
	R1A-1	I5	6-10	++
	R1A-6	I5	6-10	++
I2	R1-21(List 1)	I5	6-10	++
	R1-26(List 1)	I5	6-10	++
	R1-28(List 1)	I5	6-10	++
	R1-30(List 1)	I5	6-10	++
	R1-33(List 1)	I5	6-10	++
	I-2	I5	6-10	++
	R1D-5(List 1)	I5	6-10	++
	R2-15	I5	6-10	++
JDSC	N-1	I5	6-10	
J1	R1-21(List 1)	I5	11-15	++
	R1-26(List 1)	I5	11-15	++
	R1-28(List 1)	I5	11-15	++
	R1-30(List 1)	I5	11-15	++
	R1-33(List 1)	I5	11-15	++
	R1D-5(List 1)	I5	11-15	++
	I-2	I5	11-15	++
	R2-15	I5	11-15	++
J1A	R0D-3	I5	11-15	++
	R1A-1	I5	11-15	++
	R1A-6	I5	11-15	++
J1B	R0D-3	I5	16-20	++
	R1A-1	I5	16-20	++
	R1A-6	I5	16-20	++
J2	R1-21(List 1)	I5	16-20	++
	R1-26(List 1)	I5	16-20	++
	R1-28(List 1)	I5	16-20	++
	R1-30(List 1)	I5	16-20	++
	R1-33(List 1)	I5	16-20	++
	R1D-5(List 1)	I5	16-20	++
	I-2	I5	16-20	++
	R2-15	I5	16-20	++
KAQ	R1-28(List 1)	I5	31-35	++
KBC	R1D-3	I5	6-10	++
KCNVD	R0D-1	I5	1-5	++



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<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
KDSC	N-1	I5	11-15	++
KGDP(NRTD)	R1D-2(list 2)	I5	1-5	++
KGRD(NRTD)	R1D-2(List 2)	I5	6-10	++
KH	R1-31	E10.0	1-10	ft ² /d(m ² /s)
KHEAT	M-3(Card 2)	I5	6-10	++
KHL(IIC2)	R2-7(List 4)	7E10.0	1-70	**
KOB	R1-13	E10.0	1-10	Btu/ft-d-°F(J/m-s-°C)
KOUT	M-3(Card 1)	I5	31-35	++
KOUTD	M-3(Card 2)	I5	26-30	++
KOUTG	M-3(List 1)	I5	66-70	++
KP(NP)	R0-1(List 2)	I5	1-5, 21-25...	++
KPAQ	R1-29	I5	16-20	++
KPB	R1D-3(List 1)	I5	11-15	++
KSLVD	M-3(Card 2)	I5	16-20	++
KSWAQ	R1-29	E10.0	26-30	++
KSWB	R1D-3(List 1)	I5	21-25	++
KTPAQ	R1-29	I5	21-25	++
KTPB	R1D-3(List 1)	I5	16-20	++
KUB	R1-13	E10.0	21-30	Btu/ft-d-°F(J/m-s-°C)
KW	P-2	I5	1-5	++
KX	R1-20	E10.0	1-10	ft/d(m/s)
	R1-21(List 2)	E10.0	1-10	ft/d(m/s)
KY	R1-20	E10.0	11-20	ft/d(m/s)
	R1-21(List 2)	E10.0	21-30	ft/d(m/s)
KYY(NZ)	R1-23	E10.0	11-20	ft/d(m/s)
KZ	R1-20	E10.0	21-30	ft/d(m/s)
	R1-21(List 2)	E10.0	21-30	ft/d(m/s)
KZZ(NZ)	R1-23	E10.0	21-30	ft/d(m/s)



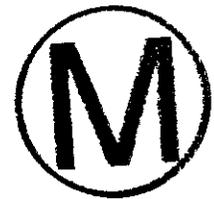
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 ** Alphanumeric

<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
K1	R1-21(List 1)	I5	21-25	++
	R1-26(List 1)	I5	21-25	++
	R1-28(List 1)	I5	21-25	++
	R1-30(List 1)	I5	21-25	++
	R1-33(List 1)	I5	21-25	++
	R1D-5(List 1)	I5	21-25	++
	I-2	I5	21-25	++
	R2-15	I5	21-25	++
K1A	R0D-3	I5	21-25	++
	R1A-1	I5	21-25	++
	R1A-6	I5	21-25	++
K1B	R0D-3	I5	26-30	++
	R1A-1	I5	26-30	++
	R1A-6	I5	26-30	++
K2	R1-21(List 2)	I5	26-30	++
	R1-26(List 2)	I5	26-30	++
	R1-28(List 2)	I5	26-30	++
	R1-30(List 2)	I5	26-30	++
	R1-33(List 2)	I5	26-30	++
	R1D-5	I5	26-30	++
	I-2	I5	26-30	++
	R2-15	I5	26-30	++
LADJ(NCP)	R0-1(List 1)	I5	26-30	++
LBIO	M-2	I5	41-45	++
LBIOR	M-2	I5	46-50	++
MAP	M-7	I5	1-5	++
	R2-13	I5	41-45	++
MAPP(1)	R2-13(List 2)	I5	5-10	++
MAPP(2)	R2-13(List 2)	I5	11-15	++
MAPP(3)	R2-13(List 2)	I5	16-20	++
MAPP(4)	R2-13(List 2)	I5	21-25	++
MASS(NCP)	R0-1(List 1)	I3	1-3	++
MAXITN	R2-11	I5	6-10	++
MDAT	R2-13	I5	46-50	++



++ Indicates a program flag, switch, option indicator, or other indicator for which dimensions do not apply.

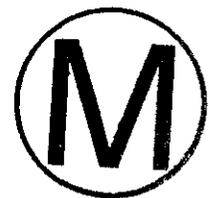
<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
MDATP	Q2-13(List 2)	I5	26-30	++
METHOD	M-3(Card 1)	I5	61-65	++
	R2-2	I5	1-5	++
MINITN	R2-11	I5	1-5	++
NABLMX	M-3(Card 1)	I5	46-50	++
NAQMAX	M-3(List 1)	I5	51-55	*
NBIOMX	M-3(Card 2)	I5	36-40	*
NCALC	R1-29	I5	1-5	++
NCALL	M-2	I5	1-5	++
	R2-11.5	I5	1-5	++
NCP	M-3(Card 1)	I5	21-25	++
NCV	R1-6	I5	1-5	++
NDT	R1-6	I5	16-20	++
NITQ	R2-3	I5	1-5	++
NORNXY	R2-14	I5	1-5	++
NORNXZ	R2-14	I5	6-10	++
NOUT	R1-4	I5	1-5	++
NP(NCP)	R0-1(List 1)	I5	21-25	++
NPLC	M-2	I5	31-35	++
NPLP	M-2	I5	21-25	++
NPLT	M-2	I5	26-30	++
NPT	R1-29	I5	6-10	++
NPTDST	R1-1.5(List 1)	I5	1-5	++
NRCHMX	M-3(Card 1)	I5	56-60	++
NREPB	M-3(Card 2)	I5	11-15	++
NRT	M-3(Card 1)	I5	26-30	++
NRTD	M-3(Card 2)	I5	21-25	++
NSD(NRTD)	R0D-2	I4I5	1-70	++
NSMAX	M-3(Card 1)	I5	41-45	++



* Dimensionless

++ Indicates a program flag, switch, option indicator, or other indicator for which dimensions do not apply.

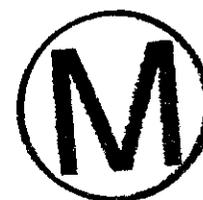
<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
NSS	R2-9	I5	1-5	++
NTIME	M-3(Card 2)	I5	1-5	++
NTIMEMX	M-3(List 2)	I5	31-35	*
NTV1	R1-6	I5	11-15	++
NTVR	R1-6	I5	6-10	++
NWT	R2-4	I5	1-5	++
NX	M-3(Card 1)	I5	1-5	++
NY	M-3(Card 1)	I5	6-10	++
NZ	M-3(Card 1)	I5	11-15	++
NZOB	R1-12	I5	1-5	++
NZUB	R1-12	I5	6-10	++
OD	R2-7(List 3)	E10.0	31-40	ft(m)
PAQ	R1-31(List 2)	E10.0	41-50	psi (Pa)
PBASE	R1-5	E10.0	1-10	psi (Pa)
PBD(NRTD)	R1D-3(List 2)	E10.0	1-10	psi (Pa)
PBWR	R1-3	E10.0	11-20	psi (Pa)
PHI	R1-20	E10.0	31-40	*
	R1-21(List 2)	E10.0	31-40	*
PHID(NRTD)	R1D-2(List 1)	E10.0	21-30	*
PHIH	R1-31	E10.0	11-20	ft(m)
PINIT	R1-16	E10.0	11-20	psi(Pa)
POROS(NZ)	R1-23	E10.0	31-40	*
POS	P-4	E10.0	21-30	psi(Pa)
POW	P-4	E10.0	11-20	psi(Pa)
PRT	M-3(Card 1)	I5	36-40	++
PRTAB	R1-27	I5	6-10	++
PRTIF	R1-29	I5	11-15	++
PSMN	P-3(Card 1)	E10.0	51-60	psi(Pa)



* Dimensionless

++ Indicates a program flag, switch, option indicator, or other indicator for which dimensions do not apply.

<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
PSMX	P-3(Card 1)	E10.0	61-70	psi(Pa)
PTD(NPT)	R1-32	E10.0	11-20, 31-40...	*
PWMN	P-3(Card 1)	E10.0	31-40	psi(Pa)
PWMX	P-3(Card 2)	E10.0	41-50	psi(Pa)
P1	R1-28(List 2)	E10.0	11-20	psi(Pa)
Q(NWT)	R2-5	7E10.0	1-70	ft ³ /d(m ³ /s)
QCC(NSS,NCP)	R2-10(List 2)	5E10.0	21-70	lb/d(kg/s)
QHH(NSS)	R2-10(List 2)	E10.0	11-20	Btu/df(J/s)
QRCH	R2-2.5	E10.0	21-30	ft/d(m/s)
QWELL	R2-6	E10.0	6-16	ft ³ /d(m ³ /s)
QWW(NSS)	R2-10(List 2)	E10.0	1-10	lb/d(kg/s)
RAQ	R1-31	E10.0	21-30	ft(m)
RCHG	R2-2.5	E10.0	21-30	ft/d(m/s)
RCMPB	R1-2.5	E10.0	21-30	psi ⁻¹ (Pa ⁻¹)
RE	R1-22	E10.0	21-30	ft(m)
RR(NX)	R1-24	7E10.0	1-70	ft(m)
RSTRT	M-2	I5	6-10	++
RSTWR	R2-13	I5	36-40	++
RWW	R1-22	E10.0	1-10	ft(m)
R1	R1-22	E10.0	11-20	ft(m)
SAD(NRTD)	R1D-2(List 2)	E10.0	11-20	ft(m)
SC(NCV)	R1-8	E10.0	1-20 21-20...	*
SCNSTR	R1A-4	E10.0	11-20	ft(m)
SDRIFT	R1A-4	E10.0	1-10	ft(m)
SINX	R1-20	E10.0	41-50	*
SINY	R1-20	E10.0	51-60	*
SWAQ	R1-31(List 2)	E10.0	61-70	*



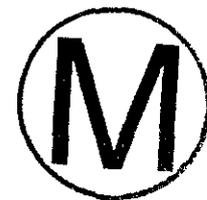
* Dimensionless

++ Indicates a program flag, switch, option indicator, or other indicator for which dimensions do not apply.

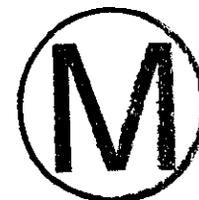
<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
SWBD(NRTD)	R1D-3(List 2)	E10.0	21-30	*
TAQ	R1-31(List 2)	E10.0	31-40	ft ² /day(m ² /s)
TBWR	R1-3	E10.0	21-30	°F(°C)
TBOTW	R2-7(List 3)	E10.0	51-60	°F(°C)
TBUD	R2-11.1	E10.0	11-20	**
TCHG	R2-12	E10.0	1-10	d(s)
TD(NDT)	R1-11	E10.0	11-20, 31-40...	°F(°C)
TD(NPT)	R1-32	E10.0	1-10, 21-30...	*
TDIS	R1-5	E10.0	21-30	ft ² /day(m ² /s)
TDS	P-4	E10.0	41-50	°F(°C)
THADD	R1-26(List 2)	E10.0	61-70	ft(m)
THETA	R2-7(List 3)	E10.0	71-80	°
THETAQ	R1-31	E10.0	31-40	°
THP(NWT)	R2-8	7E10.0	1-70	psi
TI(NTVI)	R1-10	E10.0	1-10, 21-30...	°F(°C)
TINJ	R2-7(List 2)	E10.0	21-30	°F(°C)
TIMTDST	R1-1.5	E10.0	1-10	d(s)
TIR	R1-7	E10.0	21-30	°F(°C)
TITLE	M-1	20A4/20A4	1-80	**
TMN	P-3(Card 1)	E10.0	1-10	d(s)
TMX	P-3(Card 1)	E10.0	11-20	d(s)
TO	R1-16	E10.0	1-20	°F(°C)
TOLDP	R2-G	E10.0	16-25	psi(Pa)
TOLX	R2-3	E10.0	6-15	*
TOS	P-4	E10	41-50	
TOW	P-4	E10.0	31-40	°F(°C)
TOX	P-4	E10.0	1-10	d(s)

* Dimensionless

** Alphanumeric

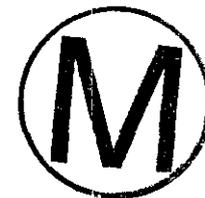


<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
TPAQ	R1-31(List 2)	E10.0	51-60	°F(°C)
TPBD(NRTD)	R1D-3(List 2)	E10.0	11-20	°F(°C)
TR(NTVR)	R1-9	E10.0	1-10	°F(°C)
TRR	R1-7	E10.0	1-20	°F(°C)
TSCALE	R2-16	E10.0	61-70	*
TSMN	P-3(Card 2)	E10.0	21-30	°F(°C)
TSMX	P-3(Card 2)	E10.0	31-40	°F(°C)
TTOPW	R2-7(List 3)	E10.0	41-50	°F(°C)
TWMN	P-3(Card 2)	E10.0	1-10	°F(°C)
TWMX	P-3(Card 2)	E10.0	11-20	°F(°C)
T1	R1-28(List 2)	E10.0	21-30	°F(°C)
T2	R1-28(List 2)	E10.0	41-50	°F(°C)
T3	R1-28(List 2)	E10.0	51-60	Btu/d-ft-°F(J/m-s-°C)
UCOEF	R2-7(List 3)	E10.0	61-70	Btu/ft ³ -°F-hr(J/m-s-°C)
UCPR	R1-21(List 2)	E10.0	61-70	Btu/ft ³ -°F(J/a ³ -°C)
UH	R1-21(List 2)	E10.0	41-50	ft(m)
UKTD	R1D-2(List 1)	E10.0	51-60	Btu/ft-°F-d(J/m-s-°C)
UKTX	R1-2	E10.0	1-20	Btu/ft-°F-d(J/m-s-°C)
UKTY	R1-2	E10.0	11-20	Btu/ft-°F-d(J/m-s-°C)
UKTZ	R1-2	E10.0	21-30	Btu/ft-°F-d(J/m-s-°C)
UTCX(NRT)	R1-2.5(List 1)	E10.0	1-10	Btu/ft-°F-d(J/m-s-°C)
UTCY(NRT)	R1-2.5(List 1)	E10.0	11-20	Btu/ft-°F-d(J/m-s-°C)
UTCZ(NRT)	R1-2.5(List 1)	E10.0	21-30	Btu/ft-°F-d(J/m-s-°C)
UTH	R1-21(List 2)	E10.0	51-60	ft(m)
VAB	R1-28(List 2)	E10.0	1-10	+
	R1-30(List 2)	E10.0	1-10	*
VCC(NCV)	R1-8	E10.0	11-20, 31-40...	cp(Pas)
VEL	I-3	E10.0	1-10	ft/d(m/s)



* Dimensionless
 + Depends on Input

<u>Variable</u>	<u>Cards</u>	<u>Format</u>	<u>Columns</u>	<u>Dimensions</u>
VISCAQ	R1-31(List 2)	E10.0	11-20	cp(Pa-s)
VISI(NTV1)	R1-10	E10.0	11-20, 31-40...	cp(Pa-s)
VISIR	R1-7	E10.0	31-40	cp(Pa-s)
VISR(NTVR)	R1-9	E10.0	11-20, 31-40	cp(Pa-s)
VISRR	R1-7	E10.0	11-20	cp(Pa-s)
VSCALE(I)	R2-16	E10.0	51-60	*
WI	R2-7(List 2)	E10.0	1-10	ft ² /d(m ² /s)
WTFAC	R2-2	E10.0	6-15	*
X	R2-7(List 1)	E10.0	1-20	ft(m)
XYXL	R2-14.5	E10.0	1-10	in
XYYL	R2-14.5	E10.0	11-20	in
XZXL	R2-14.5	E10.0	21-30	in
XZZL	R2-14.5	E10.0	31-40	in
ZT(NDT)	R1-11	E10.0	1-10, 21-30...	ft(m)

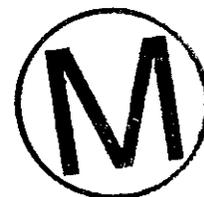


* Dimensionless

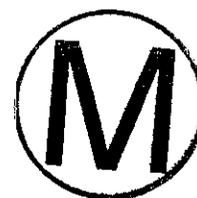
APPENDIX C

ENGLISH AND SI UNITS USED BY THE SWIFT MODEL

<u>Variable</u>	<u>English</u>	<u>SI</u>
Area	ft ²	m ²
Compressibility	l psi	l/Pa
Component mass flow rate	lb/d	kg/s
Component transmissibility	lb/d	kg/s
Concentration	fraction	fractions
Darcy velocity	ft/d	m/s
Density	lb/ft	kg/m
Diffusivity	ft ² /d	m ² /s
Dispersivity	ft	m
Distribution coefficient	ft ² /lb	m ³ /kg
Enthalpy	Btu	J
Fluid transmissibility	lb/d	kg/s
Fluid heat capacity	Btu/lb-°F	J/kg-°C
Fluid mass flow rate	lb/d	kg/s
Half-life	yr	yr
Heat flow rate	But/d	J/s
Hydraulic conductivity	ft/d	m/s
Length	ft	m
Mass	lb	kg
Porosity	fraction	fraction
Pressure	psi	Pa
Recharge	ft/d	m/s
Rock heat capacity	Btu/ft ³ -°F	J/m ³ -°C
Salt dissolution product	l/d	l/s
Temperature	°F	°C



<u>Variable</u>	<u>English</u>	<u>SI</u>
Thermal conductivity	Btu/ft-d-°F	J/m-s-°C
Thermal expansion	1/°F	1/°C
Thermal transmissibility	Btu/d-°F	J/s-°C
Time	d	s
Transmissivity	ft ² /d	m ² /s
Viscosity	cp (centipoise)	Pa-s
Volume	ft ³	m ³
Waste concentration	lb/ft ³	kg/m ³
Well flow rate	ft ³ /d	m ³ /s
Well index	ft ² /d	m ² /s



APPENDIX D

CONVERSION OF ENGLISH TO SI UNITS FOR THE SWIFT MODEL*

<u>Multiply</u>	<u>By</u>	<u>To Obtain</u>
1/psi	1.4504E-4	1/Pa
1/°F	1.800	1/°C
Btu/lbm-°F	4185.0	J/kg-°C
Btu/ft ³ -°F	67,037	J/m ³ -°C
Btu/ft-d-°F	0.07208	J/m-s-°C
ft	0.3048	m
ft ² /d	1.0753E-6	m ² /s
lbm/ft ³	16.018	kg/m ³
psi	6894.6	Pa
cp (centipoise)	0.001	Pa-s
Btu/lbm	2325.0	J/kg
ft/d	3.5278E-6	m/s
lbm	0.45359	kg
ft ³	0.028317	m ³
Btu	1054.6	J
ft ³ /d	3.2774E-7	m ³ /s
d	86,400	s
lb/d	5.2498E-6	kg/s

* To facilitate data input conversions, the order of this table follows closely the order of input to the code.
0.5556 °F - 17.78 = °C



APPENDIX E

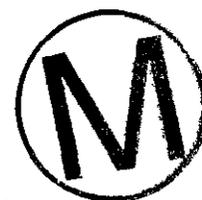
DATA INPUT ERRORS

In order to facilitate its application, the SWIFT II model performs a number of checks on the input data. If an error is detected, the code then converts to an error mode of operation. In this mode the reading of data continues through the last recurrent data set. An error summary is then written, and the run is aborted. This appendix provides an explanation of the codes that appear in the summary.

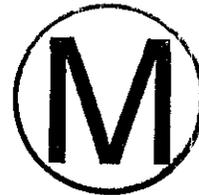
<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
1	Increment numbers are incorrectly specified: $NX < 2$, $NY < 1$, or $NZ < 1$.	M-3
3	Compressibilities assume nonphysical values: $CW < 0$ or $CR < 0$: or heat capacities are given nonphysical values: $CPW < 0$ or $CPR < 0$.	R1-1
4	Thermal conductivities are given nonphysical values: $UKTX < 0$, $UKTY < 0$, or $UKTZ < 0$: dispersivities are incorrectly specified: $ALPHL < 0$ or $ALPHT < 0$: the diffusion is erroneously defined: $DMEFF < 0$: or the dimensions of $ALPHL$ and $ALPHT$ have exceeded the dimensions ($NRTMAXM$): $NRT > NRTMAXM$.	R1-2
5	Fluid or rock densities are incorrectly specified: $BROCK \leq 0$, $BWRN \leq 0$ or $BWRI \leq 0$.	R1-3
6	Viscosities are given nonphysical values: $VISRR \leq 0$, $VISIR \leq 0$, $VCC \leq 0$, $VISR \leq 0$, or $VISI < 0$: brine concentrations are incorrectly specified: $SCC < 0$: the reference temperatures have been used a second time:	R1-7 R1-8 R1-9 R1-10



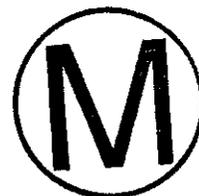
<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
	TR = TRR or TI = TIR; or NCV > NCVMX, NTVR > N RMX, NTVI > N IMX, NDT > NDTMX.	
7	The heterogeneity/geometry control is outside its permitted range: HTG < 1 or HTG > 3.	M-3
8	Initialization output is incorrectly specified: KOUT ≠ 0, 1 or 3.	M-3
9	The print orientation control is outside its permitted range: PRT < -1 or PRT > 2.	M-3
10	For the over/underburden, either the thermal conductivity is incorrectly stated: KOB < 0 with NZOB > 2; or KUB < 0 with NZUB > 2.	R1-13
11	Grid block sizes are specified incorrectly: DELX ≤ 0, DELY ≤ 0 or DELZ ≤ 0.	R1-17 R1-18 R1-19
12	Homogeneous reservoir properties are prescribed incorrectly for the permeabilities: KX < 0, KY < 0 or KZ < 0; for the porosity: PHI < 0; or for the reservoir dip angles: SINX < -1 or SINX > 1, SINY < -1 or SINY > 1.	R1-20
13	Heterogeneous reservoir properties are prescribed incorrectly for the grid-block indices: I1 < 1 or I2 > NX, J1 < 1 or J2 > NY, K1 < 1 or K2 > NZ, I1 > I2, J1 > J2 or K1 > K2: for the permeabilities: KX < 0, KY < 0, or KZ < 0; for the porosity: PHI < 0 or PHI > 1	R1-21



<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
	or for the heat capacity of the saturated rock: UCPR < 0.	
14	For the gridding of the radial coordinate, the radii are incorrectly specified: R1 ≤ RWW with R1 > 0, R1 ≥ RE, or In (RE/R1)/(NX-0.5) will cause overflow.	R1-22
15	For simulation in cylindrical coordinates, the value of the vertical increment is incorrect: DELZ ≤ 0; the values of the permeabilities are incorrect: KYY < 0 or KZZ < 0; or the value of the porosity is incorrect: POROS < 0 or POROS > 1.	R1-23
16	Radial block centers are erroneously prescribed: RR(I) > RE for 1 ≤ I ≤ NX.	R1-25
17	Block edges are incorrectly specified for the reservoir modifications: I1 < 1 or I1 > NX, J1 < 1 or J1 > NY, K1 < 1 or K2 > NZ, I1 > I2, J1 > J2, or K1 > K2.	R1-26
18	Aquifer-influence conditions are in error for the option parameter: IAQ < 0 or IAQ > 4: R1-28 or for the block edges: I1 < 1 or I2 > NX, J1 < 1 or J2 > NY, K1 < 1 or K2 > NZ I1 > I2, J1 > J2, or K1 > K2: or NPT > NPTMX	R1-27
19	The number of aquifer-influence functions (NABL) summed from the input specifications exceeds that allocated (NABLMX) in READ M-3 or the number of	R1-28



<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
	points in the table of influence function (NPT) exceeds that allocated (NPTMX).	
20	The number of recharge blocks (NRCH) summed from the input specifications exceeds that allocated (NRCHMX) in READ M-3.	R2-2.5
21	For initialization of the brine concentrations, the block indices are given incorrectly: $I1 < 1$ or $I2 > NX$, $J1 < 1$ or $J2 > NY$, $K1 < 1$ or $K2 > NZ$ $I1 > I2$, $J1 > J2$, or $K1 > K2$: or for the concentration: $CINIT < 0$.	I-2
22	For initializations of the radionuclide concentrations, the block indices are given incorrectly, as specified for Error 21.	I-4
23	Some grid-block that has a nonzero pore volume also has a zero sum of transmissibilities over its surface.	R1-21 R1-26
24	A grid-block pore volume is negative.	R1-26
25	The number of wells is specified incorrectly: $NWT < 1$ or $NWT > NWMAX$ where the latter parameter is defined internally within routine MAIN. Currently the value of this quantity is: $NWMAT = 100$.	R2-4
26	A well index I is out of range. $I < 1$ or $I > NWT$.	R2-6
27	Well locators $I1W$ and $I2W$ are outside the reservoir: $I1W < 1$ or $I1W > NX$, $I2W < 1$ or $I2W > NY$.	R2-7
28	The well-completion zone lies outside of the system: $IIC1 < 1$ or $IIC2 < 1$,	R2-7



<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
	IIC1 > NZ or IIC2 > NZ, IIC1 > IIC2, or the top block of the completion interval has zero pore volume.	
30	The well-specification option is erroneously given: IINDW1 \neq 1, ± 2 , ± 3 , or ± 4 or IINDW1 = 2, 3, 4 with NCALL greater than 4.	R2-7
23	Some grid-block that has a nonzero pore volume also has zero sum of transmissibilities over its surface.	R1-21 R1-26
24	A grid-block pore volume is negative.	R2-4
25	The number of wells is specified incorrectly: NWT < 1 or NWT > NWMAX where the latter parameter is defined internally within routine MAIN. Currently the value of this quantity is: NWMAX = 100.	R2-4
26	A well index I is out of range. I < 1 or I > NWT.	R2-6
27	Well locators IIW and IJW are outside the reservoir: IIW < 1 or IIW > NX, IJW < 1 or IJW > NY.	R2-7
28	The well-completion zone lies outside of the system: IIC1 < 1 or IIC2 < 1, IIC1 > NZ or IIC2 > NZ, IIC1 > IIC2, or the top block of the completion interval has zero pore volume.	R2-7
30	The well-specification option is erroneously given: IINDW1 X 1, ± 2 , ± 3 , or ± 4 or IINDW1 = 2, 3, 4 with NCALL greater than 4.	R2-7
32	Well index is incorrectly defined: WI \leq 0 with IINDWI \neq 1.	R2-7



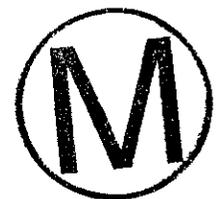
<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
35	The completion interval contains only blocks having zero pore volumes.	R2-7
37	Layer-allocation factors are incorrectly prescribed: $KHL < 0$.	R2-7
38	All layer-allocation factors, KHL, are zero. At least one KHL factor must be nonzero.	R2-7
39	A well identification number I is out of range: $I < 1$ or $I > NWT$.	R2-7
40	Differencing and matrix solution are improperly given: $METHOD < -2$ or $METHOD > 2$ $WTFAC > 1$.	R2-2
41	The number of nonlinear iterations is incorrect: $MINITN < 1$ or $MINITN > MAXITN$.	R2-11
43	Recurrent time is specified incorrectly: $TCHG \leq TIME$ where TIME is the current time.	R2-12
44	The time step is: $DT = 0$ for the first time step.	R2-12
45	The maximum time step is erroneous: $DTMAX < DTMIN$.	R2-12
46	Mapping is specified incorrectly in that one of the four digits of MAP is greater than unity.	R2-13
47	Maps are prescribed incorrectly: $I1 < 1$ or $I2 > NX$, $J1 < 1$ or $J2 > NY$, $K1 < 1$ or $K2 > NZ$. $I1 > I2$, $J1 > J2$, or $K1 > K2$: or for cylindrical geometry (HTG = 3, READ M-3) $J2 \times 1$.	R2-15
48	The number of nuclide monitor blocks encountered exceeds that allocated (NDSCMX).	R2-16



<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
50	Sink/source information contains error. The number of blocks containing sinks is greater than that allocated: NSS > NSMAX: the sink number is too large: I > NSS; or the block indices are incorrect: IIS < 1 or IIS > NX, IJS < 1 or IJS > NY, IKS < 1 or IKS > NZ.	d2-9 R2-10
51	Radioactive-component specification is incorrect. For the component number, I = 0 or I > NCP, or for the number of parents, NP < 0.	R0-1
52	The half-life is physically unreasonable DEC < 0.	R0-1
53	Branching, as specified, is incorrect. For the parent index, KP < 1 or KP > NCP, or for the branching ratio, AP < 0.	R0-1
54	The Freundlich η factor is given incorrectly: DIS(I) < 0, I \leq NCP.	R0-2
55	For the rock-type modifications, the block numbers are out of range: I1A < 1 or I1B > NX, J1A < 1 or J1B > NY, K1A < 1 or K1B > NZ. I1A > I1B, J1A > J1B, or K1A > K1B.	R1A-1
56	The salt-dissolution coefficient is prescribed erroneously: ACS < 0.	R1A-2
57	For canistered storage (ILEVEL = 1, READ R1A-3), the spacing parameters are given incorrectly: SDRIFT < 0, SCNSTR < 0, DCNSTR < 0, or HCNSTR < 0.	R1A-4
58	The specified location of the repository is unreasonable. A block number is out of range:	R1A-6



<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
	<p>I1A < 1 or I1B > NX, J1A < 1 or J1B > NY, K1A < 1 or K1B > NZ: I1A > I1B, J1A > J1B or K1A > K1B. or the allocated number of repository blocks, NREPB, is exceeded.</p>	
59	<p>For the concentration of the unleached wastes or the repository heat load, the interpolation table is given incorrectly: CTIME ≤ 0, or the values are not in ascending order.</p>	R1A-/
60	<p>For canistered storage (ILEVEL = 1 in READ R1A-3), the storage-parameter values are erroneous: SDRIFT > Max (DELX, DELY), SCNSTR > Max (DELX, DELY), or HCNSTR > DELZ.</p>	R1A-4
61	<p>Solubilities are given incorrectly: CS < 0.</p>	R1A-9
62	<p>The dual-porosity blocks are not specified correctly. Block indices are in error: I1A < 1 or I1B > NX, J1A < 1 or J1B > NY, K1A < 1 or K1B > NZ: I1A > I1B, J1A > J1B, or K1A > K1B: the local rock-type indicator is outside its permitted range: IR > NRTD; or the position control for the local unit cannot be interpreted: IFD < -3 or IFD > 3.</p>	R0D-3
63	<p>The properties of the local units have nonphysical values. For the rock compressibility: CRD < 0; for auto mesh generation the length of the local units: SAD ≤ 0 or DSD ≤ 0;</p>	R1D-1 R1D-2



<u>Error</u>	<u>Explanation</u>	<u>Card Code</u>
	for double mesh generation: $DSDO < 0$; for user defined mesh: $DS(I) \leq 0$; for permeability and porosity: $AKSD < 0$ or $PHID < 0$; for the dispersivity: $ALPD < 0$; or for the thermal conductivity and heat capacity: $UKTD < 0$ or $CPRKD < 0$.	
64	Distribution coefficients are incorrect. $D1SD < 0$.	R1D-4
65	Mesh generation is prescribed incorrectly. For single mesh generation (outer increment $DSDO = 0$), there is an insufficient number of nodes ($KGRD = 1$): $NSD \leq 3$; or for double mesh generation ($DSDO > 0$), there is an insufficient number of nodes ($KGRD = 2$): $NSD \leq 4$.	R0D-2 R1D-2
66	Grid-block volume is less than pore volume in a dual porosity block. Avoid pore volume modification R1-26 with dual porosity blocks.	
67	Modifications to dual porosity blocks are not specified correctly. Block indices are in error: $I1 < 1$ or $J1 > NY$, $K1 < 1$ or $K1 > NZ$, $I1 > I2$, $J1 > J2$, or $K1 > K2$.	

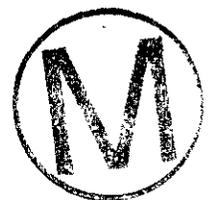
END OF GRASP-INV

APPENDIX D

Appendix E: Functionality Not Used in Performance Assessment

The following functions of GRASP-INV Version 2.01 are not used as part of the Waste Isolation Pilot Plant (WIPP) performance assessment (PA):

1. The Gaussian and Power variogram models within the CONSIM II portion of GRASP-INV for the categorical and continuous variables.
2. None of the heat and radionuclides transport subroutines or the two- and three-dimensional velocity fields within the SWIFT II portion of the GRASP-INV code.
3. None of the subroutines within the GRASP II portion of GRASP-INV related to determining the sensitivities of pressures to brine density or storativity.



Appendix F: QA Review Forms

As a convenience to users, this section contains a complete history of all the Quality-Assurance Review Forms issued during the review of this User's Manual. Review forms are issued after the User's Manual has been completed and reviewed. Thus, they are appended to the manual after it has been paginated. Their page numbers may or may not follow the sequence of the user's manual's page numbers.



NOTE: Copies of the User's Manual Reviewer's Forms are available in the Sandia WIPP Central Files.