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PORFLO-3: A Mathematical Model for Fluid Flow, Heat, and Mass Transport in Variably Saturated Geologic Media

Users Manual, Version 1.0

Prepared for the U.S. Department of Energy
Assistant Secretary for Environment, Safety and Health



Westinghouse
Hanford Company Richland, Washington

Hanford Operations and Engineering Contractor for the
U.S. Department of Energy under Contract DE-AC06-87RL10930

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ABSTRACT

This manual provides instructions for the use of the PORFLO-3 computer code. This computer code is based on mathematical formulation of fluid flow, heat transfer, and mass transport in variably saturated geologic media. The geologic medium may be heterogeneous and anisotropic and may contain linear and planar features such as boreholes and fractures. The code can be used to analyze three-dimensional problems of partially as well as fully saturated media with various types of fluid, heat, and mass sources. PORFLO-3 is written in American National Standard Fortran 77.

A summary of the theory of PORFLO-3 is provided in Chapter 2.0. The three partial differential equations that govern fluid flow, heat, transfer, and mass transport and the method of their solution are discussed. The governing equations are discretized by the method of 'Nodal Point Integration' and solved by any of the four alternate methods: Point-successive Over-relaxation, Alternating Direction Implicit Scheme, Choleski Decomposition, and Gaussian Elimination. The structure of the code and the information flow between its 89 subroutines are explained in Chapter 3.0. Certain practical suggestions for the design of the spatial grid and choice of time steps are discussed in Chapter 4.0. A format-free approach for data input is used in PORFLO-3. This aspect is discussed in Chapter 5.0 and in Appendix A. Chapter 6.0 provides detailed instructions for data input. Input and output for two example problems are shown in Appendix B. Error messages of PORFLO-3 are listed in Appendix C.

Keywords: Variably Saturated Flow, Heat and Mass Transport in Porous Media, Three-dimensional Modeling, Numerical Modeling, Fracture Flow Modeling.

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MATHEMATICAL NOTATION

All symbols are defined where they first occur in the text. Definitions of the important symbols are listed below to facilitate easy reference.

Symbol	Meaning	Dimensions	SI units ^a	FPS units ^b
B	Buoyancy parameter	----	----	----
c _f	Specific heat of fluid	L ² t ⁻² T ⁻¹	J/(kg•K)	Btu/(lbm°F)
c _s	Specific heat of solid	L ² t ⁻² T ⁻¹	J/(kg•K)	Btu/(lbm°F)
C	Species concentration in fluid	M L ⁻³	kg/m ³	lbm/ft ³
C _e	Species concentration in fluid+solid matrix	M L ⁻³	kg/m ³	lbm/ft ³
C _s	Species concentration in solid	M L ⁻³	kg/m ³	lbm/ft ³
D	Dispersion tensor	L ² t ⁻¹	m ² /s	ft ² /s
D _M	Molecular diffusivity	L ² t ⁻¹	m ² /s	ft ² /s
e	Internal energy of fluid	L ² t ⁻²	J/kg	Btu/lbm
e _e	Equivalent internal energy of fluid+solid matrix	L ² t ⁻²	J/kg	Btu/lbm
F	State variable (P, T, or C)	----- Variable dependent -----		
g	Gravitational acceleration	L t ⁻²	m/s ²	ft/s ²
J _C	Species diffusional flux	M L ⁻² t ⁻¹	kg/(m ² •s)	lbm/(ft ² •s)
J _D	Species dispersive flux	M L ⁻² t ⁻¹	kg/(m ² •s)	lbm/(ft ² •s)
k	Intrinsic permeability tensor	L ²	m ²	ft ²
k _r	Relative intrinsic permeability	L ²	m ²	ft ²
k _f	Thermal fluid conductivity	M L t ⁻³ T ⁻¹	W/(m•K)	BTU/(ft•s°F)
k _e	Effective thermal conductivity of fluid+solid matrix	M L t ⁻³ T ⁻¹	W/(m•K)	Btu/(ft•s°F)
k _s	Solid Thermal conductivity	M L t ⁻³ T ⁻¹	W/(m•K)	Btu/(ft•s°F)
k _d	Sorption coefficient	M ⁻¹ L ³	m ³ /kg	ft ³ /lbm
K	Hydraulic conductivity tensor	L t ⁻¹	m/s	ft/s
m	Rate of injection of fluid	M L ⁻³ t ⁻¹	kg/(m ³ •s)	lbm/(ft ³ •s)
mv	Fluid injection rate	t ⁻¹	m ³ /(m ³ •s)	ft ³ /(ft ³ •s)
n _E	Effective or flow porosity	----	----	----
n _D	Diffusive or connected porosity	----	----	----
n _T	Total porosity	----	----	----
N	Normal coordinate	L	m	ft
p	Thermodynamic pressure	M L ⁻¹ t ⁻²	N/m ²	lbf/ft ²

MATHEMATICAL NOTATION (Continued)

Symbol	Meaning	Dimensions	SI Units	FPS Units
P	Pressure head at reference fluid density	L	m	ft
\vec{q}_D	Dispersive energy flux	M t ⁻³	W/(m ²)	Btu/(ft ² •s)
\vec{q}_T	Conductive energy flux	M t ⁻³	W/(m ²)	Btu/(ft ² •s)
r	Radial coordinate	L	m	ft
R	Density ratio	----	----	----
R _d	Retardation factor	----	----	----
S	Area of a bounding surface	L ²	m ²	ft ²
S _c	Injection rate of species	M L ⁻³ t ⁻¹	kg/(m ³ •s)	lbm/ft ³ •s)
S _s	Specific Storativity	L ⁻¹	1/m	1/ft
ST	Injection rate of heat	M L ⁻¹ t ⁻³	W/(m ³)	Btu/(ft ³ •s)
t	Time	t	s	s
T	Thermodynamic temperature	T	K	°F
T _c	Critical temperature	T	K	°F
U	Darcy velocity in x- or r-direction	L t ⁻¹	m/s	ft/s
V	Darcy velocity in y- or θ-direction	L t ⁻¹	m/s	ft/s
\vec{V}	Total velocity vector	L t ⁻¹	m/s	ft/s
V	Volume	L ³	m ³	ft ³
W	Darcy velocity in z-direction	L t ⁻¹	m/s	ft/s
x	x coordinate	L	m	ft
y	y coordinate	L	m	ft
z	z coordinate	L	m	ft

Greek Symbol	Meaning	Dimensions	SI Units	FPS Units
α _f	Fluid compressibility	M ⁻¹ L t ²	m ² /N	ft ² /lbf
α _s	Solid compressibility	M ⁻¹ L t ²	m ² /N	ft ² /lbf
α _L	Longitudinal dispersivity	L	m	ft
α _T	Transverse dispersivity	L	m	ft
β _f	Thermal expansion coefficient for fluid	T ⁻¹	1/K	1/°F
μ	Dynamic viscosity of fluid	M L ⁻¹ t ⁻¹	kg/(m•s)	lbm/(ft•s)
ρ	Density of fluid	M L ⁻³	kg/m ³	lbm/ft ³
ρ _s	Density of solid	M L ⁻³	kg/m ³	lbs/ft ³

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θ	Volumetric moisture content	----	----	----
∂	Partial derivative	----	----	----
$\vec{\nabla}$	Gradient operator	----	----	----
ψ	Soil-water potential	L	m	ft
λ	Radioactive decay coefficient	t-1	s-1	s-1
η	porosity	----	----	----

Superscripts
& Subscripts

Meaning

e	Equivalent or effective value of a soil matrix property
s	Pertaining to the solid phase
x	Pertaining to x-direction
y	Pertaining to y-direction
z	Pertaining to z-direction
t	Pertaining to time
\approx	Tensor or matrix
*	Pertaining to a reference state of the system
→	Vector

aSI = International System of Metrics.
bFPS = Foot, Pound, Second Units.

1.0 OVERVIEW AND INTRODUCTION

1.1 INTRODUCTION

The PORFLO-3 computer code is a software package for solving problems related to fluid flow, heat transfer, and mass transport in variably saturated geologic media. The computer code is written in American National Standard Fortran 77 and is essentially independent of any specific computer hardware. Flexibility to adapt the code to a variety of problems is provided through user-selected options. To the extent possible, subroutines in PORFLO-3 are designed to perform distinct functions so that users may readily customize the code for their specific needs by replacing any module with one that is appropriate for the problem.

The objective of this user's manual is to provide detailed instructions for designing input data decks for, and analyzing outputs from, PORFLO-3. However, for successfully solving complex problems, users should have a basic understanding of the mathematical theory underlying the code. The governing differential equations, along with their boundary conditions and the numerical methods for solving them, will be described in considerable detail in a future manual.

Chapter 1.0 presents an overview of the main features of PORFLO-3. To facilitate reference, a brief summary of the theory is given in Chapter 2.0. Discussion on the structure of PORFLO-3 and its subroutines is provided in Chapter 3.0. Considerations for the design of the spatial grid and choice of time steps for obtaining stable and accurate solutions are discussed in Chapter 4.0. A summary of the input and output options is given in Chapter 5.0. Chapter 6.0 provides a detailed description of all commands.

1.2 MAIN FEATURES OF PORFLO-3

Several options are available in PORFLO-3. By choosing appropriate combinations of these options, a wide range of problems can be solved. This chapter provides a brief overview of these options. Their specific features are discussed in subsequent chapters. The following sections of this chapter give an overview of the main features of PORFLO-3.

1.2.1 Spatial Dimensionality

The code is designed to solve three-dimensional problems. However, it can be adapted to solve one- and two-dimensional problems by specifying a grid size(s) of three in the direction(s) that is to be omitted. In effect, this specification results in the solution of a pseudo-three-dimensional problem.

1.2.2 Problem Geometry

A problem can be defined in terms of either cartesian or cylindrical coordinates. In both coordinate systems, z is the direction of the vertical coordinate. The horizontal plane is represented by x - y in the cartesian system and by r - θ in the cylindrical system. In a one-dimensional problem, any of the three axes (x , y , or z) can be selected as the direction of interest. Two-dimensional problems can be solved in the x - y , x - z , or y - z plane. The computational elements can vary in size across the coordinate system, but their geometry is restricted to that of a rectangular parallelepiped.

1.2.3 Time Dependence

Either transient or steady-state problems can be solved. Except for the spatial grid, all problem parameters can change with time. The values of some parameters, such as the source terms for fluid, heat, and mass, can be assumed to change continuously with time. Such quantities can be specified in the form of tables. For other parameters, such as boundary conditions and properties of the media, the input data deck can be designed to change the data values after the specified time intervals.

1.2.4 Space Dependence

The values of most parameters are allowed to vary over the spatial grid. The model domain can be divided into zones, each zone having some distinct feature such as a material property or source concentration. The material properties can also be anisotropic.

1.2.5 Coupling of Equations

There are three main equations in PORFLO-3, one each for fluid flow, heat transfer, and mass transport. The state variables in these equations are the hydraulic head (P), temperature (T), and concentration (C), respectively. These equations can be solved either independently or in various coupled modes. Thus, problems related only to fluid flow or heat transfer or mass transport can be solved, or problems in which fluid flow is coupled to heat transfer or mass transport can be solved, or all three equations can be solved in a coupled mode. Depending on the specific problem, some of the couplings can be switched on or off (e.g., thermal buoyancy, fluid density, and viscosity effects on hydraulic properties).

1.2.6 Boundary Conditions

Varied types of boundary conditions can be specified in PORFLO-3. Dirichlet (specified values of hydraulic head, temperature, or concentration), Neumann (specified fluxes of fluid, heat, or mass), or mixed (combination of specified values and fluxes) boundary conditions can be stipulated. Different types of boundary conditions can be designated at various parts of a boundary. Combined with the time-dependence feature discussed in Section 1.2.3, this feature can be used to solve a large variety of problems with space- and time-dependent boundary conditions.

Occasionally, the domain in which the heat and mass transport equations are required to be solved is large. In such cases, and if the rates of heat and mass transport are slow, an option of solving these equations in grids that are smaller than the total domain may be used. With this option, a user can specify a location between the source and external boundary of the domain to be a temporary subdomain. This temporary subdomain can be expanded or eliminated when a specified condition is satisfied. This option can save computational time for problems that are characterized by large domain sizes and heat and/or mass sources concentrated in a small portion of the overall domain.

1.2.7 Methods for Solving Governing Equations

The governing equations are solved by first discretizing them over the spatial grid and time steps and then solving the resulting system of linear algebraic equations. The fluid flow equation is discretized based on quadratic approximating functions; these functions are equivalent to a central difference scheme. The second-order partial differential terms in the heat transfer and mass transport equations are also discretized through quadratic approximating functions. However, the first-order partial terms in these equations can be discretized by either a hybrid or an exponential scheme. The nature of these schemes is described in Chapter 2.0. The discretization method used in PORFLO-3 is based on integrating the approximating functions for each grid element. This method results in solutions that automatically conserve fluid, heat, and mass locally within every grid element, as well as for the entire model domain.

Alternate solution methods for the linear systems of algebraic equations are provided. These include the explicit method of Point Successive Over-Relaxation, and the implicit methods of Alternating Direction Implicit, Cholesky Decomposition, and Gauss Elimination.

1.2.8 Operational and Output Control

Through design of the input data deck, the user can exert extensive control over the operation of the code. For example, the execution of the code can be stopped to examine the output at any convenient point and restarted later from the point at which it was stopped. The user also has considerable control over the extent and nature of output. Output can be obtained as a tabulation or written in a file for post-PORFLO-3 processing in a graphic form. The variables to be tabulated, the size of the tables, and the times at which they are to be obtained can all be controlled by input commands.

1.2.9 Variable Saturation

Problems in which the geologic media are either fully or partially saturated, or in which some parts are fully saturated while others are partially saturated can be solved with PORFLO-3. In the partially saturated zone, liquid (water) and gas (air) are assumed to exist. However, the movement of only the liquid phase is addressed.

Consideration of heat and mass transfer is also restricted to the liquid phase; i.e., vapor transport is not considered. Consequently, PORFLO-3 is a 'single-phase' computer code.

As part of the solution, the degree of saturation is determined at each grid node of the domain. The boundary between the partially and fully saturated portions of the geologic media is the water table. The water table can be moved up and/or down only from grid node to grid node; no adjustment for water table position can be made that does not coincide exactly with node locations.

1.2.10 Special Geologic Features

In addition to the capability to consider heterogeneity and anisotropy of the porous geologic media as noted in Section 1.2.4, an option is included in PORFLO-3 that permits the user to consider planar geologic features such as fractures, faults, and clastic dikes. These features are distinguished from the parent media (soil and/or rock) by their distinctively different length scales and properties. For example, one of the three dimensions of fractures, faults, and clastic dikes is so small relative to the other two dimensions that these features behave essentially as two-dimensional (planar) elements that are embedded in the three-dimensional domain. Similarly, boreholes or other small man-made excavations are essentially one-dimensional features.

As indicated in Section 1.2.4, it is possible to treat all of these features as distinct three-dimensional zones. However, due to the different length scales involved, this treatment may result in exceedingly large grid sizes. An alternate option, to consider such features as two- or one-dimensional elements that are embedded within three-dimensional media, is available in PORFLO-3. The choice of this option will reduce the required grid sizes and computational time, but will only approximate the solutions in close proximity to the features.

1.2.11 Pore Structure

The user can define up to three types of porosities in PORFLO-3. The smallest of these is the effective or flow porosity, which consists of the pores through which fluid flow occurs. The second is the diffusive porosity. Diffusive porosity is greater than, or equal to, the effective porosity. It includes the dead-end pores that are assumed to not contribute to fluid flow, but that are assumed to facilitate the diffusion of heat and mass. The third porosity is the total porosity. Total porosity is greater than, or equal to, the diffusive porosity. In addition to the pores that comprise the effective and diffusive porosities, total porosity includes the isolated pores that are assumed to be inert to fluid flow and diffusion. These pores, however, are assumed to contribute to the conduction of heat.

1.2.12 Sources and Sinks

Several options are provided in PORFLO-3 for describing sources and/or sinks of fluid, heat, and mass. Spatially variable sources and/or sinks can be specified by identifying their zones of occurrence. The strength of the source and/or sink either can be constant or can vary with time. For mass, the sources can be limited by their inventory, solubility, or both.

1.2.13 Format-free Input

The input to PORFLO-3 is provided in a manner that is free of any format requirements. This feature is a major step toward making the code 'user friendly'. All input to PORFLO-3 is provided through the use of a keyword followed by alphanumeric data. Although the numerical data after a keyword must be entered in a specified sequence, it can be entered in any convenient format (I, E, or F) at any column location of the 80-column input-data card. In general, an input record can be designed to read like an easily understood complete sentence. A preprocessor is employed to interpret this input for internal use in the code. Chapter 6.0 describes in detail all of the key words of the input and their associated alphanumeric data. Details of the preprocessor FREEFORM (Runchal 1987a) are provided in Appendix A.

1.3 SUMMARY

Several user-selected options in PORFLO-3 provide the flexibility that makes the code suitable for solving a large variety of groundwater flow, heat transfer, and mass transport problems. The format-free means of providing the input makes the code user friendly. Internal checks built into the code help ensure that inputs are physically plausible; however, these checks are not comprehensive. Before attempting to solve a large or complex problem with PORFLO-3, the user is advised to solve either a spatially small problem with the desired time interval or a problem of the desired spatial size with a small time period. For problems that may require a lengthy computational time, the user is advised to scrutinize the output at some intermediate time step and then use the restart feature to complete the simulation.

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2.0 MATHEMATICAL BASIS

2.1 THE GOVERNING EQUATIONS

The governing equations in PORFLO-3 for fluid flow, heat transfer, and mass transport are written in terms of the hydraulic head (P), temperature (T), and mass concentration (C), respectively. These equations are based on the conservation principles of continuum mechanics (Bear 1972), except that the empirically derived Darcy's equation is used in place of the full-fledged momentum equation. A brief summary of the governing equations is provided here. The principal processes considered in developing these equations are listed in Figure 2-1.

2.1.1 Governing Equation for Fluid Flow

The equation for the conservation of a slightly compressible fluid mass in nondeforming media is

$$\partial_t(\theta\rho) + \vec{\nabla} \cdot (\rho\vec{V}) - m = 0. \quad (2.1-1)$$

The Darcy equation for nonisothermal flow is

$$\vec{V} = -(\underline{k}/\mu)(\vec{\nabla}p + \rho g\vec{z}). \quad (2.1-2)$$

Substituting Equation 2.1-2 into Equation 2.1-1, the governing equation for single-phase fluid flow for nonisothermal conditions becomes

$$\begin{aligned} S_s \partial_t P = & (1/r) \partial_x(rRK_x \partial_x P) + \partial_y(RK_y \partial_y P) + \partial_z\{RK_z(\partial_z P + B)\} \\ & + \theta\beta_f R \partial_t T + m_v. \end{aligned} \quad (2.1-3)$$

In Equations 2.1-1 through 2.1-3, the following symbols have been used:

∂ = partial derivative with respect to the subscripted variable

t = time

x, y, z = coordinates in cartesian coordinate system

\underline{k} = intrinsic permeability tensor

μ = dynamic fluid viscosity

θ = volumetric moisture content

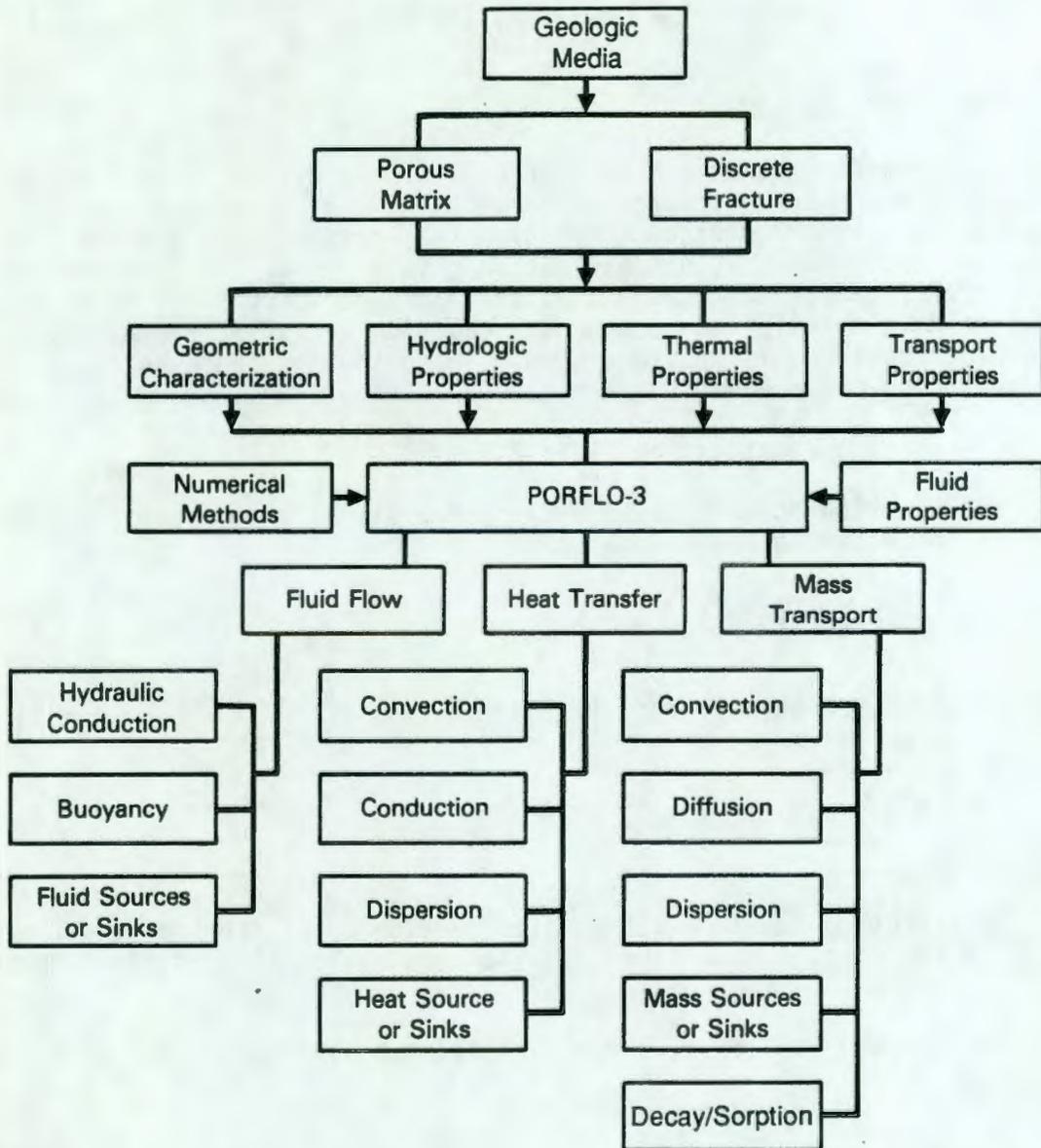


Figure 2-1. Geologic Features and Processes Addressed by PORFLO-3.

\vec{V} = Darcy velocity vector

p = fluid pressure

P = hydraulic head with respect to a reference fluid density

T = temperature of fluid-containing geologic media

S_s = fluid storage term (defined in Eq. 2.1-4a and 2.1-4b)

B = thermal buoyancy term (defined in Eq. 2.1-6)

β_f = fluid compressibility

m = fluid source term in mass units

m_v = fluid source term in volume units

K = hydraulic conductivity in the direction denoted by x, y, z subscripts (defined in Eq. 2.1-7)

$\vec{\nabla}$ = vector differential operator ($\vec{\nabla} = i\partial_x + j\partial_y + k\partial_z$)

r = radial coordinate in cylindrical coordinate system

R = ratio of fluid density (defined in Eq. 2.1-5)

g = acceleration due to gravity

i, j, k = unit vectors.

Fluid storage (S_s), density ratio (R), thermal buoyancy (B), and the hydraulic conductivity tensor (K) are defined as follows.

$$S_s = (\alpha_s + nE\alpha_f)\rho g \text{ if } \theta = nE \quad (2.1-4a)$$

$$S_s = \partial\theta/\partial\psi \text{ if } \theta < nE \quad (2.1-4b)$$

$$R = (\rho/\rho^*) \quad (2.1-5)$$

$$B = R - 1 \quad (2.1-6)$$

$$K_{ij} = \rho g k_{ij} / \mu \quad (2.1-7)$$

where, in addition to symbols already defined,

α_s = compressibility of solid media

ρ^* = fluid density at reference temperature

nE = effective or flow porosity

h = pressure head = (p/ρ^*g)

ψ = soil-moisture potential = $-h$ when $h < 0$.

In writing the above equations, the principal directions of the permeability tensor were assumed to coincide with the coordinate directions, so that only the diagonal terms of the tensor are nonzero.

The hydraulic head, P , is related to the pressure, p , as follows,

$$P = h + z - z^* \quad (2.1-8)$$

where z^* is an arbitrary datum. The pressure head, h , is larger than the atmospheric pressure head (therefore positive) for fully saturated flow and is less than the atmospheric pressure head (therefore negative) for partially saturated flow.

The volumetric moisture content, θ , is equal to the flow or effective porosity, n_E , for fully saturated flow; n_E is the porosity provided by interconnecting liquid convecting pores. In Section 1.2.1, two other porosities are noted. One of these is the diffusive porosity, n_D , which is the sum of effective porosity and the porosity provided by pores that do not convect liquid. The pores that do not convect liquid are assumed to be water-saturated, and heat and solutes are assumed to be transported into them by diffusion. The other type of porosity is the total porosity, n_T , which is the sum of effective porosity, diffusive porosity, and isolated porosity. Isolated pores are assumed to be impermeable to fluid flow and mass diffusion. However, heat is assumed to be conducted through the isolated pores.

For partially saturated flow, the soil-moisture potential, ψ , and intrinsic permeability, k , are functions of the volumetric moisture content, θ . The nature of these functions will be discussed in Section 2.1.4. The governing equation for fluid flow (Eq. 2.1-3) and Equations 2.1-12 and 2.1-14 in Sections 2.1.2 and 2.1.3, respectively, are applicable to both cartesian and cylindrical coordinates (Section 1.2.2).

2.1.2 Governing Equation for Heat Transfer

The governing equation for heat transfer in fluid-containing geologic media is based on the equation for the conservation of energy

$$\partial_t(e_e) + \vec{\nabla} \cdot (\rho \vec{V} e) = -\vec{\nabla} \cdot (\vec{q}_T + \vec{q}_D) + S_T \quad (2.1-9)$$

where

e = internal energy of the fluid per unit mass

e_e = equivalent internal energy per unit volume of the fluid-containing porous media (Eq. 2.1-10)

\vec{q}_T = rate of conductive heat transfer per unit area

\vec{q}_D = rate of diffusive heat transfer per unit area

S_T = thermal source term.

The equivalent or effective internal energy per unit mass of the fluid-containing geologic media is given by

$$e_e = [\eta_T \rho_{cf} + (1-n_T) \rho_{scs}] T \quad (2.1-10)$$

where

η_T = specific liquid volume conducting heat, $\eta_T = \theta + n_T - n_E$

n_T = total porosity of the medium

n_E = diffusive porosity

c_f = specific heat of fluid

c_s = specific heat of the media in dry condition

ρ_s = density of media in dry condition

T = temperature of fluid-containing medium.

In writing Equations 2.1-9 and 2.1-10, it was assumed that the transfer of heat is sufficiently slow that the fluid phase is always in thermal equilibrium with the solid phase. The rate of conductive heat transfer per unit area is obtained from Fourier's law as

$$\vec{q}_T = -k_e \vec{\nabla} T \quad (2.1-11)$$

and the rate of dispersion transfer is obtained from Fick's law as

$$\vec{q}_D = -\eta_D \vec{\nabla} T \quad (2.1-12)$$

where

\vec{D} = thermal dispersion tensor

η_D = specific volume of liquid diffusing heat; $\eta_D = \theta + n_D - n_E$.

The term k_e in Equation 2.1-11 is the effective thermal conductivity, which is calculated as

$$k_e = \eta_T k_f + (1 - n_T) k_s \quad (2.1-13)$$

where

k_f = thermal conductivity of fluid

k_s = thermal conductivity of dry solid.

Substituting Equations 2.1-10 and 2.1-11 into Equation 2.1-9, the governing equation for temperature is

$$c_e \partial_t T + (1/r) \partial_x (r \rho U c_f T) + \partial_y (\rho V c_f T) + \partial_z (\rho W c_f T) = \\ (1/r) \partial_x \left[r \left\{ k_e + \eta_D D_x \right\} \partial_x T \right] + \partial_y \left[\left\{ k_e + \eta_D D_y \right\} \partial_y T \right]$$

$$+ \partial_z \left[\left\{ k_e + \eta_D D_z \right\} \partial_z T \right] + S_T \quad (2.1-14)$$

where U, V, and W are the components of the Darcy velocity vector in the x, y, and z directions, respectively, D_x , D_y , and D_z are the principal components of the thermal diffusivity tensor, and c_e is the equivalent specific heat of the fluid-solid matrix defined in the same manner as k_e of Equation 2.1-13.

2.1.3 Governing Equation for Mass Transport

The equation for the conservation of mass can be written as

$$\partial_t C_e + \vec{v} \cdot (\vec{\nabla} C) = -\vec{v} \cdot (\vec{J}_C + \vec{J}_D) + S_C - \lambda C_e \quad (2.1-15)$$

where

C = concentration in fluid

\vec{J}_C = rate of mass transport due to molecular diffusion

\vec{J}_D = rate of mass transport due to hydrodynamic dispersion

S_C = mass source

λ = decay coefficient

C_e = mass per unit volume in the fluid-containing geologic medium
(see Eq. 2.1-16).

The C_e term in Equation 2.1-15 depends on the moisture content and is given by

$$C_e = \eta_D C + (1 - \eta_T) C_s \quad (2.1-16)$$

where C_s is the concentration associated with the solids. The liquid and solid phases are assumed to be in chemical equilibrium, and C and C_s are assumed to be related through a linear Freundlich isotherm (Freeze and Cherry 1979, p. 403); i.e.,

$$C_s = \rho_s k_d C \quad (2.1-17)$$

where k_d is the sorption or partition coefficient. The rates of mass transport in Equation 2.1-15 are evaluated using Fick's law as

$$\vec{J}_C = -\eta_D D_M \vec{\nabla} C \quad (2.1-18)$$

and

$$\vec{J}_D = -\theta \underline{D} \vec{\nabla} C \quad (2.1-19)$$

where

D_M = molecular diffusion coefficient

\underline{D} = hydrodynamic dispersion tensor.

Combining Equations 2.1-16 through 2.1-19 with Equation 2.1-15, the following governing equation for mass transport is obtained.

$$\eta_D R_D \partial_t C + (1/r) \partial_x(rUC) + \partial_y(VC) + \partial_z(WC) = (1/r) \partial_x\{r(\eta_D D_M + \theta D_x)\partial_x C\} + \partial_y\{(\eta_D D_M + \theta D_y)\partial_y C\} + \partial_z\{(\eta_D D_M + \theta D_z)\partial_z C\} + S_C - \eta_D R_D \lambda C \quad (2.1-20)$$

where

$$R_D = \left[1 + \frac{(1-n_T)\rho_s k_d}{\eta_D} \right]. \quad (2.1-21)$$

The term R_D of Equation 2.1-21 is the retardation coefficient.

2.2 THE AUXILIARY EQUATIONS

In addition to the governing equations discussed in Section 2.1, several auxiliary equations are employed in PORFLO-3. In general, these equations describe the dependence of soil (or rock) and fluid properties on moisture content, pressure, temperature, and concentration. These equations are summarized in the following sections.

2.2.1 Fluid Properties

The dependence of fluid density on temperature is described by three alternative equations:

$$\text{or} \quad \rho = \rho^* [(T_C - T)/(T_C - T^*)]^A \quad (2.2-1a)$$

$$\text{or} \quad \rho = A_1 + A_2 T + A_3 T^2 + A_4 T^3 \quad (2.2-1b)$$

$$\text{or} \quad \rho = \rho^* [1 + A_5 (T^* - T) + A_6 (C^* - C)] \quad (2.2-1c)$$

where

T_C = critical temperature

T^* = reference temperature

ρ^* = fluid density at T^*

A = empirically calculated exponent

C^* = reference concentration

A₁ to A₆ = empirical coefficients that depend on the nature of the fluid.

For water, T_c = 647.3 K, T* = 300 K, ρ* = 996.59 kg/m³, and A = 0.20. The fluid viscosity is similarly described by three alternative equations:

$$\mu = B_1 \exp(B_2/T) \quad (2.2-2a)$$

or

$$\mu = B_3 + B_4T + B_5T^2 + B_6T^3 \quad (2.2-2b)$$

or

$$\mu = \mu^* \exp[B_7(T^*-T) - B_8(T^*-T)^2] \quad (2.2-2c)$$

where μ* is the fluid viscosity at reference temperature, T*, and B₁ to B₈ are empirically determined coefficients. For water, the values of B₁ and B₂ are 6.4 x 10⁻⁶ kg/(m•s) and 1436 K, respectively.

2.2.2 Hydraulic Properties of Soil or Rock for Partially Saturated Conditions

Two types of functional relations are required: (1) Between moisture content, θ, and the pressure head, h (or soil-moisture tension, ψ) and (2) between relative hydraulic conductivity, k_r, and moisture content, θ (or ψ). The θ - ψ (or θ - h) relationship is a basic soil (or rock) property for partially saturated flow and is usually based on measurements. The k_r - θ relationship, on the other hand, is derived from the θ - ψ relationship. For both the θ - ψ and k_r - θ relations, three options are provided in PORFLO-3. The first option is to use the functional relations of van Genuchten (1978),

$$\theta^* = [1 + (\psi/\alpha)^n]^{-m}, \quad h < 0, \quad (2.2-3a)$$

$$\theta^* = 1, \quad h \geq 0. \quad (2.2-3b)$$

Using Mualem's predictive model (Mualem 1976), the corresponding function for k_r is

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m]^2, \quad (2.2-4a)$$

while with Burdine's model (Burdine 1953), the relation is

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m] \quad (2.2-4b)$$

in which θ* and k_r are the normalized water content and relative hydraulic conductivity respectively, which are defined as

$$\theta^* = \frac{\theta - \theta_r}{nE - \theta_r} \quad (2.2-5)$$

and

$$\frac{K}{K_s} = \frac{K_s}{K_s} k_r \quad (2.2-6)$$

where

K_{sS} = saturated hydraulic conductivity tensor

k_r = relative conductivity

θ_r = residual moisture held in small pores against large negative (suction) pressure

$m = (1 - 1/n)$.

The second option is to use the relation from Brooks and Corey (1966)

$$\theta^* = (\psi/\psi^*)^{-\beta}, \quad h < -\psi^*, \quad (2.2-7a)$$

$$\theta^* = 1, \quad h \geq -\psi^*, \quad (2.2-7b)$$

and

$$k_r = \theta^*(5/2 + 2/\beta) \quad (2.2-8a)$$

or

$$k_r = \theta^*(3+2/\beta) \quad (2.2-8b)$$

where ψ^* is the air-entry head. Again, Equation 2.2-8a is obtained using the Mualem (1976) theory and the Burdine (1953) theory leads to Equation 2.2-8b.

The third option for both the $\theta - h$ and $k_r - \theta$ relationships is to provide them in a tabular form. Linear interpolation between specified values is then used to estimate the required values.

2.2.3 Hydrodynamic Dispersion Tensor

The hydrodynamic dispersion tensor is assumed to be diagonal; i.e., its principal axes are assumed to coincide with the coordinate directions. Consequently, it has three directional components. The directional components are related to the dispersivities as

$$D_x = \alpha_L U' + \alpha_T (V'+W') \quad (2.2-9a)$$

$$D_y = \alpha_L V' + \alpha_T (W'+U') \quad (2.2-9b)$$

$$D_z = \alpha_L W' + \alpha_T (U'+V') \quad (2.2-9c)$$

where α_L and α_T are, respectively, the longitudinal and transverse dispersivities, and

$$U' = U^2/\xi; \quad V' = V^2/\xi; \quad W' = W^2/\xi \quad (2.2-10a)$$

where

$$\xi = (U^2 + V^2 + W^2)^{\frac{1}{2}}. \quad (2.2-10b)$$

2.2.4 Boundary and Initial Conditions

The boundary conditions for the three governing equations can be represented in general as

$$- a\partial F/\partial N = b(F - F_0) + c \quad (2.2-11)$$

where F represents P , T , or C , depending on the governing equation under consideration, N is a direction that is normal to the boundary, and a , b , c , and F_0 are specified constants. By selecting appropriate values of a , b , c , and F_0 , three types of boundary conditions can be represented by Equation 2.2-11. These boundary conditions are as follows.

1. Dirichlet boundary condition: Obtained by specifying $a = c = 0$ and $b = 1$. In other words, this condition is represented by

$$F = F_0 \quad (2.2-12a)$$

where F_0 is the specified value of F at the boundary. This boundary condition is also known as a fixed head, temperature, or concentration boundary condition for the P , T , and C equations, respectively.

2. Neumann boundary condition: Obtained by specifying $b = 0$. In this case, a is equal to hydraulic conductivity, thermal conductivity, or the dispersion coefficient for the fluid flow, heat transfer, and mass transport equations, respectively. Thus, this boundary condition is

$$- a\partial F/\partial N = c \quad (2.2-12b)$$

where c is the specified flux of fluid, heat, or chemical species per unit surface area of the boundary.

3. Mixed (or radiation) boundary condition: Obtained by substituting $c = 0$ in Equation 2.2-11, resulting in

$$- a\partial F/\partial N = b(F - F_0). \quad (2.2-12c)$$

In this case, ' a ' has the same meaning as in the Neumann boundary condition, ' b ' is the fluid, heat, or mass transfer coefficient, and F_0 is the equilibrium value of F . Using the heat transfer equation as an example, F_0 may be specified to be the temperature of the atmosphere to which heat is being lost from the boundary of the domain under consideration.

The initial condition can be any reasonable value of the variable under consideration. For ease of specification, a linear variation in both the initial and boundary conditions is allowed; i.e.,

$$F = a + bx + cy + dz \quad (2.2-13)$$

where a , b , c , and d are constants, and x , y , and z are the coordinates of a point either in the interior of the domain or on its boundary.

2.3 THE NUMERICAL METHOD

Numerical solution of the governing equations described above requires two steps: (1) Discretization of the equations for the grids of space and time and (2) solution of the resulting system of linear algebraic equations. A brief summary of these two steps is provided in the sections that follow.

2.3.1 Discretization Scheme

Spatial discretization is performed over a nonuniform grid that is imposed on the domain of interest. One such grid is formed by the system of cartesian coordinates illustrated in Figure 2-2. In this figure the dashed lines are the grid lines; and the solid lines are the cell (or element) boundary lines. The cell boundaries are drawn midway between the grid lines, and each cell formed by the solid lines encloses one grid node. Because of the nonuniform spacing of the grid lines, the node is not at the centroid of the cell, as indicated in the figure.

For all computations in PORFLO-3, the fluxes of fluid, heat, and mass are calculated and/or specified at the cell boundaries (solid lines). The state variables [i.e., hydraulic head (P), temperature (T), and concentration (C)] are calculated and/or specified at the nodes (with the few exceptions noted in Chapter 6.0). Each node (and cell corner) is indexed by an ordered alphanumeric triplet (i,j,k), as indicated in Figure 2-2.

The discretized form of the governing equation is obtained by integrating it over each cell. To perform this integration, a profile for the variable (P , T , or C) is assumed. When the second-order derivatives in the governing equations are integrated, a quadratic profile is assumed. This results in algebraic equations that are equivalent to a central difference scheme. For the first-order derivatives in the governing equations for T and C , two schemes are provided.

In the hybrid scheme, a quadratic profile is assumed if heat and mass are transferred primarily by dispersion. The relative importance of dispersion as a transfer mechanism is judged by calculating a grid Peclet number that is the fluid velocity divided by the dispersivity for each cell. If this number is less than two, dispersion is assumed to be the primary mode of heat and mass transfer. However, if the grid Peclet number is larger than two, an upwinding scheme is used.

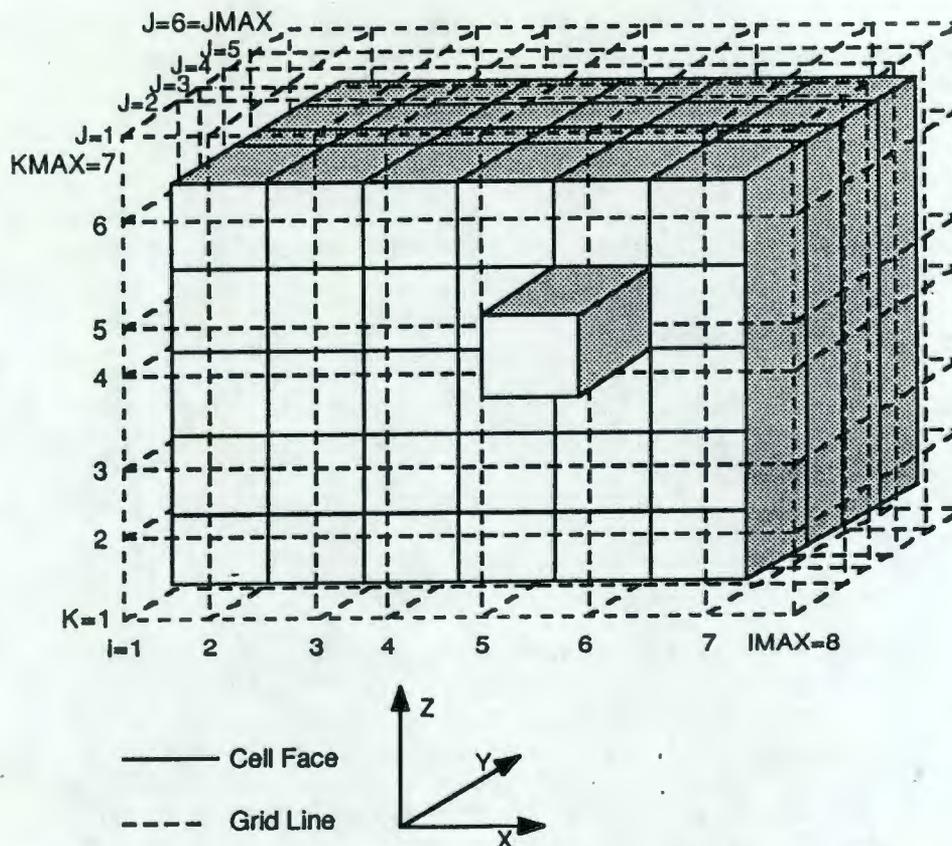


Figure 2-2. Example of a Nonuniform Grid Using Cartesian Coordinates.

In the upwinding scheme, the fluid velocity at the up-stream cell boundary of a grid node is assumed to control heat and mass transfer through that cell. Such a scheme, although efficient, can result in false diffusion (greater smearing of the concentration plume than would be expected). The alternative exponential scheme strives to correct this shortcoming by assuming piecewise exponential profiles for T and C . Because of the computation of exponential functions in this scheme, it is more expensive to use than the upwinding scheme.

The discretization in PORFLO-3 with respect to time may be either explicit or implicit. In the explicit scheme, any nodal values of the variables P , T , or C that appear in the spatially discretized equation are taken at the time step that precedes the time step for which they are being calculated. Knowing the values at the preceding time step, a straightforward calculation of the value at the new time can be made. In the implicit schemes, by comparison, some or all of the nodal values in the spatially discretized equation are taken at the new time step. Thus, each algebraic equation in this case has more than one unknown, and matrix methods are required to solve the set of equations.

Denoting by F the variable that may be P , T , or C , depending on the governing equation to be discretized, the general form of the discretized equation for a node identified by (i,j,k) is given below. In this equation, implicit discretization with respect to time has been assumed and n denotes the time step.

$$\begin{aligned}
 & A_E F(i+1,j,k,n+1) + A_W F(i-1,j,k,n+1) + A_N F(i,j+1,k,n+1) \\
 & + A_S F(i,j-1,k,n+1) + A_T F(i,j,k+1,n+1) + A_B F(i,j,k-1,n+1) \\
 & - [A_E + A_W + A_N + A_S + A_T + A_B] F(i,j,k,n+1) + S_F(i,j,k,n+1) \\
 & = A_R [F(i,j,k,n+1) - F(i,j,k,n)] \qquad (2.3-1)
 \end{aligned}$$

where S_F is the source at the (i,j,k) cell at time step $(n+1)$. The coefficients A_E , A_W , A_N , A_S , A_T , A_B , and A_R are functions of the internodal distances, cell sizes, and properties of the media. Their exact forms depend on the spatial discretization scheme adopted as well as the time step.

The method of discretization discussed above is known as the nodal point integration method. It has the advantage of conserving the fluid, energy, and mass not only within each cell, but for the entire domain. In this manner, no false sources and/or sinks of fluid, energy, and mass are created as can happen with other discretization schemes (e.g., schemes using Taylor expansion and Galerkin's approach).

2.3.2 Solution of Algebraic Equations

One equation of the type given in Equation 2.3-1 is obtained for each grid node. To solve this set of algebraic equations, four options are provided in the PORFLO-3 code.

The first option is for use with explicit equations that are obtained if the time step $(n+1)$ on the left side of Equation 2.3-1 is replaced by ' n '. In this case, there is only one unknown $[F(i,j,k,n+1)]$ per equation; therefore, the unknown is easily solved for. The solution is obtained for every node and the process is repeated until the calculated values do not change by more than a specified tolerance limit. This procedure is termed the method of point-successive over-relaxation (PSOR).

The remaining three methods are for use with implicit equations. With the first of these, the alternating direction implicit (ADI) method, solution of the set of algebraic equations is obtained in three sweeps, one each along the x -, y -, and z - coordinate directions. For each sweep, Equation 2.3-1 is written only with the values at the grid nodes in that direction, at the advanced time step $(n+1)$. All other values are taken at the previous time step (n) . In this manner, each equation has only three unknowns, which gives rise to a tri-diagonal system of equations that are solved by standard means.

The second method of solving implicit equations is by Choleski decomposition. This method is applicable only to those systems of equations, such as for the fluid flow equation, that produce symmetric coefficient matrices. For the heat transfer and mass transport equations, symmetric matrices result if transport does not occur by fluid convection. Therefore, the application of this method is rather limited. In this method, the symmetric coefficient matrix of the algebraic equations is decomposed into a special form that consists of a diagonal matrix and lower and upper triangular matrices. Once the decomposition is done, the solution is obtained by back substitution.

Standard Gauss elimination without any preconditioning is the third method of solving implicit equations. This method is applicable to both symmetric and nonsymmetric matrices and, therefore, to all three governing equations of PORFLO-3.

Finally, the Reduced System Conjugate Gradient (RSCG) method that is useful for sparse systems is available in PORFLO-3. This method provides an accelerated iterative solution and is described in detail by Kincaid et al. (1982).

2.4 SUMMARY

Continuum mechanics provides the mathematical basis for the PORFLO-3 code. The governing equation for fluid flow, written in terms of the hydraulic head, P , employs the nonisothermal form of the Darcy equation. The governing equation in terms of temperature, T , includes heat transfer by conduction, hydrodynamic dispersion, and convection. Similarly, the governing equation in terms of chemical concentration, C , includes mass transport by molecular diffusion, hydrodynamic dispersion, and convection. All three governing equations are coupled through the fluid velocity term (U , V , and W) because of the temperature and concentration dependence of fluid properties. The fluid flow equation is nonlinear for partially saturated conditions, and its solution is obtained through iterations. Two alternate methods for discretizing the convective term in the heat transfer and mass transport equations and four alternate methods for solving the discretized equations are provided.

3.0 CODE STRUCTURE

3.1 SUBROUTINES AND THEIR FUNCTIONS

The PORFLO-3 computer code has 89 subroutines. To the extent possible, each subroutine has been assigned a single, distinct function. The names of these subroutines and their assigned functions are listed in alphabetical order in Table 3-1. A brief description of the information flow between subroutines is given in the next section.

Table 3-1. PORFLO-3 Subroutines and Their Primary Functions.
(sheet 1 of 5)

No.	Subroutine	Function
1.	ADATA	Read and interpret format-free input data.
2.	AFLOW	Provide coordination and operational control.
3.	ARCHIV	Read and write headers and grid information for the data archive.
4.	ARCHV2	Read and write field arrays for the data archive.
5.	ARRAYS	Initialize two-dimensional field arrays.
6.	BCDCAY	Adjust boundary conditions to account for radioactive decay.
7.	BCDFLT	Assign default boundary conditions for the governing equations.
8.	BCEDGE	Calculate boundary values at the corners of the domain.
9.	BCFO	Perform preliminary operations on boundary conditions.
10.	BCPOST	Compute boundary values after matrix inversion.
11.	BCPRE	Modify coefficient matrix for boundary values.
12.	BCUSER	Implement user-specified boundary conditions.
13.	BCUVW	Calculate boundary values for velocity components.
14.	BUGSET	Incorporate user-specified data on active debugging options.

Table 3-1. PORFLO-3 Subroutines and Their Primary Functions.
(sheet 2 of 5)

No.	Subroutine	Function
15.	CYCLE	Incorporate periodic boundary conditions.
16.	DATTIM	Call system time and date routine.
17.	DELXYZ	Calculate fracture length between grid nodes.
18.	DENSTY	Calculate the thermal buoyancy term for the pressure equation.
19.	DIFH	Compute hydraulic and thermal conductivities and mass diffusivities at the cell faces.
20.	DISPER	Calculate dispersion coefficients for the porous matrix.
21.	DOMAIN	Calculate the subdomain of interest for the heat and concentration equations.
22.	ERROR1	Print error conditions for FORTRAN INTEGER variables.
23.	ERROR2	Print error conditions for FORTRAN REAL variables.
24.	ERROR3	Print error conditions for specification of planar elements and sources.
25.	EXIST	Detect the presence of a modifier on a user command.
26.	EXPM	Determine the value of the exponential function.
27.	FDS	Compute matrix coefficients for the heat and concentration equations.
28.	FDSEXP	Calculate matrix coefficients for the exponential scheme.
29.	FDSP	Store coefficient matrix for the pressure equation.
30.	FIX	Fix values of variables at user-specified internal grid nodes.
31.	FLOW	Compute fluid flow through cell faces.
32.	FLUX	Calculate convective and diffusive fluxes of heat and mass through cell faces.

Table 3-1. PORFLO-3 Subroutines and Their Primary Functions.
(sheet 3 of 5)

No.	Subroutine	Function
33.	FLUX1	Perform the repetitive calculation required by FLUX.
34.	GEODEF	Define the default geometry for the problem.
35.	GEOM	Calculate lengths, areas, and volumes associated with computational elements.
36.	GETROW	Obtain elements of a selected row from the coefficient matrix.
37.	GRID	Calculate default values or user-specified values of x and y coordinates.
38.	HARMON	Compute the harmonic mean of a variable.
39.	HISTRY	Interpret user-supplied specifications for time-dependent output.
40.	HISTR2	Prepare data for time plots and tabular output.
41.	INIT	Provide default and initial values.
42.	INPUT	Coordinate reading of user-specified input data.
43.	INPUT2	Call satellite module for INPUT.
44.	INPUT3	Read tabular input on unsaturated properties.
45.	INTABL	Calculate the value of a variable by linear interpolation.
46.	INVERT	Invert nonperiodic tri-diagonal matrices.
47.	IOFILE	Extract the file name and format from input data.
48.	IOUNIT	Open the operating system files for I/O operations.
49.	LOCNP	Transform grid indices from 3-D to 1-D space and vice versa.
50.	OPENIO	Open an I/O file.
51.	OUTALL	Coordinate printing of tables for two-dimensional field arrays.

Table 3-1. PORFLO-3 Subroutines and Their Primary Functions.
(sheet 4 of 5)

No.	Subroutine	Function
52.	OUTF1	Set output options for field variables based on input data.
53.	OUTF2	Select default options for the output of field variables.
54.	OUTSAV	Coordinate the reading and writing of data archives.
55.	OUTVAR	Process user-specified options for the output of field variables.
56.	PECFNC	Calculate the Peclet number function for the exponential scheme.
57.	PLALFA	Compute the storage term for planar and linear elements.
58.	PLAREA	Calculate the area of plate elements.
59.	PLPRF	Incorporate the effects of planar and linear elements into the temperature and concentration equations.
60.	PLPRF2	Call satellite module for PLPRF.
61.	PLPRP	Incorporate effects of 1-D and 2-D elements into the pressure equation.
62.	PORFLO	Coordinate memory allocation and call AFLOW.
63.	PRINT	Print out record of key variables and parameters at the reference node.
64.	PRNTZN	Print component and matrix properties for each zone.
65.	PROPER	Calculate volumetric and effective properties of soil/water matrix.
66.	PROPZ	Define zonal properties from user input.
67.	PROPO	Incorporate default values for density and viscosity.
68.	PUTF	Perform internal three-dimensional array manipulations.
69.	RESDU2	Calculate the residual error in the solution of a variable.
70.	ROUND	Round off numeric labels on plots.
71.	SLVADI	Solve the equation by the ADI method.

Table 3-1. PORFLO-3 Subroutines and Their Primary Functions.
(sheet 5 of 5)

No.	Subroutine	Function
72.	SLVCHL	Solve the equation by the method of Cholesky decomposition.
73.	SLVGSE	Solve the equation by method of Gaussian elimination.
74.	SLVSOR	Solve the equation by the PSOR method.
75.	SOLVE	Coordinate the solution of the set of algebraic equations.
76.	SORCIN	Incorporate source information into appropriate arrays.
77.	SOURCE	Compute the current value of source and sink terms.
78.	SOURC9	Compute the current value of the inventory-limited source term.
79.	TABLES	Set up format for the printing of 3-D field variables.
80.	TABLE2	Print tables of the 3-D field variables.
81.	TSTAT	Calculate time of computation.
82.	USPIN	Compute the hydraulic conductivity of unsaturated media.
83.	USPRP	Process soil properties for unsaturated media.
84.	VEL	Calculate Darcy velocity components and stream function.
85.	WINDOW	Incorporate the input specification of a window or sub-domain.
86.	XALFA	Calculate the volumetric storage term for the general equation.
87.	XYPLOT	Produce time-history printer plots.
88.	ZNAME	Initialize the names of two-dimensional arrays.
89.	ZONE	Assign a zone-designation index to various regions of flow.

3.2 INFORMATION FLOW BETWEEN SUBROUTINES

The main subroutine is named PORFLO-3. The sizes of various arrays are declared in this subroutine. The problem title, user identification,

and grid size are read from the input file and the AFLOW subroutine is called to start the solution. Normal termination of the program occurs in this subroutine.

The sequence of the solution process is controlled by AFLOW. First, the initial or default values of various parameters (properties of fluid and matrix, computational cell size, time step, program execution controls, and output tables) are assigned by calling the subroutine INIT. Some or all of these default values subsequently change because of the user-supplied data. The default values are discussed in Chapter 6.0. Some of the information required to control the execution of the program is read within AFLOW. This information includes the frequency and nature of tabular output, creation of a restart file, time steps, and criteria to end calculations. The remaining problem-related information is obtained by calling the INPUT subroutine to read the user-supplied data.

All user-supplied data are obtained in the form of 80-character input records created by the user in the input file. These records, which are identified by the keywords defined in Chapter 6.0, have no format requirements. Each input record is interpreted by the ADATA subroutine before storing it for internal use in the code. Several subroutines are called, either from AFLOW or INPUT, to read the entire data set. These subroutines include BCUSER for reading boundary condition data, PROPZ for fluid and matrix properties, USPIN for hydraulic properties of partially saturated media, SORCIN for defining sources of fluid, heat, and mass, PLZONE for data on linear or planar geologic features, and OUTF1 for obtaining the names of variables for tabular output.

Data processing begins by calling the GEOM subroutine, in which the internodal distances, cell sizes, surface areas, and volumes are calculated. Then, a check is made in the AFLOW subroutine to determine which of the three governing equations are to be solved. The sequence of equation solution is: (1) Fluid flow, (2) heat transfer, and (3) mass transport. Solution of the fluid flow equation begins by calling the DIFH subroutine in which the zonal hydraulic conductivities are assigned to appropriate nodes. From the nodal values, hydraulic conductivities at the cell faces are calculated in the HARMON subroutine. Also in HARMON, these hydraulic properties are appropriately combined with internodal distances and cell sizes to obtain preliminary values of coefficients of the algebraic equations (see Section 2.2). These coefficients are modified for linear or planar geologic features in the PLPRP subroutine. Thermal buoyancy terms are calculated in the DENSITY subroutine. The final values of the coefficients are calculated in the FDSP subroutine. The fluid source term is assigned in the SOURCE subroutine. At this stage, the SOLVE subroutine is called to solve the system of algebraic equations. Before the actual solution, however, boundary conditions are incorporated into the equations by the BCPRE subroutine. In accordance with the choice of a solution method, the SOLVE subroutine directs the flow of information to the SLVADI (ADI), SLVCHL (Choleski decomposition), SLVGSE (Gauss elimination), or SLVSOR (PSOR) subroutine for the actual solution. The

values of the hydraulic head at domain boundaries are calculated in the BCPOST subroutine. Fluid mass balances are checked in the RESDUE subroutine.

The solution of the heat transfer and mass transport equations proceeds in a similar manner through the same subroutine, except that the hydrodynamic dispersion coefficients are calculated in the DISPER subroutine, and the final values of the coefficients of the algebraic equations are obtained in the FDS subroutine. Compared to the fluid flow equation, an additional term is accommodated in FDS because of the first-order derivatives in the heat transfer and mass transport equations.

An example of a typical flow of information in PORFLO-3 is depicted by Figure 3-1. The two larger subroutines, AFLOW and INPUT, are shown in segments, each having a distinct function. To the left of AFLOW in the figure, the subroutines used to produce output are grouped for easy reference.

3.3 INPUT AND OUTPUT FILE UNITS

PORFLO-3 employs six I/O units, whose input functions are assigned by default. Their names, default assignments, and functions are listed in Table 3-2. The user has the option of attaching the first four of these units to alternative files (or devices).

3.4 DIMENSION PARAMETERS

The PORFLO-3 code employs FORTRAN PARAMETER statements to change the dimensions of various arrays. Twelve parameters completely define the dimensions of these arrays (Table 3-3). The user must ensure that the dimensions set by these parameters are equal to, or larger than, those required for the problem to be solved. For example, the parameters LX, LY, and LZ should be equal to, or greater than, the number of grid nodes in the x- or (r-), y- (or θ), and z-coordinate directions.

3.5 SUMMARY

PORFLO-3 is composed of 89 subroutines. The AFLOW subroutine controls the flow of information between subroutines. Storage is allocated in the main subroutine, PORFLO-3. All of the storage is allocated in named common blocks. Variables whose values are stored at every grid node (or cell face) are termed field variables. Twenty-one field variables are present in PORFLO-3; they use most of the storage.

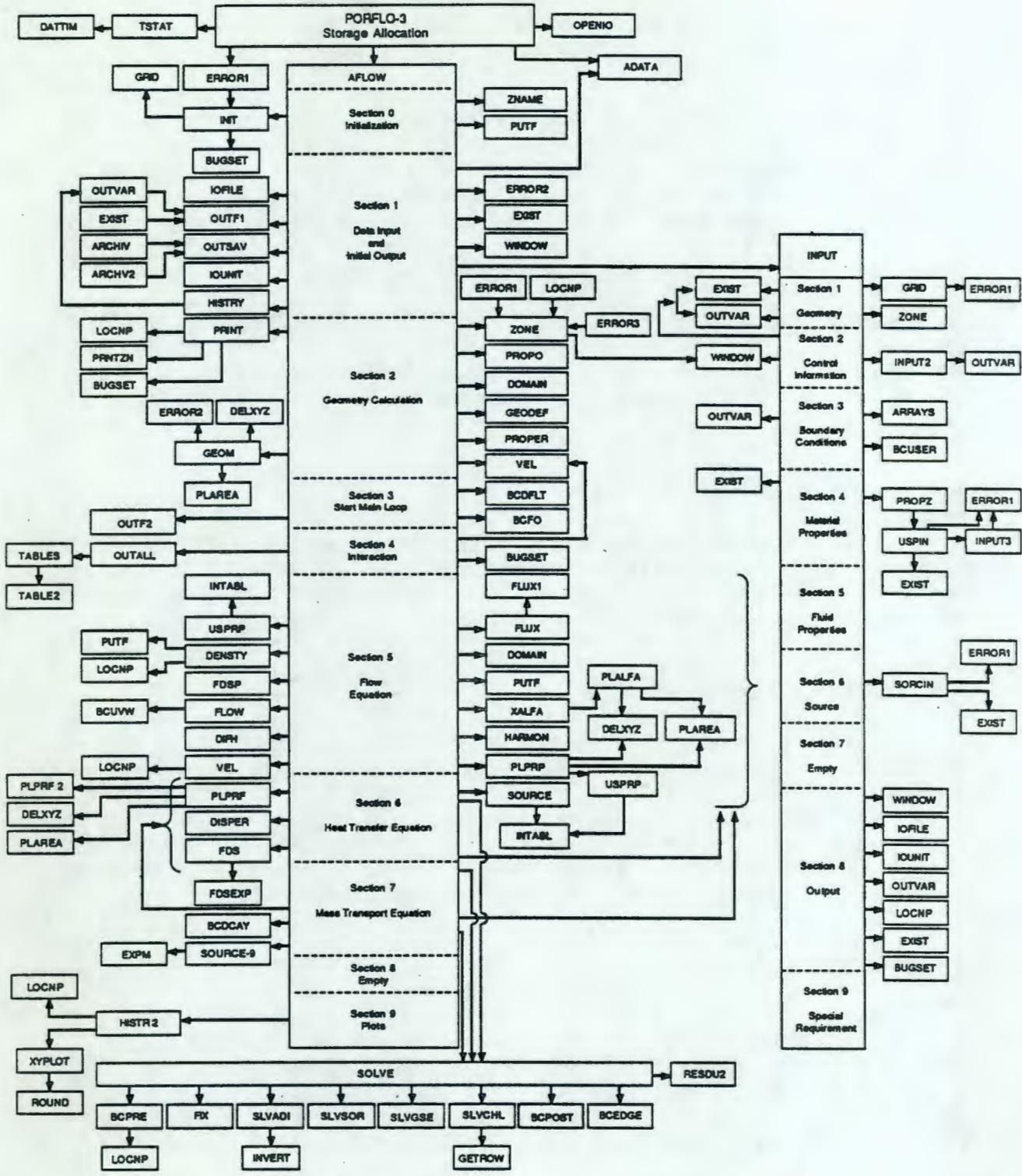


Figure 3-1. Information Flow within PORFLO-3.

Table 3-2. I/O File Units of PORFLO-3.

Unit No.	Symbolic name	Default assignment		Input function
		File name	Data type	
1	NUNIT1	RESTART	Unformatted	Read input data for restart option.
2	NUNIT2	ARCHIVE	Unformatted	Write data file for restart, archive, and post-processor.
3	NUNIT3	TIMEHIS	Unformatted	Write time-history data.
4	NUNIT4	ZONEFLX	Unformatted	Write data for fluxes crossing a zone boundary.
5	IRD	Console	Formatted	Read user input commands.
6	IWR	Printer	Formatted	Write output from PORFLO-3.

Table 3-3. Description of Dimension Parameters.

Parameter	Description
LX	Maximum number of grid coordinates in the x-direction.
LY	Maximum number of grid coordinates in the y-direction.
LZ	Maximum number of grid coordinates in the z-direction.
LMX	Largest of LX, LY, and LZ.
LSS	Maximum number of sources in an equation.
LSO	Maximum number of values in a time-source table.
LUS	Maximum number of values in a table of properties of the unsaturated zone.
LFLD	Maximum size of the matrix of algebraic equations.
LBC	Maximum number of locations where boundaries are specified.
LZN	Maximum number of zones.
LSR	Maximum number of elements in the tabular input for the source (or sink) of fluid, heat, or mass.
LSZ	Maximum number of zones (for each variable) in which a source (or sink) may be present.

4.0 SPATIAL GRID AND TIME STEPS

The design of the spatial grid and choice of time steps for a given problem may depend on several competing objectives. A need for detailed and accurate solutions suggests the use of a fine-mesh spatial grid and small time steps, but limitations on computer resources (memory and execution time) restrict their use. In practice, considerations of computational cost, accuracy and stability of numerical solution, output needs with respect to locations and times, and accommodation of special physical features (boundaries, heterogeneities, and sources) influence design of the spatial grid and choice of time steps.

4.1 DESIGN OF SPATIAL GRID

The spatial grid in PORFLO-3 is composed of elements (or cells) that are rectangular parallelepipeds. For a cartesian coordinate system, the size of an element enclosing a node (i,j,k) is written as $(\Delta x_i, \Delta y_j, \Delta z_k)$. For a cylindrical coordinate system, they are written as $(\Delta r_i, \Delta \theta_j, \Delta z_k)$. The values of these element sizes depend on the factors described in the following sections.

4.1.1 Scale of Heterogeneity

The spatial variation in hydraulic, thermal, and mass transport properties should be adequately represented by the grid. The material properties are specified at grid nodes (see Section 2.3.1) and are assumed to remain constant within a cell. If these properties change in a discontinuous manner, as commonly would occur in layered media, spatial grids should be designed such that a cell face coincides with the boundary between two layers with differing characteristics. For problems with continuously varying properties, the cell size should be smaller in regions where the variation in properties is relatively rapid, and larger where the variation occurs more gradually. All other factors being equal, a uniformly accurate solution may be expected if the properties of interest vary uniformly across the cells of interest.

To design the grid, it is helpful to sketch the domain and all of the zones in which the properties have different values. Then, cell faces should be located wherever properties are expected to change abruptly. Because a cell face is located midway between two nodes, the two nodes on either side of the cell face should then be located.

4.1.2 Scale of Resolution

For a variety of reasons, in specific parts of the domain solutions may be needed at a finer scale than in other parts. For example, interest may be focused on those areas where temperatures or chemical concentrations are high. In such areas, smaller cells should be used.

4.1.3 Scale of Geologic Features

Geologic or man-made features such as fractures and clastic dikes, and bore holes, wells, and tunnels, respectively, are distinguishable from the geologic continuum by distinctive contrasts in their physical properties and scales. To accurately represent these features, cell sizes that are comparable to the sizes of these features (i.e., to the sizes of their openings, thicknesses, and diameters) should be used.

However, if the solution in close proximity to these features is not of interest, they may alternatively be represented as two-dimensional planar elements and one-dimensional line elements. Fractures and clastic dikes can be considered to be planar features because the dimension orthogonal to the plane defined by their dip and strike is considerably smaller than their dimension in that plane. Thus, fluid flow, heat transfer, and mass transport can be assumed to occur in only two-dimensions in these features. Similarly, only one dimension needs to be considered for boreholes, wells, and tunnels. If these features are represented using reduced dimensionality, the choice of cell sizes is not affected by them.

4.1.4 Sources and Sinks

Hydraulic head, temperature, and chemical concentrations are expected to change relatively rapidly close to sources and/or sinks of fluid, heat, and mass. Unacceptable errors may occur in the solution if large cells are used in such areas. As a general principle, finer-mesh grids should be used in areas where the values of the state variables are expected to change rapidly.

4.1.5 Boundary Conditions

Some boundaries are natural geologic features. For instance, a river may form a boundary at which it is appropriate to specify hydraulic heads. Cell sizes should be comparatively small in close proximity to these boundaries. Other boundaries do not represent natural geologic features and are usually located at large distances (in theory, at infinite distance) from the area of interest. Near these boundaries, coarse-mesh grids can be used. In problems with boundaries at infinity, it is advisable to discern whether the boundaries are indeed located at distances sufficiently far that they do not affect the solution.

4.1.6 Memory Requirements

The amount of computer memory required for solving a problem is directly proportional to the number of computational cells. Consequently, an upper limit to the number of computational cells is imposed by the capacity of the available computer memory. An estimation of appropriate cell size, based on considerations discussed in Sections 4.1.1 to 4.1.5, may require subsequent adjustment to remain within this limit.

4.1.7 Computation Time

The time required to solve a problem is a nonlinear function of the number of grid cells. The time of computation increases in a ratio that varies from the square to the cube of the number of cells. In some cases, the maximum allowable computation time may restrict the maximum number of computational cells.

4.2 CHOICE OF TIME STEPS

The size of time steps is determined by the time scales characteristic of the propagation of pressure, diffusion, and convective transients. These time scales depend on the cell sizes discussed in Section 4.1 and the material properties discussed in the following sections.

The choice of time steps is also influenced by considerations of numerical stability. In general, a stable numerical scheme controls the growth of numerical error as the solution advances with time. Two types of instabilities may be encountered: (1) Weak instability in which the solution oscillates about a mean value and (2) strong instability in which divergence from the true solution increases monotonically. Both types of instabilities can be removed by shortening the time steps. However, for strong instability, alternate solution methods (see Section 2.3.2) may be more economical.

4.2.1 Time Scale of Pressure Transient

Let ΔL represent the length of one edge of a computational cell; ΔL can be equal to Δx , Δy , or Δz , depending on the coordinate direction under consideration. Similarly, let K_L represent the hydraulic conductivity in the L direction of the cell under consideration (L could be in the x , y , or z direction). The characteristic time scale (δt_{pL}) for the propagation of transient pressure (or hydraulic head) effects in the L direction for that cell is given by

$$\delta t_{pL} = S_s \Delta L^2 / K_L. \quad (4.2-1)$$

Similar equations can be written for all cells. The smallest of these characteristic time-scale values for all cells in the grid represents the time scale for pressure transients (δt_p). The term δt_p is an approximation of the time required to propagate a pressure change across a cell. If the computational time step, Δt , is much larger than δt_p , then it is possible that the variation of pressure with time will be missed across some of the cells in the grid. Therefore, for problems in which prediction of time-dependent pressures (or hydraulic heads) is important, δt_p can be used as a guide in selecting appropriate time steps. For the PSOR method (see Section 2.3.2) of solution, stability considerations require that Δt be less than δt_p . For other methods of solution, there is no theoretical limit on Δt for stability, but for physically accurate solutions, Δt should be kept less than ten times δt_p .

Pressure transients may be thought of as consisting of waves of different frequencies. As the high frequency components pass across the computational grid, the severity of pressure transients decreases. Therefore, it is possible to gradually increase the size of the time step as the solution advances with time.

4.2.2 Time Scale of Diffusion. A time scale for diffusion is defined in a manner similar to the time scale for pressure transients that was discussed in Section 4.2.1.

$$\delta t_D = \Delta L^2 / (2D_L) \quad (4.2-2)$$

where D_L is the diffusion coefficient in the L direction (which can be in the x, y, or z direction.) The term D_L is the sum of the molecular diffusion coefficient and the coefficient of hydrodynamic dispersion (see Section 2.2.3). For reasons analogous to those discussed in Section 4.2.2, the smallest value of δt_D in the grid is selected. For problems in which diffusion and dispersion are major considerations, the choice of size of the time step should be guided by the value of δt_D . For the PSOR method to be stable, the computational time step size, Δt , should be less than δt_D . For other methods, Δt should be less than ten times δt_D .

4.2.3 Time Scale of Convection

The time scale of convection is based on the flow velocity of fluid and is defined as

$$\delta t_C = \Delta L / U_L \quad (4.2-3)$$

where U_L is the fluid velocity in the L direction (in which L can be in the x, y, or z direction). The constraint on size of the computational time step, Δt , based on Equation 4.2-3, is often stated in terms of the Courant number, Co , which is defined as,

$$Co = \Delta t / \delta t_C = (U_L \Delta t) / \Delta L. \quad (4.2-4)$$

For the PSOR method to remain stable, Co must not exceed unity. For other methods, Δt must not exceed ten times δt_C .

4.2.4 Other Time Scales

The time scales defined in Sections 4.2.1 through 4.2.3 are the most common ones. However, in certain problems, other time scales may apply. These other time scales occur whenever time-dependent phenomena are included in the problem. For example, time-varying sources and sinks and time-dependent boundary conditions would inherently have time scales associated with them. The general rule in such cases is that the size of the computational time step, Δt , be kept less than any other time scale of a problem. The basis for this rule is that the effect of the variation of time on any phenomena with a time scale less than Δt will not manifest itself in the solution.

4.3 : SUMMARY

Rules for the design of a spatial grid and choice of a size for the computational time step should be treated only as guidelines. In practice, grid design and selection of the size of the time step are iterative processes. Trial runs of the computer code may be required before a satisfactory grid and time step are obtained. The number of trials required will depend on user experience and the complexity of the problem.

To design a grid, judgments must be made on what is most important in a specific problem. Some of these judgments may subsequently be shown to be incorrect as the solution is developed; consequently, grid and/or time-step modifications may be required.

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5.0 COMMAND STRUCTURE FOR DATA INPUT

The method of providing input data to PORFLO-3 is based on the FREEFORM command language, details of which are discussed in Appendix A. Each input command starts with a "keyword" that identifies the nature of the data to follow. The keyword is followed by alphanumeric data. The following is the notational convention for the input commands of PORFLO-3.

- BOLD** The keywords of PORFLO-3 are shown in upper-case characters in bold type-face. The string of keyword characters may be specified by the user in upper or lower case. Bold face is used here only for notational purposes; it must not be used as operator input.
- CAPS** Upper-case characters in standard type-face are modifiers of the PORFLO-3 keywords that are significant for machine interpretation of user input. The string of characters shown may be specified by the user in either upper or lower case.
- char** Lower-case characters denote information on keyword commands that is not significant for machine interpretation of user input, but improves the clarity or readability of the input. The string of characters shown may or may not be specified by the user, or may be replaced by other characters. These strings of characters may also be provided in either lower or upper case.
- |** Vertical bar indicates a choice; only one of the items separated by the bar (and enclosed in braces or square brackets) may be specified.
- { }** Braces indicate that the enclosed item (or one of the enclosed items separated from other enclosed items by vertical bars) is required and must be specified.
- []** Square brackets indicate that the enclosed item is optional.
-** Ellipses (in horizontal or vertical format) indicate that other, similar items may follow those shown.
- Nn** The n-th numeric value is associated with an input command.

5.1 KEYWORD-BASED INPUT COMMANDS

All input data for PORFLO-3 are associated with a keyword. Up to four characters comprise a keyword; i.e., a keyword can be one, two, three, or four characters long. The characters can be any from A to Z in upper or lower case. A keyword always begins in the first column of an

80-column record. The keywords of PORFLO-3 and their functions are summarized in Table 5-1. The keywords are abbreviations of commonly used words. Details are provided in Chapter 6.0.

Table 5-1. Keywords of PORFLO-3 and Their Functions.
(sheet 1 of 3)

No.	Keyword ^a	Input function	Type ^b
1.	BAL ance	Activate postprocessing output option.	F
2.	BOUND ary	Override built-in boundary conditions.	C
3.	CHAR acteristic	Characteristic constants for unsaturated soil.	C
4.	CONV ergence	Specify convergence criterion.	C
5.	CYL indrical	Select cylindrical (axisymmetric) geometry.	F
6.	DEBU g	Specify debug options.	C
7.	DENS ity	Select options for mass density of fluid.	C
8.	DISA ble	Disable specific built-in default options.	F
9.	END	End of a problem. More problems may follow.	F
10.	FIXE d	Fixed values of state variables.	F
11.	FLUI d	Physical properties of the principal fluid.	C
12.	FLUX	Activate output option for flux balance.	C
13.	FOR	Specify zone designation for property input.	C
14.	GRID	Number of grid nodes in the x and y directions.	F
15.	HALF life	Half-life of radioactive decay.	C
16.	HIST ory	Provide time-history output at selected nodes.	F
17.	HYDR aulic	Hydraulic properties of porous matrix.	C
18.	INIT ial	Initial conditions for state variables.	F
19.	INTE gration	Index for selection of integration profile.	C
20.	MATR ix	Specify option for matrix inversion.	C
21.	OUTP ut	Frequency and extent of tabular output.	C

Table 5-1. Keywords of PORFLO-3 and Their Functions.
(sheet 2 of 3)

22.	PAUSE	Cause a temporary pause in processing.	C
23.	PERIodic	Specify periodic boundary conditions.	F
24.	PROPerty	Option for mode of property specification.	F
25.	R	Radial coordinates for cylindrical geometry.	F
26.	READ	Read initial conditions from archive file.	F
27.	REFERENCE	Reference node for diagnostic output.	C
28.	RELAX	Relaxation factors for governing variables.	C
29.	ROCK	Material properties of soil or rock.	C
30.	SAVE	Frequency of output to archive file.	C
31.	SCALE	Internal scaling of specified input.	F
32.	SCREen	Echo some of the diagnostic output to screen.	F
33.	SOIL	Material properties of soil or rock.	C
34.	SOLVE	Start of solution of equations.	C
35.	SOURCE	Specify source, injection, or withdrawal terms.	F
36.	SUBDomain	Select subdomain option for solution.	F
37.	THERmal	Thermal properties of soil or rock.	C
38.	THETA	Tangential coordinate in angular units.	C
39.	TIME	Set initial time for simulations.	C
40.	TITLE	Problem title specification.	C
41.	TRANsport	Transport properties of porous matrix.	C
42.	UNSAturated	Selection of unsaturated soil functions.	C
43.	USER	User identification for input and output files.	C
44.	VISCosity	Select fluid viscosity option.	C
45.	WINDow	Set subdomain for output purposes.	C

Table 5-1. Keywords of PORFLO-3 and Their Functions.
(sheet 3 of 3)

46.	X	X-direction grid coordinates.	F
47.	Y	Y-direction grid coordinates.	F
48.	Z	Z-direction grid coordinates.	F
49.	ZDATum	Datum for vertical (z) distance	F
50.	ZONE	Specify matrix zones for input specification.	F

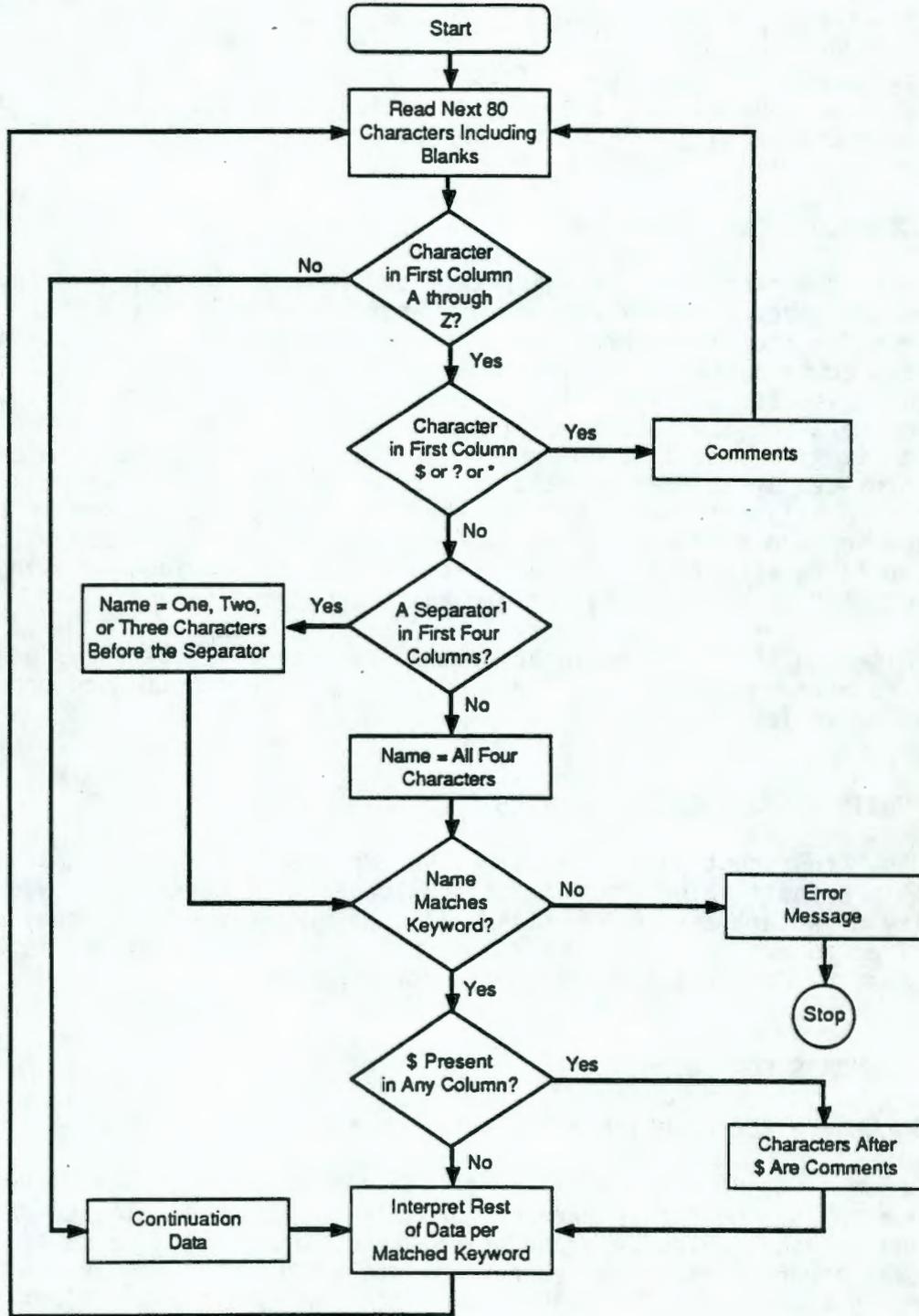
^aKeywords are abbreviations of commonly used names.

^bThe letter 'F' indicates that the data specified through that command is fixed and cannot be changed during simulations. In contrast, the letter 'C' indicates that data associated with that command can be modified by the user during simulations.

A simplified logic for interpreting a given keyword-based data input is given in Figure 5-1. As indicated by this figure, 80 characters, including blanks, are read at one time. Characters in the first four columns are analyzed to identify the keyword. This identification is compared to the keywords of Table 5-1. If a match is obtained, the remaining data (those data before another keyword is encountered) are interpreted. If a match is not obtained, a mistake (most likely in typing) is assumed to have been made, an error message is printed, and program execution is stopped.

In addition to the keyword, there are three other categories of data: (1) Modifier, (2) separator, and (3) numeric. A modifier is a string of characters that modifies the interpretation of the data associated with a keyword. Various modifiers associated with a keyword are defined in Chapter 6.0. Separators (identified in Figure 5-1 and explained in detail in Appendix A) are characters that enable distinction between different strings of characters and numeric data. Numeric data are numerical values of parameters associated with a particular keyword.

Any number of additional characters can be appended to the end of a keyword. For example, WIND may be typed as WINDOW without any change in meaning because only the first four characters will be matched with the standard keywords, as indicated in Figure 5-1. However, keywords consisting of fewer than four characters cannot be extended in this manner. For instance, if X is written as XCOORDINATE, an error message will be displayed and the program execution will be stopped because a match to the first four characters, in this case XCOO, will not be obtained. One way to extend keywords of fewer than four characters is to add a blank space as a separator; e.g., X COORDINATE.



¹Separator Characters are: blank, =, :, ;, ' (,), .

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Figure 5-1. Interpretation of Keyword-Based Input.

The numeric data following a keyword must be entered in a fixed sequence, but they can be typed in any format; there are no fixed-column numbers associated with them. This flexibility for entering format-free numeric data coupled with the keyword feature provides a user-friendly means for preparing the input for PORFLO-3.

5.2 ORDER OF INPUT COMMANDS

With few exceptions, the input records may be specified in any convenient order. The exceptions are as follows: (1) TITLE, USER, and GRID must be the first three commands. A user may elect to omit the TITLE and USER command, but the GRID command must be provided. (2) The SOLVE command initiates problem solution and must follow all commands that provide data for that problem. (3) The END command terminates the solution and must be the last command. In addition, if a command refers to data provided by another command, the referenced command must be used first. An illustration of this is the HYDRauiic property command that may be used to read hydraulic property data on a zone-by-zone basis. For this command to be effective, zone definitions must be provided by using the ZONE command prior to using the HYDRauiic property command.

Although the order of input commands is largely arbitrary, a natural order is recommended to facilitate debugging. The recommended order is indicated in Table 5-2.

5.3 UNITS OF PHYSICAL QUANTITIES

Any consistent set of units may be employed for input. However, all built-in default values for dimensional physical properties (e.g., for density of water) are in SI units. If other units are used, they must be specified as part of the input data. Units are not identified for output; they must be inferred from the units for input.

5.4 COMMANDS FOR OUTPUT

5.4.1 General Description of Output Commands

Five commands are available for diagnostic output. These are the BALANCE, DEBUg, OUTPut, REFERENCE, and WINDow commands. The BALANCE command provides output of convective and diffusive flux terms and residual errors of mass and energy balance in the solution of the governing equations. The DEBUg command can be used for troubleshooting. It provides a trace-back function and initiates diagnostic output from different parts of the code. The OUTPut command allows currently active variables to be written in tabular form to the output file unit, IWR (see Section 3.3). The REFERENCE command provides a means to monitor the time-history of dependent variables and residuals of the governing equations from one iterative step to the next, at a user-specified grid node. The

Table 5-2. Functional Units of PORFLO-3 Commands and Recommended Order of Input.

Order	Function	Related keyword command
1.	Identification	TITLe, USER
2.	Grid specification	GRID, R, SCALe, THETA, X, Y, Z
3.	Type of geometry	CYLIndrical, ZONE
4.	Initial and boundary conditions	BOUNDary, INITIal, PERIodic, READ, TIME
5.	Fluid properties	DENSity, VISCosity, FLUID
6.	Soil and/or rock matrix properties	CHARacteristic, FOR, HYDRaulic, PROPERty, ROCK, SOIL, THERmal, TRANSport, UNSAturated
7.	Source and/or sink specifications	HALF, SOURce
8.	Solution options	DISAbLe, INTEgration, MATRIx, RELAx, SUBDomain
9.	Output control	BALANCE, DEBUg, FLUX, HISTory, OUTPut, REFERENCE, SAVE, SCREEn WINDow
10.	Operational control	CONVergence, SOLVe, PAUSE, END

WINDow command, in conjunction with the BALANCE and OUTPut commands, provides output of only a subregion of the master arrays.

5.4.2 Commands for Tabular Output of Field Variables

The user may obtain tabular output of up to seven variables at various stages of the calculations. Table 5-3 lists these variables in the order they are written to the output file. The output file is written to the file unit, IWR (see Table 3-2). The extent and frequency of this output are controlled by a combination of the OUTPut and WINDow commands. The OUTPut command specifies the variables to be written to the output device and their frequency of output. The WINDow command specifies a subregion for printing as output.

Table 5-3. Field Variables Obtainable in Tabular Format.

Output order	Fortran name	Mathematical symbol	Description
1.	U	U	X-direction velocity component.
2.	V	V	Y-direction velocity component.
3.	W	W	Z-direction velocity component.
4.	P	P	Pressure head at reference density.
5.	T	T	Temperature.
6.	C	C	Mass concentration of species in fluid.
7.	TH	θ	Saturation fraction for soil.

5.4.3 Commands for Creating Archive File

Using the **SAVE** command, the user may generate an archive file consisting of basic problem specifications and the values of up to 30 variables (including those listed in Table 5-3). This archive file may subsequently be used either for restarting a simulation or for other postprocessing purposes; i.e., to produce contour, raster, surface, or vector plots on a console screen or pen plotter.

The archive file is self-documenting. It contains an identifier and the problem title specified by the user. The time and date of creation, the basic grid information, and the names of variables stored in the file are also included in the information written to this file. The archive information is written to file unit NUNIT2 (see Section 3.4) in either unformatted or formatted records. By default, NUNIT2 is assumed to be unit 2, the file is given the name ARCHIVE, and the data records are written in an unformatted mode.

Through the **SAVE** command, the user can select the variables to be archived, their frequency of output, the file name, and the nature of the data records (formatted or unformatted). The output to the archive file consists of several records for each data set. Whenever these records are written in the archive file, informational messages appear in the standard output file that identify the information being transferred to the archive file.

5.5 SEQUENTIAL CONTROL OF DATA DURING SIMULATIONS

In the PORFLO-3 computer code, calculations are initiated as soon as the SOLVe command is encountered. Once the computations specified in a SOLVe command are completed, the program is ready to execute additional commands until an END command is encountered, at which time the execution is terminated. This feature can be used to exert greater control over the simulations. Any given simulation may be partitioned into convenient segments. For each segment, those input commands that are not fixed (see Table 5-1) may be repeated to alter data and to restart computations by using the SOLVe command. Thus, any time-dependent or sequential aspects of the input or output requirements may be changed between the segments.

In general, all specifications relating to problem geometry are considered to be independent of time. The remaining input, including that relating to the physics of the problem, the operational control, the output requirements, and the boundary conditions, may be changed during simulations. The keywords that may be employed to specify time-varying requirements of input and output are identified in Table 5-1 by a letter 'C' in the column headed 'Type'.

An illustration of the specifications for a two-segment calculation sequence is given in Table 5-4. In this illustration, the output requirements for both the archive file and the tabular output are changed after 50 time steps. In Table 5-4, keywords are shown in bold-face type for emphasis only; in actual practice, standard-face type must be used.

Example problems are presented in Appendix B. Details of the structure of each input command of Table 5-1 are given in Chapter 6.0.

5.6 SUMMARY

All input data, output requirements, and control information are provided to PORFLO-3 via commands that begin with a keyword. The numeric and other information following the keyword need not be typed in any specific format, but it must follow a fixed sequence that is described in the next chapter. The nature and extent of output from the code can be determined largely by the code operator. Within certain limitations, the code operator may also choose to read new input data after one segment of a problem has been solved.

Table 5-4. Example of Input Arrangement for a Multisegment Calculation.

```

TITLE ILLUSTRATION OF A TWO SEGMENT CALCULATION WITH OUTPUT OPTION CHANGES
GRID 11 BY 12 BY 5
X type=2, range = 100, grid spacing increment ratio = 1.1
Y type=3, Ymin = 0, Ymax = 120, geometric ratio = 2
Z type=1, coordinates = 10, 20, 30, 40, 50
/
ZONE = 1 from (1,1,1) to (11,12, 5)
/
INITIAL P = 1. from (2,2,2) to (4,4,4)
INITIAL T = 1. from (2,2,2) to (4,4,4)
INITIAL C = 1. from (2,2,2) to (4,4,4)
/***** Comment: P, T, C will be initialized to 0 at all remaining nodes
ROCK density = 1., Porosity = 0.4
HYDRaulic properties: storativity 0.1; conductivity x = 1., y = 1., z = 2
OUTPut for P (pressure) at this stage      $ Print initial values of P
/***** Comment: Start of first segment of calculations
SOLVE for 50 years in time step of 1.0 year
/
OUTPut for variables P and T
SAVE variables U, V, P
/
/***** Comment: Start of second segment of calculations*****/
SOLVe for 25 years in time step of 0.5 year
/
OUTPut for variables U, V, W, P, T and C
SAVE variables U, V, W, P, T and C
/
END

```

6.0 DETAILED DESCRIPTION OF PORFLO-3 KEYWORD COMMANDS

The sequence of numeric and other data that follow a keyword is described in this chapter. The notation given at the front of this manual is used in the description that follows. Reference should be made to Appendix A for the structure and syntax of the FREEFORM command language that are used to interpret the format-free input.

The data following a keyword can be typed in any format and in any column, but strict adherence must be made to the required sequence of data entry. For example, if five numeric values (N_1 , N_2 , N_3 , N_4 , and N_5) are associated with a keyword, then they must be typed in the sequence, N_1 , N_2 , N_3 , N_4 , and N_5 . If some of these values; e.g., N_2 , and N_3 , are not required for a problem, 'dummy' values must be provided for them. The descriptions that follow are listed in alphabetical order.

6.1 BALANCE COMMAND

6.1.1 Purpose

The purpose is to obtain output of convective and diffusive fluxes of heat and mass crossing the boundaries of the user-specified rectangular subregion within the flow domain.

6.1.2 Syntax

For this command to be effective, a character string must be provided. This character string determines the governing equation to which this command is applied. Seven numeric fields can be associated with this command as follows.

BALA {character string}, [N_1 , N_2 , N_3 , N_4 , N_5 , N_6 , N_7]

character string: One of the character strings: C, P or T. The flux-balance output will be obtained for the corresponding variable (i.e., mass, fluid, or heat). One, and only one, character string must be specified for each command.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 IMAX	1	The starting I-node index for flux computations.
N2	1 JMAX	1	The starting J-node index for flux computations.
N3	1 KMAX	1	The starting K-node index for flux computations.

N4	N1 IMAX	IMAX	The ending I-node index for flux computations.
N5	N2 JMAX	JMAX	The ending J-node index for flux computations.
N6	N3 KMAX	KMAX	The ending K-node index for flux computations.
N7 at	>0	1	The frequency (in terms of the number of steps) which the fluxes are printed to the output file

6.1.3 Comments

Only one flux-balance zone may be specified for each of the dependent variables.

6.1.4 Examples

In the first example, the boundary is the entire domain and, by default, the frequency is every time step .

BALANCE calculations for T
 BALANCE calculations for P: subregion (2,2,2) to (5,7,10) every 5 steps
 BALANCE for C; subregion (2,3,3) to (5,3,4) print every 20 steps

6.2 BOUNDARY CONDITION COMMAND

6.2.1 Purpose

The purpose is to specify boundary conditions at the external boundaries of the domain of interest. As explained in Section 2.2.4, the user may choose from three types of boundary conditions (Dirichlet, Neumann, and mixed). The general form of the boundary condition is,

$$- a\partial F/\partial N = b(F - F_0) + c, \tag{6.2-1}$$

where F is the dependent variable (C, P or T), N is the coordinate x (or r), y (or q) or z (whichever is normal to the boundary), and 'a', 'b', 'c' and F₀ are constants.

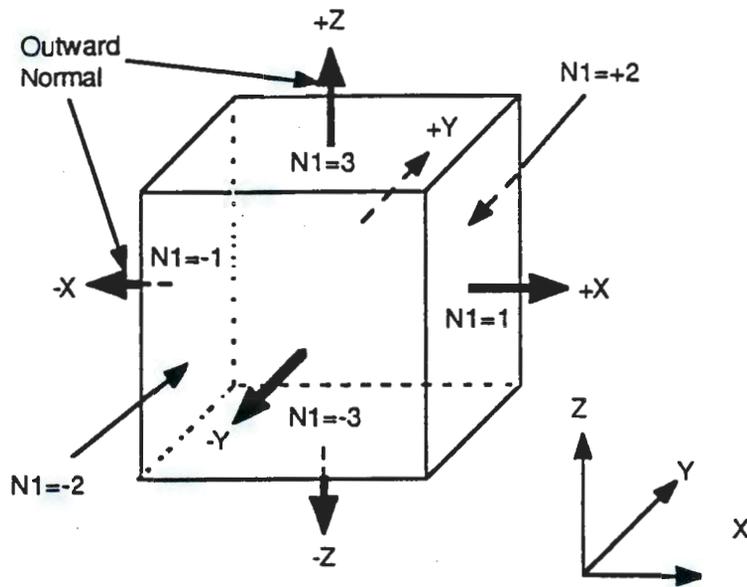
6.2.2 Syntax

The character string indicates the governing equation for which boundary conditions are being specified. Thirteen numerical values are interpreted with this command. Of these, the first must be provided. The form of this command is,

BOUN {character string}, {N1}, [N2, N3, ..., N13]

character string: One of the character strings: C, P, or T. It denotes the dependent variable for which the boundary condition is being specified. One, and only one, character string must be specified for each command.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	None		Orientation index of the external boundary. See Figure 6-1 for index notation.
	-1		The y-z plane at I=1. The outward normal at boundary is along the negative direction of x.
	1		The y-z plane at I=IMAX. The outward normal at boundary is along the positive direction of x.
	-2		The z-x plane at J=1. The outward normal at boundary is along the negative direction of y.
	2		The z-x plane at J=JMAX. The outward normal at boundary is along the positive direction of y.
	-3		The x-y plane at K=1. The outward normal at boundary is along the negative direction of z.



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Figure 6-1. Illustration of Boundary Index Notation.

Numeric field	Numeric value	Default value	Remarks and explanations
		3	The x-y plane at K=KMAX. The outward normal at boundary is along the positive direction of z.
N2		0	Index for type of boundary conditions.
	0		Dirichlet boundary condition ($a = c = 0, b = 1$ in Eq. 6.2-1) is specified at a boundary grid node.
	1		Dirichlet boundary condition is specified at the wall of a boundary cell (see Fig. 2-2).
	2		Neumann boundary condition ($b = 0$ in Eq. 6.2-1) is specified at the wall of the boundary cell.
	3		Mixed boundary condition at the wall of a boundary cell ($c = 0$ in Eq. 6.2-1).

Numeric field	Numeric value	Default value	Remarks and explanations
N3	Any	0	Value of variable (F_0 of Eq. 6.2-1) for a Dirichlet boundary, flux (the term c of Eq. 6.2-1) for a Neumann boundary, and equilibrium value of a variable (F_0 of Eq. 6.2-1) for mixed boundary conditions. For the latter two boundary conditions, the term 'a' is the diffusion coefficient for the variable. It is internally computed from other input data; a separate specification is not required. Units for F_0 are the same as those for F ; units for flux are those of fluid velocity, heat, and mass for P , T , and C , respectively.
N4	Any	0	The term 'b' is the heat or mass transfer coefficient of Equation 6.2-1, if $N2 = 3$; otherwise, this input is ignored. A value must be explicitly specified if any of the numeric fields, $N5$ through $N10$, are not zero. Units for b are t^{-1} for P , $(ML^{-1} T^{-1} t^{-3})$ for T , and Lt^{-1} for C .
$N5, N6,$ and $N7$	1 NMAX	See below	Starting (I,J,K) indices of boundary plane. NMAX denotes the maximum grid nodes (IMAX, JMAX, or KMAX in the corresponding direction).
$N8, N9,$ and $N10$	See remarks	See below	Ending (I,J,K) indices of boundary plane. The numerical values must be such that: $N8 \geq N5$, $N9 \geq N6$, and $N10 \geq N7$. Also, $N8, N9,$ and $N10$ must not exceed the IMAX, JMAX, and KMAX, respectively.
$N11, N12,$ and $N13$	Any	0	The gradients of the boundary value in the x, y, and z-directions, respectively. This command is used to modify the F_0 or c terms specified above (e.g., in Eq. 6.2-1) according to the equation: $\text{boundary value} = N3 + N11*x + N12*y + N13*z$ <p>where x, y and z are the coordinates of the boundary node. The values are modified for the subregion explicitly defined by $N5$ through $N10$, or for the whole of the region by default.</p>

6.2.3 Comments

By default, the specification is assumed to apply to the whole of the boundary plane identified by the boundary index, as shown in Figure 6-1. In this instance, the domain is assumed to be rectangular. However, this command may be used to specify an active nonrectangular subregion within the overall domain by suitable choice of N5 through N10. The boundary conditions are then applied at the nodes specified by N5 through N10 and the region enclosed by these nodes becomes the active region.

6.2.4 Examples

A few illustrations of boundary condition specification are given below.

```
//      Next command specifies a Dirichlet boundary for P at I=1 plane
BOUNDary for P: boundary index = -1, type = 0
//      Next command specifies a Neuman boundary for C at I=IMAX plane
BOUNDary for C: index = 1 type=2, value=20
//      Next command specifies a mixed boundary for T at J=jMAX plane
BOUNDary for T: at 2 type=3 value=5 h=0.5
//      Next command specifies bilinear Dirichlet boundary condition (T =
1 + x/2 + y)
//      at K = 1 (x-y) plane for the subregion (2,3,1) to (5,7,1)
BOUNDary T: -3, Type 1, value=1., 0., (2,3,1) to (5,7,1) xgrad=0.5,
ygrad=1
```

6.3 CHARACTERISTIC COMMAND

6.3.1 Purpose

The purpose is to specify values of empirical constants for the soil-moisture characteristic curves of the unsaturated soil or rock zone. Relations for both the soil-moisture tension and hydraulic conductivity can be specified by this command. Options for functional specification and tabular readout are available. The following functional relationships are available (for definition of symbols and more discussion, see Section 2.2.2),

(a) van Genuchten (1978) relations:

$$\theta^* = [1 + (\psi/\alpha)^n]^{-m}, \quad h < 0, \quad (6.3-1a)$$

$$\theta^* = 1, \quad h \geq 0, \quad (6.3-1b)$$

$$m = (1 - 1/n) \quad (6.3-1c)$$

and

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m]^2; \quad (6.3-2a)$$

or

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m]. \quad (6.3-2b)$$

(b) Brooks and Corey (1966) Relations:

$$\theta^* = (\psi/\psi^*)^{-\beta}, \quad \psi < -\psi^*, \quad (6.3-3a)$$

$$\theta^* = 1, \quad \psi \geq -\psi^*, \quad (6.3-3b)$$

and

$$k_r = \theta^{*(5/2 + 2/\beta)} \quad (6.3-4a)$$

or

$$k_r = \theta^{*(3+2/\beta)}. \quad (6.3-4b)$$

The third option for both the $\theta - h$ and $k_r - \theta$ relationships is to provide them in a tabular form. Linear interpolation between specified values is then used to estimate the required values.

Any of the three options can be selected through the use of the UNSaturated command.

6.3.2 Syntax

CHAR {N1, N2, N3, N4}, [N5, N6, ..., Nn] [character string]

character string: The character string is CONDuctivity or blanks. In the presence of COND, it is assumed that the characteristic curve for the hydraulic conductivity is being specified. In the absence

of conductivity, the data are assumed to be for moisture content.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>0	See remarks	Three possible interpretations of N1 are: (1) In the absence of FOR command and properties specified in a tabular form, N1 = smallest zone number to which the property specification applies; (2) If FOR command is used and properties are in a tabular form, then N1 = number of data sets in the table; (3) If properties are specified as functions, then N1 = α , Equation 6.3-1, if van Genuchten (1978) relations are selected; and N1 = ψ^* for Brooks and Corey (1966) relations of Equation 6.3-3. The units of α and ψ^* must be the same as that of head, ψ .
N2	0	See remarks	If FOR command is not used, and properties are in a table, then N2 = the highest zone number to which the property specification applies. However, if material properties are specified by the FOR command and properties are in a table form, then N2 = first value in the property table, which is θ^* in the absence of modifier HEAD on the UNSaturated command and ψ in its presence; N2 = n of Equations 6.3-1 or β of Equations 6.3-3, if properties are specified as functions. With the last option, it has a default value of 2.
N3	0	None	In the absence of FOR command and tabular property specification, N3 = the interval in the zone number designation. With the material zones defined in the FOR command and tabular specification, N3 = second value in the table, which is ψ in the absence of modifier CONDUCTivity on the UNSaturated command and is K_r in its presence. With FOR command and properties as functions, no value need be specified for N3. Without the FOR command and functional specification, N3 must be specified as 0.

Numeric field	Numeric value	Default value	Remarks and explanations
N4	0	None	If FOR command is not used for zone designation and properties are in a table, N4 = number of data values in the tabular specification. With the FOR command and tabular properties, this is the next value in the table. For functional specification, N4 should be specified as N3 above.
N5	0	None	If FOR command is not used and the properties are in a table, N5 = first value in the table. If FOR command is used and property specification is tabular, N5 = next value in the table. For functional specification with FOR command, no value is needed. In the absence of FOR command and functional specification, N5 = the smallest zone number to which functional specification applies.
N6	0	None	For tabular specification, N6 is the next value in the property table. For functional specification and zones not specified in FOR command, N6 is the highest zone number to which specification applies.
N7	0	None	Continuation of property values for tabular specification. N7 = interval in the zone number designation if FOR command is not used and properties are in a function form.
N8 Nn	0	None	Continuation of tabular values till property specification is complete.

6.3.3 Comments

This command works in conjunction with the UNSaturated and FOR commands. The saturation fraction, q , and the relative hydraulic conductivity, K_r , must be normalized to values between 0 and 1, and the pressure head, ψ , must be positive (see the UNSaturated command). It should be noted that the UNSaturated command must precede the CHARACTERISTIC command.

6.3.4 Examples

CHARACTERISTIC values: air entry = 5 , n = 0.5, 0., 0., for zones 3,6,2
 CHAR: # of sets 4: (0, 1.1 E+06), (0.1, 1.1 E+03), (0.9, 1.1 E+02), (1., 1.)

6.4 CONVERGENCE COMMAND

6.4.1 Purpose

The purpose is to specify the convergence criterion for solution of the system of algebraic equations obtained from the discretization of a governing equation (see Section 2.3.1). Two options are provided. In the first option, convergence is checked with respect to the sum of absolute values of residuals at all grid nodes. In the second option, the criterion is the maximum residual at any node of the grid.

6.4.2 Syntax

CONV [character string], {N1}, [N2, N3]

character string: One of the character strings: C, P, or T. It denotes the dependent variable for which the convergence will be monitored. By default, the convergence is monitored for the pressure equation.

Numeric field	Numeric value	Default value	Remarks and explanations
N1		2	An index for choice of convergence criterion options.
	1		Convergence is judged by the criterion: $R_1 = \sum Ax - b \leq N_2, \quad (6.4-1)$ where the summation is over all internal nodes and $Ax = b$ is the matrix of equations being solved.
	2		Convergence is judged by the criterion: $R_2 = \max (1 - F_p^{n+1} / F_p^n) \leq N_2, \quad (6.4-2)$ where the superscripts, $n+1$ and n , represent the values of the variable, F , at node P for successive iterations. The maximum is taken over all internal nodes.
N2	>0	0.001	The convergence factor of Equations 6.4-1 or 6.4-2.
N3	>0	1	Maximum number of iterations for convergence.

Numeric field	Numeric value	Default value	Remarks and explanations
N4	>1 E-20	1 E-07	The minimum value of the variable for which the convergence criterion of option 2 (N1 = 2) is applicable. If the value of the variable is less than this value, then its variations are ignored. This input is ignored if N1 = 1.

6.4.3 Comments

This command is used in two ways. If the steady state-mode of solution is invoked by the SOLVE command, then the criteria of this command are used to check convergence of the steady state. However, if a transient solution is invoked, then the criteria of this command are used to monitor convergence of the solution at each time step. The latter is especially important for solution of the nonlinear unsaturated flow equations in the transient mode.

6.4.4 Examples

CONvergence for P: option 2: acceptable error = 1 E-04
 CONvergence for T variable: option 1: acceptable error = 1 E-04
 CONvergence option 2, error value = 0.01
 CONV for C: option 2, value = 1 E-04, ignore if variable less than 1 E-05

6.4.5 Status

Convergence option 1 (specified by N1 above) for this command is not currently active in some installations of PORFLO-3.

6.5 CYLINDRICAL COMMAND

6.5.1 Purpose

The purpose is to select a cylindrical geometry. Cylindrical geometry can also be specified by the R command for specifying radial coordinates. If R is used, then CYLI need not be used.

6.5.2 Syntax

No numerical value is interpreted with this command.

CYLI

6.5.3 Comments

Cartesian geometry is the default. Hence, either a CYLI command or an R command must explicitly be specified if cylindrical geometry is to be selected.

The axial coordinate of cylindrical geometry is assumed to coincide with the z-axis, the radial axis is assumed to be coincident with the x-direction, and the angular (θ) direction is assumed to be coincident with the y-direction. In this mode, an additional restriction is placed on the choice of the x- or r-coordinate values; the radial location of the cell boundaries must all be non-negative. This restriction implies that:

$$r_i > 0; i = 2,3, \dots, \text{IMAX}. \quad (6.5-1a)$$

r_1 may be less than zero, but it must satisfy

$$r_1 \geq -r_2. \quad (6.5-1b)$$

Equation 6.5-1b ensures that the first cell (between nodes at $I = 1$ and $I = 2$) has a positive r coordinate. For problems where the first cell boundary is to be the axis of symmetry, r_1 should be equal to $-r_2$ so that the first element boundary in the r-direction is located at $r = 0$.

6.5.4 Examples

CYLINDRICAL geometry for this problem

6.6 DEBUG COMMAND

6.6.1 Purpose

The purpose is to obtain debug output and messages for diagnostics and trouble shooting.

6.6.2 Syntax

The string of characters is either FINA or blanks.

DEBU {N1}, [N2, N3, N4], [character string]

Character string: If a character string beginning with FINA is present anywhere on the command line, then the debug output specified by N1 is obtained at the final step of the iterative procedure in addition to the output obtained from N2 through N4, as explained below.

Numeric field	Numeric value	Default value	Remarks and explanations
N1		0	An index for level of debug output. The default setting suppresses all debug output.
	1		A road-map (trace) of all subroutines called during execution is produced.
	2		Matrix coefficients from the INVERT subroutine are printed.
	3		Output of all active output variables (see the OUTPUT command for name of variables) is obtained just before solution of the pressure equation.
	4		Output of all active output variables is obtained just before solution of the temperature equation.
	5		Output of all active output variables is obtained just before solution of the concentration equation.
N2	0	1	The first step of the iterative solution procedure at which the debug output specified by N1 is initiated.

Numeric field	Numeric value	Default value	Remarks and explanations
N3	0	N2	The last step at which the debug output is obtained. If no value is specified, then a default value equal to N2 is assumed.
N4	0	1	The step increment, between N2 and N3, for output.

6.6.3 Comments

This command generates extensive output. It must therefore be used with due caution. Some types of output from this command that produce a printout of the field arrays are also subject to control by the **OUTPUT** and **WINDOW** commands. Multiple types of debug output, each with its own step sequence, may be specified.

6.6.4 Examples

DEBUG level 1: from step 1 to 100 in increments of 3 steps
DEBUG level 2: from step 25 to 31
DEBUG level 2: at step 50
DEBUG level 2: only at FINAL step
DEBUG level 2: at FINAL step and steps 25 through 50 in steps of 5

6.6.5 Status

This command is not fully operational in all installations of PORFLO-3.

6.7 DENSITY COMMAND

6.7.1 Purpose

The purpose is to specify the option and constants employed for calculation of fluid density as a function of temperature and/or concentration of species (also see Section 2.2.1).

6.7.2 Syntax

The first numeric field indicates the choice of option and must be specified.

DENS {N1}, [N2, N3, N4, N5, N6, N7, N8]

Numeric field	Numeric value	Default value	Remarks and explanations
N1		0	An index for mode of density calculations.
	0		Constant fluid density.
	1		Density changes according to the equation: $\rho = \rho^* [(T_c - T)/(T_c - T^*)]^A. \quad (6.7-1)$
	2		Density changes according to the equation: $\rho = A_1 + A_2 T + A_3 T^2 + A_4 T^3. \quad (6.7-2)$
	3		Density changes according to the equation: $\rho = \rho^* [1 + A_5(T^* - T) + A_6(C^* - C)]. \quad (6.7-3)$
N2	Any	0	Reference temperature, T*. Ignored if Equation 6.7-2 is used.
N3	Any	0.2	Coefficient A1 or A5. The default value is appropriate when fluid is water and Equation 6.7-2 is to be used.
N4	Any	374.15	Coefficient Tc, A2, or C*. The default value is appropriate when the fluid is water and Equation 6.7-2 is to be used.
N5	Any	0	Coefficient A3 or A6.
N6	Any	0	Coefficient A4.

Numeric field	Numeric value	Default value	Remarks and explanations
N7	0	0	The effect of $\partial T/\partial t$ is ignored in computing the pressure source term (see Eq. 2.1-3).
	1		The effect of $\partial T/\partial t$ is retained.

6.7.3 Examples

DENSITY type 1 \$ Use equation 6.7-1 with default values
 DENSITY type 1, TREF = 20: Exponent = 0.25, Tc = 374.15 K
 /NOTE: In the following, do not use symbols A1, A2 etc. because 1 and 2 /
 will be read as numeric values.
 DENSITY type 2 T=20, aone=1,000., atwo=0.05, athree=0., afour=3 E-05
 DENSITY type 3 TREF = 20 Degrees, Beta=1.0 E-04
 DENSITY type 3 TREF = 20., beta=1 E0-4, CREF=0., betas= -1 E-03
 DENSITY type 1, 5*0, SP=1 \$ default values; include T effect in P
 equation

6.8 DISABLE COMMAND

6.8.1 Purpose

The purpose is to disable solution of one or more equations.

6.8.2 Syntax

DISA [P, T, or C]

- P: By default, the flow (or pressure) equation is always solved. To disable flow calculations, this command modifier must be used.
- T: The temperature equation is activated if thermal properties are specified. By using the modifier T on this command, the T equation will not be solved.
- C: With modifier C present on this command, the concentration equation is not solved.

6.8.3 Examples

DISAbLe P equation

6.9 END COMMAND

6.9.1 Purpose

The purpose is to signify the end of a problem.

6.9.2 Syntax

No numeric values are supplied with this command.

END

6.9.3 Comments

This command signifies the end of a problem; the input for a new problem may be continued with a new problem specification after this command. For each problem, this command must be employed as the last command. Failure to do so may cause a loss of some or all of the data and output files, depending on the host operating system.

6.9.4 Examples

END

END of problem number 1

6.10 FIXED COMMAND

6.10.1 Purpose

The purpose is to specify fixed pressure, temperature, or species concentration in a region within the domain of the calculation. This command works in conjunction with the INITIAL command. The nodes on which a variable is to be fixed are identified by this command; the values of the variable itself are provided by the INITIAL command. In essence, the FIXED command is invoked to indicate that the values specified by the INITIAL command at the specified nodes are not to change during calculations.

6.10.2 Syntax

FIXEd {character string}, {N1, N2, N3, N4, N5, N6}

character string: One of the character strings: C, P, or T. It denotes the dependent variable whose value is fixed for the region specified by N1 to N61.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	2 IMAX-1	None	The starting I-node Index of the region.
N2	2 JMAX-1	None	The starting J-node index of the region.
N3	2 KMAX-1	None	The starting K-node index of the region.
N4	2 IMAX-1	None	The ending I-node index of the region.
N5	2 JMAX-1	None	The ending J-node index of the region.
N6	2 KMAX-1	None	The ending K-node index of the region.

6.10.3 Comments

This command defines a region for fixing the value of a variable inside the flow domain; the values at the domain boundary cannot be fixed by this command (the boundary values may be fixed by the BOUNDARY command). The FIXED command, for example, may be used to specify a fixed pressure region, such as a river passing through the domain of the calculations. Similarly, this command may be used to fix temperature or

concentration due, for example, to a source of infinite quantity. More than one **FIXEd** command may be used for each variable. The actual value to be assigned may differ from one grid node to another within the specified region. The fixed value, itself, is specified by the **INITIAL** command. Once specified, it remains constant during the calculations.

6.10.4 Examples

FIXEd P for nodes defined by (3,4,3) to (5,4,8)
FIXEd T in the region (2,2,5) to (3,5,5)
FIXEd C at (3,4,5) to (3,4,5)

6.11 FLUID COMMAND

6.11.1 Purpose

The purpose is to specify the physical properties of the principal fluid.

6.11.2 Syntax

FLUID [N1, N2, N3]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	0	997	Reference mass density of fluid.
N2	0	4182	Specific heat of the fluid per unit mass.
N3	0	0.603	Thermal conductivity of fluid.

6.11.3 Comments

These fluid properties are employed only if the default mode of property specification by weighted averages of component values is active. In this case, the effective (or equivalent) properties of the soil (or rock) (see Eq. 2.1-13) and matrix containing the fluid are calculated internally within the code. Alternatively, through the PROPERty command, the user may choose the option of specifying the effective (or equivalent) properties directly. In this latter case, all inputs except that of mass density are ignored.

6.11.4 Examples

FLUID density = 1., specific heat = 4.2, thermal K = 1

6.12 FLUX COMMAND

6.12.1 Purpose

The purpose is to compute and obtain output of convective and diffusive fluxes of water, heat or the chemical species across user-specified planes within the problem domain. A single plane is specified by one FLUX command. Up to 20 FLUX commands can be used to monitor flux across different planes.

6.12.2 Syntax

The flux plane is specified by the indices of its southwest and northeast corners. The last numeric value is the frequency in terms of the number of time steps at which flux is to be calculated.

FLUX {character string} {N1, N2, ..., N7} {XY, YX | YZ, ZY | ZX, XZ}

character string: One of the character strings: C, P or T. The flux output will be obtained for the corresponding variable.

XY or YX: Horizontal plane at a fixed K-node index.

YZ or ZY: Vertical plane at a fixed I-node index.

ZX or XZ: Vertical plane at a fixed J-node index.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 IMAX	1	The starting I-node index of flux plane.
N2	1 JMAX	1	The starting J-node index of flux plane.
N3	1 KMAX	1	The starting K-node index of flux plane.
N4	N1 IMAX	IMAX	The ending I-node index of flux plane.
N5	N2 JMAX	JMAX	The ending J-node index of flux plane.
N6	N3 KMAX	KMAX	The ending K-node index of flux plane.

N7	>0	1	The frequency (in terms of number of steps) with which the fluxes are written to the output file unit.
----	----	---	--

6.12.3 Comments

Fluxes across up to 20 planes may simultaneously be monitored in Version 1.0 of PORFLO-3. The flux command would be used the same number of times as the number of planes to be specified. However, the frequency with which the flux is computed is the same for all the planes. If the output frequency (N7) is specified by more than one command, then the first value will prevail.

6.12.4 Examples

FLUX calculations for XY plane defined by (2,2,2) to (8,9,2)
FLUX for YZ plane (2,2,2) to (2,11,15) print every 20 steps

6.13 FOR COMMAND

6.13.1 Purpose

The purpose is to select the soil or rock zones to which the property information following the FOR specification applies.

6.13.2 Syntax

In the following, LZN is a dimension parameter for the maximum number of zones (see Table 3-3).

FOR {N1}, [N2, N3]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 LZN	1	The smallest zone number to which the property specification applies. LZN is the dimension parameter (see Section 3.4).
N2	N1 LZN	1	The highest zone number to which property specification applies. If N2 is not specified, then it is assumed to be equal to N1.
N3	1 LZN	1	The interval in the zone number designation. The specification will be effective for N1 to N2 at increments of N3, in the manner of a FORTRAN DO loop. If N3 is not specified, then it is taken to be 1.

6.13.3 Comments

The zone numbers specified by this command must denote an active zone; that is, they must previously have appeared on a ZONE command. Therefore, a ZONE command must precede a FOR command. The property information to which this command applies is specified through the CHARACTERistic, HYDRaulic, ROCK, SOIL, THERmal, and TRANsport commands. Therefore, the FOR command must precede these commands. A FOR command remains in effect until a subsequent FOR command is encountered. If the keyword command for the relevant property explicitly specifies the zones to which the information applies, then the FOR command is ignored.

As stated above, the zone number can be specified directly with the CHARACTERistic, HYDRaulic, ROCK, SOIL, THERmal, and TRANsport commands. However, by using the FOR command, the zone number may be specified once for all, for all of the properties of that zone.

6.13.4 Examples

FOR zone 3 properties are specified by the following commands

FOR zones 1 through 5

FOR zone numbers 1 through 9 in steps of 3

6.14 GRID COMMAND

6.14.1 Purpose

The purpose is to specify the number of grid lines in the x- (or r-), y- (or θ -), and z-directions. The z-direction is assumed to be vertical.

6.14.2 Syntax

LX, LY, and LZ in the following are dimension parameters defined in Table 3-3.

GRID [N1, N2, N3]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	3 LX	5	The number of grid nodes in the x- (or r-) direction.
N2	3 LY	5	The number of grid nodes in the y- (or θ -) direction.
N3	3 LZ	5	The number of grid nodes in the z-direction.

6.14.3 Comments

The three numeric fields of this command specify the number of grid nodes in the x-, y-, and z-directions, respectively, in rectangular cartesian coordinates. The corresponding directions in the cylindrical coordinate system are r-, θ -, and z-directions. A minimum of three grid nodes in each direction are required. The maximum number of nodes must not be larger than the corresponding value of the dimension parameter (LX, LY, or LZ, as appropriate; see Section 3.4).

This command must be specified and it must precede all other commands except the TITLE and USER specifications. The values of N1, N2, and N3 specified by this command are referred to in this manual as IMAX, JMAX, and KMAX, respectively. Much of the specification of physical properties and output requirements is made in terms of the grid node indices. Due care must therefore be taken that, in the input of data, no reference is made to grid node indices beyond values of IMAX in the x- (or r-) direction, JMAX in the y- (or θ -) direction, and KMAX in the z-direction.

A two-dimensional problem may be simulated by specifying the minimum of three nodes in the third dimension. Similarly, a one-dimensional problem results if the number of nodes in two of the dimensions is three.

However, all problems are treated as inherently three-dimensional. Therefore, even with one- and two-dimensional problems, full data specification for the three-dimensional problem is required.

6.14.4 Examples

GRID use default values
\$ by default 5, 5 and 5
GRID is 31 by 25 by 12
\$ IMAX = 31; JMAX = 25, KMAX = 12

6.15 HALF-LIFE COMMAND

6.15.1 Purpose

The purpose is to specify the half-life of radioactive decay or chemical reaction rate for the species under consideration. This command specifies the coefficient λ of Equation 2.1-15.

6.15.2 Syntax

Only one numeric field is specified by this command.

HALF {N1}

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>0	1 E+20	The half-life of radioactive decay or chemical reaction for the species under consideration. The default value ensures that no decay occurs, provided the simulation time is much smaller than 1 E+20 time units.

6.15.3 Comments

The actual rate of decay for a species, C, is calculated from the relation:

$$R_C = 0.69314718 / N1, \tag{6.15-1}$$

where the numeric constant on the right side of the equation is the negative of the value of the natural logarithm of 0.5. This relation follows from the definition of half life when the decay is exponential.

6.15.4 Examples

HALF life for iodine is 1.59 E+07
 HALF life for technetium is 2.13 E+05
 HALF life for selenium is 6.50 E+04
 HALF life is 5,730 for carbon fourteen

6.16 HISTORY COMMAND

6.16.1 Purpose

The purpose is to specify and control graphical and tabular output of time history for variables shown in Table 5-3, at specified nodes.

6.16.2 Syntax

HIST [character string, TABLEs], {N1, N2, N3}, [N4, N5,, Nn], Nn
 character string:
 One or more of the strings of characters: C, P, T, U, V, or W. It denotes the variable for which the time-history output is to be obtained. By default, the output is obtained for all six variables.

TABLEs: The time-history data are automatically displayed in a graphical form at the end of simulations. If a tabulation of this data is also required, then a character string beginning with "TABL" must be specified somewhere on the command line.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 IMAX	None	I grid index of the first time-history node.
N2	1 JMAX	None	J grid index of the first time-history node.
N3	1 KMAX	None	K grid index of the first time-history node.
N4 Nn-1	As above	None	The grid indices of the 2nd through last time-history node in the manner of N1, N2, and N3 above. The maximum number of grid nodes that may be plotted is 20.
Nn	0	1	The frequency index for tabular output. The output is obtained every Nn steps; for example, a specification of Nn=10 will result in output at the 10th, 20th, 30th, etc. steps. A value of 0 is interpreted to be equal to 1.

6.16.3 Comments

The plot file is generated on unit number NUNIT3.

6.16.4 Examples

HISTory at (2,2,2), (2,5,7), (5,2,7), (11,17,19) and (17,11,12)

HISTory for U and C at (2,2,2), (2,5,2), output every 10 steps

HISTory for U and C at (2,2,2), (2,5,2), frequency =10: print TABLEs also

6.17 HYDRAULIC COMMAND

6.17.1 Purpose

The purpose is to specify the hydraulic properties of the host porous matrix, or those of the planar or linear features.

6.17.2 Syntax

LZN is a dimension parameter defined in Table 3-3.

HYDR [N1, N2, N3, N4, N5, N6, N7]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	0	1	<p>The reference value of the effective specific storativity, S_s^* of the equation:</p> $S_s = S_s^* (\rho / \rho^*), \quad (6.17-1)$ <p>The density, ρ, is calculated according to the options selected by the user (see the DENSITY command).</p>
N2	0	0	<p>The reference value of the x-directional hydraulic conductivity, K_x^* of the equation:</p> $K_x = K_r K_x^* (\rho \mu^* / \rho^* \mu), \quad (6.17-2)$ <p>where K_x^* is a reference value at density ρ^* and viscosity μ^*. The term, K_r, is the relative conductivity. It is unity for saturated zone and between 0 and 1 for unsaturated zone (see CHARACTERISTIC and UNSATURATED commands). The viscosity is calculated according to the options selected by the user (see the VISCOSITY command).</p>
N3	0	0	<p>The reference value of the y-directional hydraulic conductivity, K_y^*, in the manner of the N1 field, as described above.</p>
N4	0	0	<p>The reference value of the z-directional hydraulic conductivity, K_z^*, in the manner of the N1 field, as described above.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N5	1	1	These three values select the zones to which N1 through LZN N4 apply. Their interpretation is identical to N1, N2, and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, then the input is assumed to apply to zone number 1.
N7			

6.16.3 Examples

HYDRaulic properties: $ss = 0.2$, $Kx^* = 2$, $Ky^* = 0.2$, $Kz^* = 0.2$ ft per day
 HYDRaulic $ss = 0.2$, $Kx = 2$; $Ky = 0.2$, $Kz = 4$. for zone 5
 HYDRaulic $ss = 0.2$, $Kx = 2$; $Ky = 0.2$, $kz = 4$. for ZONE 1 through 5
 HYDRaulic $ss=0.2$, $Kx=2$; $Ky=0.2$, $Kz=0.2$ for ZONE 1 to 5 in step of 2

6.18 INITIAL CONDITION COMMAND

6.18.1 Purpose

The purpose is to specify the initial values of field variables C, P, T, U, V, and W. The default initial values are zero for these variables in the entire domain. User selected initial values may be specified either on a node by node basis or as a linear space function according to the following equation,

$$F(I,J,K) = F_0 + a \cdot X(I) + b \cdot Y(J) + c \cdot Z(K), \quad (6.18-1)$$

where $F(I,J,K)$ represents any of the six variables named above at the grid node (I,J,K) , F_0 , a , b , and c are constants, and X , Y , and Z are the grid coordinates for the node (I,J,K) . If a , b , and c are specified as zero, then the initial condition is equal to the constant F_0 . The domain may be divided into zones through the ZONE command to specify variable initial conditions, or the subregions may be read directly through the INITIAL command as indicated below.

6.18.2 Syntax

A maximum of one hundred numeric values can be interpreted by this command. The INITIAL command may be repeated as many times as necessary to complete the specification.

INIT {character string}, [N1, N2, ..., Nn]; $n \leq 100$

character string: One or more of the character strings: C, P, T, U, V, or W. It denotes the variable for which initial conditions are specified.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	0	0	The constant, F_0 , of Equation 6.18-1 if $N8 \leq 1$. This input is ignored if $N8=2$.
N2	0 IMAX or LZN	1	N2 is taken to be the zone number if N3 is zero, otherwise it is the I-grid index of the subregion for which the initial condition is being defined.
N3	1 JMAX	1	The starting J-grid node index of the subregion.
N4	1 KMAX	1	The starting K-grid node index of the subregion.

Numeric field	Numeric value	Default value	Remarks and explanations
N5	N2 IMAX	IMAX	The ending I-grid node index of the subregion.
N6	N3 JMAX	JMAX	The ending J-grid node index of the subregion.
N7	N4 KMAX	KMAX	The ending K-grid node index of the subregion.
N8	0		An index for mode of initial value assignment.
		1	The values are assigned according to Equation 6.18-1.
		2	The values are assigned on a node-by-node basis. The order of specification of values is from (I=N2, J=N3, K=N4) to (I=N5, J=N6, K=N7) in the manner of increasing I, J, and K, in that order.
N9	Any	0	The a of Equation 6.18-1, if $N8 < 1$. The initial value of the variable at the first node in the subregion (I=N2, J=N3, K=N4), if $N8=2$.
N10	Any	0	The b of Equation 6.18-1, if $N8 < 1$. If $N8=2$, then this factor is taken to be the initial value of the variable at the second node in the subregion (node with indices I=N2+1, J=N3, K=N4 if $N5 < N2$ or I=N2, J=N3+1, K=N4 if $N5=N2$, or I=N2, J=N3, K=N4+1, if $N5=N2$ and $N6=N3$).
N11	Any	0	The c of Equation 6.18-1, if $N8 < 1$. If $N8=2$, then N11 is the initial value of the variable at the third node in the subregion.
N12	Any	0	The values of the 4th through the last nodes in the subregion defined by N2 through N7, above, if $N8=2$. This input is ignored if $N8 \geq 1$.
Nn			

6.18.3 Comments

The subregion may be as small as a single element or as large as the entire domain. It may be explicitly specified in terms of either the grid-index coordinates (N2 through N6, above) or zones (N2, above). If the subregion is not explicitly specified, then the input is assumed to apply to all of the flow field.

6.18.4 Examples

INITIAL P is 0.1 everywhere

INITIAL T is 1.E-3 from (2,2,2) to (7,9,4)

INITIAL C 0.1 from (1,1,1) to (11,08,5); model =1, grads: x=0, y=0.2, z=-0.2

INITIAL P 0. from (2,2,2) to (2,7,2); mode=2: 0.1, 0.2, 0.3, 0.4, 0.5, 0.6

INITIAL C is 1 E-02 for zone 16

6.19 INTEGRATION PROFILE COMMAND

6.19.1 Purpose

The purpose is choice of discretization scheme for integration of the heat and mass transport equations. The convective term in the heat and mass transport equations may be discretized using either the hybrid or the exponential scheme (see Section 2.3.1). The default option is the hybrid scheme, which employs the central difference scheme for low grid Peclet numbers and upwinding for high Peclet numbers.

6.19.2 Syntax

This command contains no numeric field.

INTE {C | T}, {HYBRid | EXPOntial}

- C:** The profile specification will be effective for the solution of the concentration equation.
- T:** The profile specification will be effective for the solution of the temperature equation.
- HYBRid:** The hybrid scheme is employed for integration. This is the default option.
- EXPOntial:** A tabulated version of the exponential scheme is employed for integration.

6.19.3 Comments

The default option should be adequate for most applications. However, if the local grid Peclet number (see Section 2.3.1) significantly exceeds a value of 10, then the exponential scheme may be desirable.

6.19.4 Examples

INTEgration for C by EXPOntial scheme
 INTEgration for T by profile: HYBRid (same as default)

6.20 MATRIX COMMAND

6.20.1 Purpose

The purpose is to select the manner of solution of the matrix of equations. Five options: ADI, Choleski Decomposition, Gaussian Elimination, PSOR, and RSCG are available (see Section 2.3.2).

6.20.2 Syntax

MATR [direction], [character string] [N1, N2, N3], [Option]

direction: is one or more of the strings of characters: X, Y, Z. It denotes the direction in which the matrix will be swept, if the ADI scheme is selected. For example, a specification of X will cause the matrix equations to be solved along the x-direction nodes, in increasing order of the I-index, for fixed values of the J and K indices. By default, the matrix is swept along all three directions.

character string: One or more of the character strings: C, P, or T. It denotes the variable(s) for which specification is being made. A single MATRix command is sufficient, if the same solution option (see below) is to be used for all equations being solved. However, if different equations are to be solved using different options, then more than one MATRix command should be used.

Option	Meaning
ADI	Matrix is solved by the ADI method. <u>This is the default option.</u>
SOR	Matrix is solved by the PSOR method.
GAUS	Matrix is solved by Gaussian elimination.
CHOL	Matrix is solved by Cholesky decomposition.
RSCG	Matrix is solved by the RSCG method.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>0	see remarks	If the ADI option is selected, N1 is the number of matrix sweeps using the ADI method for the variable denoted by the first character string. In this case, its default value is 1. With the selection of the RSCG method, N1 = number of maximum iterations allowed for solution during one time step. The default value of N1 for the RSCG method is 100. This input is ignored for other methods.
N2	>0	see remarks	For the ADI method, it is the number of matrix sweeps (default value of 1) for the variable denoted by the second character string. For the RSCG method, N2 = stopping criteria for check on solution convergence. N2 depends on the word-length on the computer; the larger the word-length, the smaller N2 can be. Its default value is 5 E-06 which is suitable for 32-bit machines. This input is ignored if another option is chosen.
N3	>0	1	Number of matrix sweeps for the variable denoted by the third character string. This input is ignored for all the other options.

6.20.3 Examples

MATRIX sweeps in X direction only
 MATRIX sweeps in X and Y directions: P=3
 \$ Sweep pressure equation 3 times
 MATRIX sweeps: P=3, T=1, C=2
 MATRIX for P to be solved by the SOR method
 MATRIX for P to be solved 3 times by the ADI method
 MATRIX P Eqn to be solved by RSCG method, iter = 50, conv = 1 E-04

6.21 OUTPUT COMMAND

6.21.1 Purpose

The purpose is to select the field arrays (see Table 5-3) to be written to the output file unit, IWR (see Table 3-2), and to specify the manner and frequency of output.

6.21.2 Syntax

OUTP [character strings], [plane], [NARRow | WIDE], [NOW], [N1]

character string: One or more of the character strings: C, P, T, THET, U, V, and W. Each character string represents a corresponding variable in Table 5-3 for which the output is desired (see Section 5.7 for further information).

plane: One of the character strings: XY, XZ or YZ. Because three-dimensional arrays are printed in a two-dimensional tabular format, the user has the option of selecting the plane of presentation. By default, the tables are printed for XY planes.

NARRow: The output tables are produced in an 80-column format.

WIDE: The output tables are produced in a 132-column format. This is the default mode.

NOW: The output tables are produced as soon as the command is encountered.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1	See below	The frequency index for tabular output. The output is obtained every N1 steps; for example, a specification of N1=10 will lead to output at the 10th, 20th, 30th, etc. steps. By default, tabular output is obtained automatically at the end of simulations for all active variables.

6.21.3 Comments

If an OUTPut command is specified without any of the attributes given in the syntax above, then the output of field arrays is completely suppressed. If no OUTPut command is specified, then output for the active

variables is automatically produced at the end of simulations. The active variables consist of all variables for which the equations are solved, the three velocity components (U, V, W) if the pressure equation is solved, and the saturation fraction (θ) if the unsaturated mode of PORFLO-3 is used. Successive **OUTPut** commands may be employed to accommodate changing output requirements at various stages of simulation.

6.21.4 Examples

OUTPut: U, N, W in **NARRow** tabular format

OUTPut: U, N, C, and P in **WIDE** tabular format **NOW**

OUTPut: U, N, C, P, and **THETa** by XZ planes in **WIDE** tabular format **NOW**

OUTPut: U, N, P and T in **NARRow** format **NOW** and every 20 steps

OUTPut tables for N, W, P, and **THETa** by YZ planes every 15 steps

OUTPut for none of the variables

6.22 PAUSE COMMAND

6.22.1 Purpose

The purpose is to cause a temporary halt in the calculations.

6.22.2 Syntax

This command supports no numeric fields.

PAUS

6.22.3 Comments

Operator intervention is required to restart the calculation process. This command has been inserted in PORFLO-3 Version 1.0 for future use in developing interactive execution.

6.22.4 Examples

PAUSe and await operator action

6.23 PERIODIC COMMAND

6.23.1 Purpose

The purpose is to select the periodic option for boundary conditions in the x, y, or z direction of the domain. This command is required for three-dimensional cylindrical coordinate geometry when symmetry with respect to the θ coordinate does not exist.

6.23.2 Syntax

PERI [X, Y, Z]

- X: The boundary conditions for the r-direction boundaries are determined automatically from the requirement of periodicity of the solution. Any boundary condition specification through the BOUNDary command (with a boundary index of -1 or +1) is ignored.
- Y: The boundary conditions for the θ -direction boundaries are determined automatically from the requirement of periodicity of the solution. Any boundary condition specification through the BOUNDary command (with a boundary index of -2 or +2) is ignored.
- Z: The boundary conditions for the z direction boundaries are determined automatically from the requirement of periodicity of the solution. Any boundary condition specification through the BOUNDary command (with a boundary index of -3 or +3) is ignored.

6.23.3 Examples

PERIodic boundaries in X
PERIodic boundaries in Y
PERIodic boundaries in X and Z
PERIodic boundaries in X, Y and Z

6.23.4 Status

This command is not currently active in some installations of PORFLO-3.

6.24 PROPERTY COMMAND

6.24.1 Purpose

This command has dual purposes. First, it is used to input effective (or equivalent) properties of the host porous matrix (soil or rock), or those of the planar or linear features. The effective or equivalent properties are those that account for the presence of fluid in the porous matrix (see Sections 2.1.2 and 2.2.3). By default, fluid and matrix properties are provided separately and the effective properties are calculated internally in the code. However, the PROPerTy command used in conjunction with the THERmal and TRANsport commands provides an option to read directly the effective properties.

The second purpose of this command is to provide instruction for the manner in which the material properties are to be calculated at the cell (or element) interfaces. All material properties specified through the HYDRaulic, THERmal, TRANsport, and UNSaturated commands are at grid node locations. However, some of these properties (e.g., hydraulic and thermal conductivities) are needed at the cell interfaces. Through the PRPO command, the user can provide instructions to use harmonic, geometric, or arithmetic mean of the nodal values for the cell interface. Harmonic mean is the default mode.

6.24.2 Syntax

No numeric field is required with this command.

PROP {character string} [EFFEctive], [HARMonic | GEOMetric |
 ARITHmetic | UPWInd]

character string: One of the characters, C, P, or T for which the PROPerTy specification applies.

EFFEctive: If the modifier EFFE is encountered on the PROP command, then it is assumed that the properties read through the THERmal and TRANsport commands are effective (or equivalent) properties. That is, it is assumed that the existence of fluid in the pores of the porous matrix has already been accounted for by the user in specifying the properties. If EFFE is not encountered, then the properties read by the THERmal and TRANsport commands are assumed to be for the solid portion of the porous matrix only, and the effective properties are calculated internally.

HARMonic: Property across a cell interface is computed as the harmonic mean of the property values for the two nearest grid nodes. This is the default option.

- GEOMetric:** Property across a cell interface is computed as the geometric mean between the two nearest grid nodes.
- ARITHmetic:** Property across a cell interface is computed as the arithmetic mean between the two nearest grid nodes.
- UPWInd:** Property across a cell interface takes on the value specified at a node that is upstream of the interface.

6.24.3 Comments

By default, the properties of the host media are computed as weighted averages of specified properties read via the **FLUId**, **THERmal**, and **TRANsport** commands. The input values of specific heats are interpreted to be in mass units [such as $J/(kg \cdot K)$], and the input value of **N1** of the **TRANsport** command is assumed to be the partition coefficient, k_d . However, if this command is encountered, then the input values are assumed to be the effective properties of the matrix. No internal manipulation is performed. The input specific heats are assumed to be in terms of volume units [such as $J/(m^3 \cdot K)$] and the input value of **N1** for the **TRANsport** command is assumed to be the retardation factor, R_d . The values specified by any **FLUId** command are ignored, except for the mass density.

Since the effective properties depend on the amount of fluid present in the porous matrix, for partially saturated problems, direct reading of effective properties should be avoided.

The default option for calculating the properties at the location of cell faces is the Harmonic mean. If this option is acceptable, then no action need be taken. The default option is recommended for fully saturated problems.

By using multiple **PROPerty** commands, different options may be selected for **P**, **T**, and **C** equations.

6.24.4 Examples

PROPerty mode: **EFFEctive** matrix values directly specified for **T** Eqn
PROPerty: use **GEOMetric** mean for cell interface values for **P** Eqn
PROPerty: **EFFEctive**, **ARITHmetic** for **P**

6.25 R COMMAND

6.25.1 Purpose

The purpose is to specify the grid locations of the radial (r) coordinates for cylindrical geometry.

6.25.2 Syntax

R {N1}, [N2, N3, ..., Nn]; n=IMAX

6.25.3 Comments

This command is an alternative to the X command. The interpretation of N1 through Nn is identical to that for the X command. The only difference between the two commands is that if the R command is used instead of the X command, then cylindrical geometry is automatically selected; it is not necessary to use the CYLindrical command.

As explained in the CYLindrical command description, an additional restriction is placed on the choice of r-coordinates: the interface radii (the element boundary r-coordinates) must all be positive. This requirement implies that:

$$N_1 \geq -N_2; \quad N_i > 0 : i = 2, 3, \dots, \text{IMAX}. \quad (6.25-1)$$

For problems in which the first cell (boundary between nodes at I=1 and I = 2) is to be the axis of symmetry, N₁ should be equal to -N₂, so that the first element boundary in the r-direction is located at r=0.

6.25.4 Examples

See X command.

6.26 READ COMMAND

6.26.1 Purpose

The purpose is to read the archive file for basic problem information and initial conditions. This command can be used to restart a problem from a previous point at which the archive file was created.

6.26.2 Syntax

READ [N1], ['fname'], [FORM|UNFO]

'fname': A character expression that specifies the file (or device) name from which the input is read. If it is present, it must be the first character-string expression that is enclosed in single quotes, although not necessarily the first character expression on the command line. It may consist of any valid characters allowed by the operating system. The file name may be up to 32 characters long, consisting of any characters accepted by the operating system as valid I/O file names. By default, the input data file is assumed to be named **RESTART** (see Table 3-2).

FORM or UNFO The character expression 'FORMatted' or 'UNFOrmatted' defines the nature of the data in the restart file. If this specification is omitted, then the file is assumed to be unformatted (see Table 3-2).

Numeric field	Numeric value	Default value	Remarks and explanations
N1	0	1	The data-set number to be read from the archive file. If no data-set number is specified, then the first set is read from the archive file. A data set in this context consists of several records, as explained in Section 5.4.3.

6.26.3 Examples

READ from archive file
READ record number 3
READ from 'EXAMPLE1.SAN'
READ record number 5 from 'EXAMPLE2.SAN' in FORMatted mode

6.27 REFERENCE COMMAND

6.27.1 Purpose

The purpose is to specify the option for diagnostic printout of the values of variables at a reference node. The variables printed are C, P, T, U, V, and W. In addition, the convergence rate or residuals are also printed.

6.27.2 Syntax

REFE {N1, N2, N3}, [N4]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>1 <IMAX	none	The I-grid index of the reference grid node.
N2	>1 <JMAX	none	The J-grid index of the reference grid node.
N3	>1 <KMAX	none	The K-grid index of the reference grid node.
N4	>0	32,000	The frequency of diagnostic output in terms of time steps. A value of 0 is treated as identical to that of 1. The output can be suppressed by specifying a large value of N4.

6.27.3 Comments

No default value is provided for N1, N2, and N3. No diagnostic results will be printed, in the absence of the REFERENCE command.

6.27.4 Examples

REFERENCE node (4,8,3) \$ Diagnostic printout every step
 REFERENCE node (7,2,5) print every 10 steps
 REFERENCE node (11,7,5) every 32000 steps\$ suppress step-by-step printout

6.28 RELAXATION COMMAND

6.28.1 Purpose

The purpose is to specify the relaxation factors for iterative solution of the matrix of equations in the steady-state mode.

6.28.2 Syntax

RELA [character string=N1], [character string=N2], [character string=N3]

character string: One of the character strings: P, T, and C which correspond to the variables, pressure, temperature, and concentration, respectively.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>0	1	The relaxation factor for the variable that is denoted by the character string immediately preceding the value.
N3	<2		

6.28.3 Comments

This command is effective only if the steady-state mode of solution is activated by the SOLVE command; otherwise it is ignored. The relaxation factor affects the convergence of the numerical solution. If the solution shows instability, then a value less than unity may help obtain a stable solution. Alternatively, if the convergence rate is too slow, then a value greater than unity may result in more rapid convergence. A value less than 0 or greater than two will, almost always, lead to exponentially unstable growth of the solution. A more complete discussion of the role of the relaxation parameter is given in standard text books (see, for example, Varga 1962).

6.28.4 Examples

RELAXation factor for P = 0.7
 RELAXation factors: T = 1.2, C= 0.9
 RELAXation factors: P = 0.7, T=0.7, C= 0.9

6.29 ROCK COMMAND

6.29.1 Purpose

The purpose is to specify the density and porosity of the host porous matrix (soil or rock) or those of the planar and linear features. Different porosities are defined in Section 2.1.1.

6.29.2 Syntax

ROCK [N1, N2, ..., N7]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>0	1	The density of dry, solid component, r_s .
N2	0 1	1	The effective (or flow) porosity, n_E .
N3	0 1	1	The total porosity, n_T .
N4	0 1	1	The connected (or diffusive) porosity, n_C .
N5	1	1	These three values select the zones to which N1 through N4 apply. Their interpretation is identical to that of N1, N2, and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command. If no FOR command was previously specified, then the input is assumed to apply to zone number 1.
N7	LZN		

6.29.3 Comments

In the absence of a PROPERty command, the density and porosity input are employed to weight the matrix properties of specific heat, thermal conductivity, retardation coefficients, and molecular diffusivities as functions of component properties of the dry solids and the fluid, as appropriate. However, if a PROPERty command is present, then the porosity input is used only for computing the dispersion coefficient; the density input is ignored.

6.29.4 Examples

ROCK density = 1; porosities: effective = 0.1, total 0.2, diffusive 0.15
ROCK density 2,200, porosities: 3*0.15 for ZONE number 2
ROCK density 2,200, porosities: 0.2, 0.25, 0.21 for zones 1 thru 5
ROCK rho 2,200, porosities: 0.10, 0.20, 0.15 for zone 1 to 5 in step of 2

6.30 SAVE COMMAND

6.30.1 Purpose

The purpose is to write the output to restart, plot, and archive files.

6.30.2 Syntax

SAVE [character strings], ['fname'], [fmt], [NOW], [REST], [N1]

- character string: One or more of the strings of characters: C, P, T, THET, U, V, and W. Each character string represents a corresponding variable in Table 5-3 for which the output is desired (see Section 5.7 for additional information) to be written in the files.
- 'fname': The file (or device) name to which the output is written. See the "fname" description in the READ command for the manner of this specification. By default, the archive file is assumed to be named ARCHIVE (see Section 5.3).
- fmt: The character expression, 'FORMatted' or 'UNFORMatted', that defines the nature of the data on the archive file. By default, the file is assumed to be unformatted.
- NOW: The archive output is produced immediately.
- REST: In addition to the archive file, a special file named restart.0 is created. On this file, only the output from the last time step is saved. The size of this file is much smaller than that of the archive file. It can be used to restart computations. When archive files are very large, this option may prove to be more efficient for restarts.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1	See below	The frequency index for output to be archived. The output to be archived is obtained every N1 steps. For example, a specification of N1=10 will result in output at the 10th, 20th, 30th, etc. steps. By default, output to the archive file is automatically obtained at the end of simulations for all active variables.

6.30.3 Comments

If the **SAVE** command is specified without any attributes, then writing of the field arrays to the archive file is completely suppressed. If no **SAVE** command is specified, then output to the archive file of the variables for which the equations are solved is automatically produced at the end of simulations. Successive commands may be employed to accommodate changing output requirements.

6.30.4 Examples

SAVE U, N, W on file 'DEMO.PLT' in FORMatted mode
SAVE U, N, P, THETA, and C every 100 steps
SAVE W, P, and C NOW
SAVE U, T, and C NOW and every 20 steps
SAVE none of the variables

6.31 SCALE COMMAND

6.31.1 Purpose

The purpose is to allow internal scaling of the specified input according to the following equation.

$$Q_{in} = a \cdot Q + b, \quad (6.31-1)$$

where Q_{in} is the internal representation of a variable, Q is the value specified by the user, and a and b are user-specified constants.

6.31.2 Syntax

SCAL [N1, N2]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	Any	1	The multiplier, a , of Equation 6.31-1. It is automatically set to 1 at the end of each application.
N2	Any	0	Addend, b , of Equation 6.31-1. It is automatically set to 0 at the end of each application.

6.31.3 Comments

This command can be used for internal scaling only in conjunction with the CHARACTERISTIC, SOURCE, X, Y, and Z commands.

6.31.4 Examples

SCALE multiply by 3.3 and add 10
 SCALE multiply by 0.3048

6.32 SCREEN COMMAND

6.32.1 Purpose

The purpose is to echo some of the diagnostic output obtained from the REFERENCE command to the user's screen.

6.32.2 Syntax

SCRE

6.32.3 Comments

This command is useful when the output (written to the output unit, IWR; see Section 3.3) is being directed to a printer or file. This command allows the user to monitor the progress of the solution procedure on the screen.

6.32.4 Examples

SCREen echo for diagnostic output

6.33 SOIL COMMAND

6.33.1 Purpose

The purpose is to specify the density and porosity of the host porous matrix (soil or rock) or that of embedded planar or linear features.

6.33.2 Syntax

SOIL [N1, N2, ..., N7]

6.33.3 Comments

This command is identical to the ROCK command.

6.33.4 Examples

See the ROCK command.

6.34 SOLVE COMMAND

6.34.1 Purpose

The purpose is to begin solution of the governing equations and to select the transient or steady-state mode of solution.

6.34.2 Syntax

SOLV [N1, N2, N3, N4], [STEADy], [RETURn]

STEADy: The transient mode is the default. If a string of characters beginning with "STEA" is present anywhere on the command line, then the equations are solved in their steady-state mode; i.e., the time-derivative terms of Equations 2.1-3, 2.1-14, and 2.1-20 are set to zero.

RETURn: If a string of characters beginning with "RETU" is present anywhere on the command line, then solution to the governing equations is not performed. However, the input data on geometry and properties are processed, and output in a tabular form can be obtained for checking purposes.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	0	0 or 32,000	In case of transient run (STEADy absent), it is the incremental time (default value = zero time units) for which the solution of the governing differential equations is desired. If STEADy is present in the command, then N1 represents the maximum number of iterative steps (default value = 32,000 steps) for solution of the governing equations.
N2	0	None or 10	In the transient mode, N2 is the beginning time step (see Section 4.2) to be used in the current segment of calculations. This time step may be changed during calculations either by an N3 specification or by a subsequent SOLVe command. There is no default value of N2 in this case. In the steady-state mode, N2 is the minimum number (default value = 10) of iterative steps to be performed on the matrix.

N3	0	1	The factor for increasing the time step in the transient mode. Each time step will be multiplied by this value to obtain the next time step until a maximum value specified by N4, below, is reached. This input is ignored in the steady-state mode.
N4	0	1 E+20	The maximum permissible time-step value in the transient mode. This input is ignored in the steady-state mode.

6.34.3 Comments

The code is designed to initiate the solution procedure of the governing equations as soon as this command is encountered. It should, therefore, be specified only after complete input has been supplied. However, the sequence of calculations may be subdivided into as many segments as desired and a SOLVe command specified for each segment. Any sequential or time-dependent features can thus be accommodated by these segmented calculations. An illustration of the segmented calculations is given in Table 5-4.

6.34.4 Examples

SOLVe for 50 yr in steps of 2
 SOLVe for 50 yr, initial step=0.2 yr, multiplier 1.1, max=10 yr
 SOLVe for 1 E+06 yr, DT=0.2, factor=1.1, max=1 E+03
 SOLVe in STEAdy state mode: maximum steps 200
 SOLVe in STEAdy mode: maximum steps 500; minimum steps 20

6.35 SOURCE COMMAND

6.35.1 Purpose

The purpose is to specify location, type, and magnitude of the sources (or sinks) for fluid, heat, or chemical species.

6.35.2 Syntax

SOUR {character string}, [EXPO, VOLU] | [SOLU], {N1, N2}, [N3, ..., Nn]

character string: One of the character strings: C, P, T. It denotes a corresponding variable in Table 5-3 for which the source is specified.

EXPO: By default, the source rate is assumed to be constant or specified as a tabulated function of time. However, if a character string beginning with EXPO is present anywhere on the command line, then the source is assumed to be specified as an exponential decay function made up of one or more components according to the equation:

$$S_F = \sum_{n=1}^N s_n \exp(-f_n t), \quad (6.35-1)$$

where S_F is the value of source at time t for the variable under consideration, and s_n and f_n are the strength and time constant for the n -th component.

VOLU: By default, the source units are assumed to be per unit time [e.g., m^3/s for fluid, W (J/s) for heat, and kg/s for chemical species]. However, if a string of characters beginning with VOLU is present anywhere on the command line, then the source units are taken to be per unit time per unit volume of the composite porous media [e.g., $m^3/(m^3s)$ for fluid, W/m^3 for heat, and $kg/(m^3s)$ for chemical species]. This type of source occurs, for example, for radioactive species in which the heat of decay is typically stated in terms of unit volume.

SOLU: If a string of characters beginning with SOLU is present anywhere on the command line, then the source for chemical species is assumed to be solubility limited. That is, the source is specified as the total initial mass of a chemical species, and the solubility of the species in the fluid phase is limited to a maximum saturation value, C_s . This type of source is allowed only for chemical species, C. With this option, only one source of the species may be specified, and this source may not coexist with any other type of source for the same species.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 LZN	None	The numerical designation for the source zone. All internal nodes of the field of interest (i.e., excluding the boundary nodes) with a zone designation equal to N1 are identified as the source nodes. The zone number must denote an active zone; that is, it must have previously appeared on a ZONE command. The cumulative number of zones for all SOURCE commands must not exceed the specified value of the LSZ dimension parameter (see Section 3.4).
N2	0	0	Number of sets (either time - release rate sets if a table is being specified or $s_n - f_n$ sets of Eq. 6.35-1) of values that will follow. The cumulative number of sets for all SOURCE commands must not exceed the specified value of the LS0 dimension parameter (see Section 3.4).
N3	0	0	The time at which the source becomes active (time at which release begins) in the absence of the EXPO modifier; the first time constant, f_n , of Equation 6.35-1, if the EXPO modifier is present.
N4	Any	0	The strength of source or s_n of Equation 6.35-1. The strength may be scaled according to Equation 6.31-1 by the SCALE command.
N5 through Nn			Repetition of (N3, N4) sets, except when the modifier SOLU is present. In the presence of the SOLU modifier, N5 is the saturation limit, C_s , of the chemical species and all values following N5 are ignored.

6.35.3 Comments

Multiple exponential and tabulated kinds of sources may coexist; however, only one solubility-limited source may be specified and it may not coexist with any of the other source types.

6.35.4 Examples

SOURCE for P: zone 1; # sets = 1: time=0., value=100 ft³/day
SOURCE for T: zone 1: set 1: T=10., S=10 W per unit VOLUME
SOURCE for T: zone 2: EXPONENTIAL type; 3 terms (.5,1) (.05,.1) (.001,.01)
SOURCE: T: zone 3: 5 sets: (0,50) (50,900) (100,1000) (500,1000), (5000,0)
SOURCE for C: zone 7: set 1: T=100, S=0.2 kg/day
SOURCE for C: zone 5: SOLUBILITY limited: set 1: T=0., S=100 kg; Cs=0.05

6.36 SUBDOMAIN COMMAND

6.36.1 Purpose

The purpose is to specify a region smaller than the total domain for starting the solution of temperature and concentration equations. The subdomain is expanded as the thermal and concentration pulses propagate. This command may be useful when the total domain is large and thermal and concentration sources are limited to a small region.

6.36.2 Syntax

SUBD {C | T}, {N1, N2, N3}, [N4, N5, N6], [N7]

C: The subdomain specification is effective for the concentration equation.

T: The subdomain specification is effective for the temperature equation.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 IMAX	1	The starting I-node index of the subdomain.
N2	1 JMAX	1	The starting J-node index of the subdomain.
N3	1 KMAX	1	The starting K-node index of the subdomain.
N4	N1 IMAX	IMAX	The ending I-node index of the subdomain.
N5	N2 JMAX	JMAX	The ending J-node index of the subdomain.
N6	N3 KMAX	KMAX	The ending K-node index of the subdomain.
N7	>0	1 E-07	The minimum absolute difference between value at the current boundary of the subdomain and the value at the node that is two grid nodes inside of the subdomain boundary, that triggers an automatic expansion of the subdomain boundaries.

6.36.3 Comments

An expanding zone of computation for concentration and temperature often proves economical if changes in these quantities are due solely to a source whose influence increases with time.

6.36.4 Examples

SUBDomain for C initially from (1,1,1) to (5,3,3)

SUBDomain for T initially from (5,3,3) to (7,5,5) change if del >1 E-05

6.37 THERMAL COMMAND

6.37.1 Purpose

The purpose is to specify the thermal properties of the host porous matrix (soil or rock) or those of the planar and linear features.

6.37.2 Syntax

ThER [N1, N2, ..., N7]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>0	1	Specific heat (c_s or c_e , see Section 2.1.2) of material. By default, N1 is taken to be specific heat of solids, c_s ; however, if the PROPERty command is present, then it is taken to be the effective (or equivalent) specific heat, c_e .
N2	0	0	Thermal conductivity (k_s or k_e , see Section 2.1.2) of material. By default, N2 is taken to be the thermal conductivity of the solids, k_s ; however, if the PROPERty command is present, then it is taken to be the effective (or equivalent) thermal conductivity, k_e .
N3	0	0	Longitudinal dispersivity (α_L) of material.
N4	0	0	Transverse dispersivity (α_T) of material.
N5 through N7	1	1	These three values select the material zones to which N1 through N4 apply. Their interpretation is identical to that of N1, N2, and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, then the input is assumed to apply to zone number 1.

6.37.3 Examples

ThERmal specific heat = 1, conductivity = 45. dispersivity: 3, 1.5
ThERmal properties cp=26, kt=45 alpha=0.2, alphas=0.1 for ZONE 3

THERmal props cp = 26, kt = 45. alphas: 0.2, 0.15 for ZONE 1 through 3
THERmal props cp = 26, kt = 45. alphas: 2*0. for zones 1 through 5 in
steps of 2

6.38 THETA COMMAND

6.38.1 Purpose

The purpose is to specify the grid locations of the y-coordinates for cylindrical geometry in angular units.

6.38.2 Syntax

THET [DEGRees], {N1}, [N2,, Nn]; $n \leq JMAX + 1$

DEGRees: By default, the angular input is assumed to be in radians.
However, if a string of characters beginning with "DEGR" is present anywhere on the command line, then the input values are taken to be in degrees.

6.38.3 Comments

The N1 through Nn of this command are interpreted in a manner identical to those for the Y command. A maximum of JMAX+1 numerical fields may be specified.

This command is an alternative to the Y command. The only difference between the two commands is that, if the keyword THETA is used instead of Y, cylindrical geometry is automatically selected; it is not necessary to use the CYLindrical command. (Also see the X command.)

6.38.4 Examples

THETA type=1: 0, 5, 15, 25, 35, 45, 60, 75, 90, 105, 120 degrees

THETA type=2: range = 6.28 radians

THETA type=3: min = 0, max = 3.14 radians

THETA type=2: range 360 degrees

6.39 TIME COMMAND

6.39.1 Purpose

The purpose is to specify the initial time of simulation for a problem. Normally the value of the time variable, t , at the beginning is assumed to be zero. With this command, the initial value of time may be specified to be any other suitable value.

6.39.2 Syntax

TIME {N1}

Numeric field	Numeric value	Default value	Remarks and explanations
N1	Any	0	The starting time for simulations.

6.39.3 Examples

TIME = 50 years at start of simulations

6.40 TITLE COMMAND

6.40.1 Purpose

The purpose is to specify the problem title.

6.40.2 Syntax

TITL followed by character information

6.40.3 Comments

The specification must be restricted to one 80-character record. If present, this command must occur before the GRID command.

6.40.4 Examples

TITLe ILLUSTRATIVE PROBLEM - Default SET UP - 07/30/87:ACRi/akr

6.41 TRANSPORT COMMAND

6.41.1 Purpose

The purpose is to specify the transport properties of the host porous media (soil or rock) or those of the planar and linear features.

6.41.2 Syntax

TRAN [N1, N2, ..., N7]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	Any	0 or 1	Partition coefficient, k_d , or retardation factor, R_d . By default, N1 is taken to be k_d ; however, if the PROPERty command is present, then it is taken to be R_d . The default value for N1 is 0 for k_d and 1 for R_d .
N2	0	0	Molecular diffusivity, α_M , for species, C, in water.
N3	0	0	Longitudinal dispersivity, α_L , of the porous matrix.
N4	0	0	Transverse dispersivity, α_T , of the porous matrix.
N5 through N7	1	1	These three values select the zones to which through N4 apply. Their interpretation is identical to that of N1, N2, and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, then the input is assumed to apply to zone number 1.

6.41.3 Examples

TRANsport properties: $k_d=1$, $D_m=5.24$, $\alpha_L=10$, $\alpha_T=1$
 TRAN: $K_d=0$, $d_m=1 \text{ E-03}$, $L=10$, $T=1$, for ZONE 1
 TRANsport $K_d=1.1 \text{ E-03}$, $d_m=0.$, $L=10$, $T=1$, for zones 1 to 5
 TRANsport $R_d=21$, $d_m=0.$, $L=10$, $T=1$, for ZONE 1 to 5 in step 2

6.42 UNSATURATED COMMAND

6.42.1 Purpose

The purpose is to specify the nature of the characteristic curve for unsaturated soil or rock zones. This command works in conjunction with the CHARACTERISTIC and FOR commands (see Section 2.2.2).

6.42.2 Syntax

UNSA [[TABU], [HEAD] | [VAN | BROO], [BURD | MUAL], [NETC], [N1, N2, N3]

TABU: The unsaturated soil (or rock) characteristics are specified as a table. This is the default option.

HEAD: By default, it is assumed that the conductivity characteristic for the tabulated option is specified relative to normalized moisture content θ^* . However, if the modifier HEAD is present anywhere in the command, then the conductivity characteristic is taken to be specified as tabulated values of ψ relative to k_r .

VAN: The unsaturated properties are calculated according to van Genuchten (1978) formulae:

$$\theta^* = [1 + (\psi/\alpha)^n]^{-m}, \quad h < 0, \quad (6.42-1a)$$

$$\theta^* = 1, \quad h \geq 0, \quad (6.42-1b)$$

$$m = (1 - 1/n) \quad (6.42-1c)$$

and

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m]^2; \quad (6.42-2)$$

BROO: The unsaturated properties are calculated according to the Brooks and Corey (1966) relations:

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m] \quad (6.42-3a)$$

$$\theta^* = (\psi/\psi^*)^{-\beta}, \quad \psi < -\psi^*, \quad (6.42-3b)$$

$$\theta^* = 1, \quad \psi \geq -\psi^*, \quad (6.42-3c)$$

and

$$k_r = \theta^*(5/2 + 2/\beta) \quad (6.42-4)$$

It should be noted that Brooks and Corey employed the Burdine (1953) theory for computing K_r from soil moisture characteristics. Equation 6.42-4 employs the Mualem (1976) theory. The original form can be recovered by specifying the modifier, BURD, as explained below.

BURD: The k_r term in Equation 6.42-2 is derived according to Mualem (1976). However, if a string of characters beginning with "BURD" is present anywhere on the command line, then K_r is calculated according to the Burdine (1953) theory. Equation 6.42-2 is replaced by:

$$k_r = \theta^2 [1 - (1 - \theta^{1/m})^m] \quad (6.42-5a)$$

and

$$k_r = \theta^{(3+2/\beta)} \quad (6.42-5b)$$

NETC: By default, species concentration is calculated based on the quantity of pore liquid. If NETC is present anywhere on the command line, species concentration is provided in terms of the total control volume, including the soil.

Numeric field	Numeric value	Default value	Remarks and explanations
N1 - N3	1 LZN	None	N1 to N3 have the same interpretation as in the FOR command. If zones are being specified by the FOR command, then N1 to N3 need not be specified.

6.42.3 Comments

This command must be specified to trigger the variably saturated mode. In the absence of this command, the soil is assumed to be fully saturated.

6.42.4 Examples

- UNSAturated properties in TABUlated form for zone 2 to 6 in steps of 2
- UNSAturated prop: TABUlated form; HEAD versus relative K specification
- UNSAturated prop: VAN genuchten with BURDine theory
- UNSAturated BROOKs and COREY with MUALem theory

6.43 USER COMMAND

6.43.1 Purpose

To specify user identification for purposes of archiving.

6.43.2 Syntax

USER followed by character information

6.43.3 Comments

The specification must be restricted to one 10-character record. All output produced by the user, including the archive files, contains the user identification. If present, this command must occur before the GRID command.

6.43.4 Examples

USER John Doe
USER 5C380

6.44 VISCOSITY COMMAND

6.44.1 Purpose

The purpose is to specify the option and constants employed for calculation of fluid viscosity as a function of temperature. The viscosity, in turn, is used to modify the hydraulic conductivity (see HYDRauiic command).

6.44.2 Syntax

VISC {N1}; [N2, N3, N4, N5, N6]

Numeric field	Numeric value	Default value	Remarks and explanations
N1		0	An index for mode of viscosity calculations.
	0		Constant fluid viscosity.
	1		Viscosity changes according to the equation: $\mu = B_1 \exp[B_2/(T+\alpha)] \quad (6.44-1)$
	2		Viscosity changes according to the equation: $\mu = B_3 + B_4T + B_5T^2 + B_6T^3 \quad (6.44-2)$
	3		Viscosity changes according to the equation: $\mu = \mu^* \exp[B_7(T^*-T) - B_8(T^*-T)^2] \quad (6.44-3)$
N2	Any	0	The reference temperature, T^* , at which the reference viscosity is μ^* (Equation 6.44-3).
N3	Any	See remarks	The coefficient B_2 of Equations 6.44-1, B_3 of Equation 6.44-2, or B_7 of Equation 6.44-3. Default value is 1436 if $N1=1$; otherwise, it is zero.
N4	Any	See remarks	The coefficient α of Equation 6.44-1, B_4 of Equation 6.44-2, or B_8 of Equations 6.44-3. Default value is 273.15 if $N1=1$; otherwise it is zero.
N5	Any	0	The coefficient B_5 of Equation 6.44-2; this input is ignored for all other choices of $N1$.

Numeric field	Numeric value	Default value	Remarks and explanations
N6	Any	0	The coefficient B_6 of Equation 6.44-2; this input is ignored for all other choices of N1.

6.44.3 Examples

VISCosity type 2: $T^* = 25$, $a=1.1 \text{ E-04}$, $b=5.5 \text{ E-05}$, $c=0.00$, $d=3.3 \text{ E-09}$

VISCosity type=3: TREF 30, first coeff = 1.1 E-05 , second coeff = 1.1 E-07

6.45 WINDOW COMMAND

6.45.1 Purpose

The purpose is to specify a window or subdomain within the domain of simulations for which the output is desired. The window is defined by specifying two corners: the ones with the lowest and the highest (I,J,K) indices.

6.45.2 Syntax

WIND [N1, N2, ..., N9]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 IMAX	1	The starting I-node index of the subdomain.
N2	1 JMAX	1	The starting J-node index of the subdomain.
N3	1 KMAX	1	The starting K-node index of the subdomain.
N4	N1 IMAX	IMAX	The ending I-node index of the subdomain.
N5	N2 JMAX	JMAX	The ending J-node index of the subdomain.
N6	N3 KMAX	KMAX	The ending K-node index of the subdomain.
N7	1	1	The x-direction node interval for output. For example, a specification of 3 will result in the printout at I=1,4,7,10, etc. grid nodes.
N8	1	1	The y-direction node interval for output.
N9	1	1	The z-direction node interval for output.

6.45.3 Comments

This command works in conjunction with the OUTPUT command to produce tabular output. The WINDOW command, once specified, stays in effect for all subsequent outputs until another WINDOW command is encountered.

6.45.4 Examples

WINDow is the total calculation domain

WINDow from (2,4,2) to (10,9,5)

WINDow from (2,4,7) to (10,9,11) skip I = 2, J = 3, K = 2

6.46 X COMMAND

6.46.1 Purpose

The purpose is to specify the grid locations for the x-coordinates.

6.46.2 Syntax

X {N1}, [N2, ..., Nn]; $n \leq \text{IMAX} + 1$

Numeric field	Numeric value	Default value	Remarks and explanations
N1		2	An index of the type of coordinate specification.
	1		Coordinate values are explicitly specified by the user.
	2		Only the range of coordinates is specified. The coordinates are calculated internally, with a geometric ratio between the successive grid intervals.
	3		As for option 2, except that the minimum and maximum values of the x-coordinates are specified.
N2	Any	1	The value of the first x-coordinate; i.e., X(1), if N1=1 or N1=3. The value of the desired range (must be > 0), if N1=2.
N3	Any	1	The second coordinate value if N1=1. The value of the geometric ratio by which the intervals between successive grid nodes change, if N1=2. The maximum value of the x-coordinate, X(IMAX), if N1=3.
N4	Any	1	The value of the third coordinate point, if N1=1. The value of the geometric ratio by which the intervals between successive grid nodes change, if N1=3. This input is ignored if N1=2.

Numeric field	Numeric value	Default value	Remarks and explanations
N5 through Nn	Any		The values of the successive grid node coordinates, from fourth node onwards, if N1=1. A total of IMAX values (see GRID command) must be specified (including N2 and N3 above) in an algebraically ascending order. These values are ignored if N1 is not equal to 1.

6.46.3 Examples

X type=1: -5, 5, 15, 25, 35, 45, 55, 65, 75, 85, 95, 105
 X type=2, range = 10., ratio = 1.2
 X type=2 \$ uniform values over a range of unity
 X type=3, minimum = 0., maximum = 10
 X type=3, minimum = 0., maximum = 10.; ratio = 1.1
 X coordinates by default \$ uniform values over a range of unity

6.47 Y COMMAND

6.47.1 Purpose

The purpose is to specify the grid locations for the y-coordinates.

6.47.2 Syntax

Y [DEGRees], {N1}, [N2; ..., Nn]; $n \leq \text{JMAX} + 1$

DEGRees: If a character string beginning with "DEGR" is present anywhere on the command line, then the values N2 through Nn are taken to be in degrees and the cylindrical geometry option is automatically activated.

6.47.3 Comments

The N1 through Nn numeric fields of this command are interpreted in a manner identical to that for the X command. A maximum of JMAX+1 numerical fields may be specified that are interpreted to pertain to the y-coordinate in a manner identical to that for the X command.

6.47.4 Examples

Y type=1: 0, 5, 15, 25, 35, 45, 60, 75, 90, 105

Y type=2: range = 100 meters

Y type=2: range 360 DEGRees; geometry is cylindrical

Y type=3: min = 0, max = 2,000 m

6.48 Z COMMAND

6.48.1 Purpose

The purpose is to specify the grid locations for the z-coordinates.

6.48.2 Syntax

Z {N1}, [N2, ..., Nn]; $n \leq JMAX + 1$

6.48.3 Comments

The N1 through Nn of this command are interpreted in a manner identical to that for the X command. A maximum of KMAX+1 numerical fields may be specified that are interpreted to pertain to the z-coordinate in a manner identical to that for the X command.

6.48.4 Examples

See the X command.

6.49 ZDAT COMMAND

6.49.1 Purpose

ZDAT command provides for specification of the datum (z^* of Equation 2.1-8) from which all vertical distances are measured. While datum can be chosen arbitrarily, it is common to take it at the water table, ground surface, or mean sea level. z^* can be conveniently taken to be zero by locating the $z = 0$ coordinate at the datum. The value of z^* is of importance in the unsaturated flow problems only.

In addition to the datum, two other limiting quantities are read by this command as explained below.

6.49.2 Syntax

ZDAT {N1, N2, N3}

Numeric field	Numeric value	Default value	Remarks and explanations
N1	any	$z(1)$	Datum, the value of z^* of Equation 2.1-8. The default value is the z-coordinate of the K= 1 node.
N2	>0	1 E+15	The maximum value of the soil-moisture tension.
N3	>0	1 E-12	The minimum value of the relative hydraulic conductivity.

6.49.3 Comments

The maximum value of the soil-moisture tension and the minimum value of the relative hydraulic conductivity is used to avoid underflow during execution.

6.49.4 Examples

ZDATum zstar = 0.0, maxpsi = 1 E+20, minkr = 1. E-20

6.50 ZONE COMMAND

6.50.1 Purpose

The purpose is to define a zone (or subdomain) of the calculation domain that has unique hydraulic, thermal, or transport properties, linear or planar features, or other unique characteristics such as sources or sinks, fixed values of variables, etc.

6.50.2 Syntax

ZONE {N1}, [N2, N3, ..., N9] [FRACTure or PLANar | BOREhole or LINE]

FRACTure: The zone being defined is a planar feature that may be a fracture or some other feature.

PLANar: The zone being defined is a planar feature that may be a fracture or some other feature.

BOREhole: The zone being defined is a one-dimensional borehole or some other linear feature.

LINE The zone being defined is a one-dimensional borehole or some other linear feature.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 LZN	1	The zone designation index; LZN is a dimension parameter (see Section 3.4).
N2	1 IMAX	1	The starting I-node index of the zone.
N3	1 JMAX	1	The starting J-node index of the zone.
N4	1 KMAX	1	The starting K-node index of the zone.
N5	N1 IMAX	IMAX	The ending I-node index of the zone.
N6	N2 JMAX	JMAX	The ending J-node index of the zone.
N7	N3 KMAX	KMAX	The ending K-node index of the zone.

Numeric field	Numeric value	Default value	Remarks and explanations
N8	Any	None	Width of the planer feature, if FRAC or PLAN is encountered; outer diameter of the linear feature, if BORE or LINE is encountered; otherwise N8 is ignored.
N9	Any	None	Inner diameter of the linear feature, if BORE or LINE is encountered, otherwise, these data are ignored.

6.50.3 Comments

The ZONE command is employed to partition the domain of calculations into subdomains, each with its distinctive or unique features and properties. A subdomain may be as small as a single element or as large as the entire calculation domain. It may be a single, contiguous region, or it may consist of several noncontiguous regions. A zone may be specified by a single ZONE command or it may be specified by a series of ZONE commands with the same zone index (N1), but with different grid index values (N2 through N7).

Only one of the character strings, FRACture or PLANar feature, needs to be used. Similarly, only one of the BOREhole or LINE element symbols needs to be used. A planar feature may lie in the XY (N3 = N6), YZ (N1 = N4), or ZX plane (N2 = N5). Similarly, the linear feature may be in the X- (N2 = N5, N3 = N6), Y- (N1 = N4, N3 = N6), and Z- (N1 = N4, N2 = N5) direction.

The area of the linear element is calculated as

$$\text{Area} = (\pi/4) \cdot (D^2 - d^2) \tag{6.49-1}$$

The value for D (outer diameter) is N8 and that of d (inner diameter) is N9.

6.50.4 Examples

```

ZONE 1  $ total domain
ZONE 3  from (1,1,1) to (11,7,5)
ZONE 3  from (6,10,2) to (31,19,7)
    
```

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APPENDIX A

DESCRIPTION OF FREE-FORMAT COMMAND LANGUAGE

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DESCRIPTION OF FREE-FORMAT COMMAND LANGUAGE

The user interface with PORFLO-3 is through the FREEFORM command language developed by Analytic & Computational Research, Inc. (Runchal 1987a). This command language reduces user input to a set of conversational, English-like commands. These commands are largely free (with some exceptions) of any requirements of format and hierarchy. The modules that implement the commands are written in FORTRAN 77. These modules provide for interactive input or emulate the interactive input in batch mode.

1.0 THE FREEFORM INPUT RECORDS

Input is specified through three types of records: KEYWORD, CONTINUATION, and COMMENT, as described in the sections below.

1.1 THE KEYWORD RECORD :

Function: The function of a keyword record is to specify the numeric and character data.

Structure: The keyword has the following attributes.

- A keyword record must begin with a keyword.
- Only one keyword per record is allowed.
- The keyword may be followed by modifiers and numerical fields.
- The keyword, the modifiers, and the numerical fields must be separated from one other by comment, separator, or terminator fields.
- Any character or numeric data in a keyword record after the first occurrence of a terminator are ignored.

1.2 THE CONTINUATION RECORD

Function: A continuation record continues the input of numeric and character data started by the preceding keyword record.

Structure: The following rules are to be followed.

- A continuation record must begin with either a separator or a numeric character as the first character of the record. It must not begin with an alphabetic ('A' through 'Z' or 'a' through 'z') character as the first character of a record.

- A continuation record must always occur after a keyword record for that group.
- A continuation record must consist only of a combination of modifiers and numerical fields separated from each other by separators.
- Any character or numeric data in a continuation record after the first occurrence of a terminator is ignored.
- Any number of continuation records may follow a keyword record.

1.3 THE COMMENT RECORD

Function: The function of a comment record is to enhance the clarity and readability of the input.

Structure: The following properties apply to the comment record.

- A comment record must begin with a back-slash (\), asterisk (*), or dollar (\$) character in the first column of a record. Any combination of characters may follow the first character.
- A comment record is not processed. No numerical or character data are extracted; the record is merely written to the output file.
- A comment record cannot be extended by a continuation record.
- A comment record can be inserted anywhere in the input.

2.0 ELEMENTS OF INPUT RECORD

One or more of the following six basic elements comprise an input record: KEYWORD, MODIFIER, NUMERIC, SEPARATOR, TERMINATOR, and COMMENT. These elements are described in the sections below.

2.1 THE KEYWORD

Function: The keyword identifies the input group.

Structure:

- The keyword may consist of any characters except separator (Section 3.4) or terminator (Section 3.5) characters. However, the first character of a keyword must be alphabetic ('A' through 'Z' or 'a' through 'z'). To this extent, the concept of a keyword is similar to that of a variable name in FORTRAN.

- The keyword may be in upper or lower case.
- A keyword must begin in the first column of a record.
- The keyword is terminated with the first occurrence of a valid separator or terminator character.
- The keyword may consist of 1 to 80 characters. However, if there are more than four characters, only the first four are machine-identifiable.

Examples:

ABCD, A123, A&B+, A&B. are all valid examples of a keyword. The keyword specifications of ABCD, abcd, ABCDEFGH, AbCd123, ABCDxxxxxxxxxxx (where x can be any character) are all equivalent because only the first four characters are significant and the input is case-insensitive.

1ABC, 567, (abc, 'abc, .abc are all invalid keyword specifications. In all of these examples the first character is not alphabetic.

Note that a specification of ABC), ABC', or ABC\$, although valid, is equivalent to that of ABC because the last character in all of these examples is either a separator (Section 3.4) or a terminator (Section 3.5).

2.2 THE MODIFIER

Any character information in an input record following a keyword, except that embedded in a numeric or comment field (see Sections 3.3 and 3.6) is treated as modifier(s).

Function: The modifier contains character data that help to interpret the other data in the record.

Structure:

- A modifier in any input group, if present, must follow the keyword.
- The modifier is identical to the keyword in its structure. It may consist of any characters, except separator and terminator characters, of which the first character must be alphabetic.
- A modifier must not start in the first column of a record. It can be from 1 to 79 characters in length; however, if it is longer than four characters, only the first four are significant.

- The modifier must be separated from the keyword, other modifiers, and numeric data by a valid separator, terminator, or comment field.

Examples: The structure of the modifier is identical to that of a keyword, except that it must not start in the first column of a record. Examples are given in Section 2.1.

2.3 THE NUMERIC FIELD

Any numeric characters in a continuation or keyword record that follows a keyword, except those embedded in a keyword, modifier, or comment field (see Sections 3.1, 3.2 and 3.6) are treated as numeric data.

Function:

A numeric field contains numeric data for input variables.

Structure:

- A numeric field is a continuous string of characters that must begin with the numeric character set. In this context, the numeric character set consists of the numerals (0-9), the decimal point (.), and the plus (+) and minus (-) operators.
- A numeric field must consist only of the numeric character set defined above, the asterisk (*), and the exponent in lower (e) or upper (E) case. It must not contain any other character.
- The plus (+) or minus (-) sign, if present, must immediately precede the numerical value without any intervening blank or other characters.
- The asterisk (*) or the exponent (E or e), if present, must be embedded; the numeric field must not begin or end with one of these characters.
- A numeric field must be separated from the keyword, modifiers, and other numeric fields by a valid separator, terminator, or comment field.
- A numeric field may be located anywhere on a keyword or continuation record.
- The numeric values may be specified in any of the following formats:
 - Integer, (e.g., 999),
 - Real (e.g., 999.0, 999.)
 - Exponent (e.g., 9.99 E+02, 99.9 E+01)

- Successive, repetitive, identical numeric values may be specified by the asterisk (*) option. Thus, (30., 30., 30.) may be represented as (3*30. or 3*3.0E+1); embedded separators or non-numeric characters must not appear in such specification.

Examples: The input character strings, 1, 0.1234, .567, +123., -1.0005, 1.2e00, 1.35E0, and 3*1.2 are all valid examples of a numerical field. Input specifications of 123, 123., 1.23e02, +0.123E+3, 1.23E2, 1*123, 1*1.23E02 are all equivalent.

The strings 1ABC, 11X11, 1+2, 11., 1+1.E1 are all invalid numeric specifications. In the first three, non-numeric characters follow a leading numeric character, and in the last three, a valid numeric character occurs in an invalid, embedded location.

Note that a specification of 1.2)2. or 1.2=2, although valid, will be equivalent to a specification of two numeric fields, 1.2 and 2, because of the embedded separator (Section 3.4) in both cases. A specification of 1.2\$2 is equivalent to a specification of 1.2 because the 2 following the \$ will be ignored (Section 3.5).

2.4 THE SEPARATOR FIELD

Function: A separator field separates the keyword, the modifiers, and the numeric fields of an input record.

Structure: Any continuous string of characters in an input record that consists only of the characters from the separator character set is treated as a separator field. The valid separator characters are the comma (,), the space (), the equal (=), the colon (:), the semi-colon (;), the apostrophe ('), the left parenthesis '(', and the right parenthesis ')' characters.

Examples: The sequence of characters, ';;:)', =====, =', and (;) are all valid separator fields. However, the characters (a) or (1) are not valid separator fields. In the first case, the character, 'a', will be processed by FREEFORM as a modifier; in the second, the character, '1', will be processed as a numeric field.

2.5 THE TERMINATOR FIELD

Function: A terminator ends all input to a keyword or continuation record. It also provides a vehicle for the user to insert comments in these records.

Structure:

- The dollar (\$) character is the only valid terminator.
- The terminator ends the input for the keyword or continuation record in which it occurs; input associated with that particular keyword may continue in a continuation record that follows.
- The terminator may appear anywhere in a record.
- Any characters following the terminator in that input record are not processed; rather, they are treated as comments and are merely written to the output file.

Examples: The character sequences 'XYZ \$comments now', '\$ any comments here', and '123.456\$789.123' are all examples of sequences with embedded terminators. In the first sequence, XYZ will be treated as valid character data (either keyword or modifier, depending on its starting position on the input record), whereas the characters following \$ will be ignored. In the second example, the total sequence will be treated as comments and ignored. In the third example, 789.123 will be ignored, whereas 123.456 will be treated as numeric data.

2.6 THE COMMENT FIELD

Function: A comment field provides a vehicle for the user to insert comments in input to enhance the clarity and readability of the input.

Structure:

- A comment field may be in the form of an embedded comment or a comment record.
- An embedded comment field is a field that occurs in a keyword or continuation record. It must begin with a terminator (\$) character; any combination of characters may follow the terminator. The comment field is terminated at the end of the 80th character in that record (Section 3.5).
- A comment field in a comment record may consist of any combination of characters. In this case, the comment field begins with the back slash (/), asterisk (*), or a terminator (\$) character and terminates with the 80th character.

Examples: In the input record,

```
ARRAY = 1., 2., 3., 4., 5.  $ EXAMPLE 1
```

the character string, '\$ EXAMPLE 1', is an example of an embedded comment in a keyword record. Input processing stops with the \$ character; all characters in that record following, and including, the \$ character are ignored.

The following are examples of comment records:

```
/ARRAY = 1., 2., 3., 4., 5.  $ EXAMPLE 1  
*ARRAY = 1., 2., 3., 4., 5.  - another EXAMPLE  
$****///// ARRAY = 1., 2., 3., 4., 5.  $ still another example
```

All of these strings of characters will be treated as comment records and no processing will be done because one of the identifier characters of the comment field appears as the first character of the input record.

3.0 REFERENCES

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APPENDIX B

ILLUSTRATIONS OF PORFLO-3 INPUT AND OUTPUT

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```

TITLE CASE 3 - VERTICAL INFILTRATION WITH RAINFALL
/
GRID 3 BY 3 BY 16
/
SCREEN ECHO
Z MODE 3: min =-30, max 0
/
ROCK DENSITY 1, POROSITY = 0.52
HYDRAULIC PROPS SS = 1.E-7, (KX,KY,KZ) --> 3*3.125
VISCOSITY GEOMETRIC MEAN OPTION
/
UNSATURATED FLOW CHARACTERISTICS: COREY & BROOKS
CHARACTERISTIC: HREF=5.4, LAMDA=0.2
CONVERGENCE FOR P: MODE 2; VALUE=0.00001 MAX ITERATIONS = 20
/
INITIAL P -130.54 everywhere (6*0) mode 1: gradx=0, grady=0, gradz=1
/
BOUNDARY CONDITIONS FOR P: INDEX -1, TYPE 2
BOUNDARY CONDITIONS FOR P: INDEX +1, TYPE 2
BOUNDARY CONDITIONS FOR P: INDEX -2, TYPE 2
BOUNDARY CONDITIONS FOR P: INDEX +2, TYPE 2
BOUNDARY CONDITIONS FOR P: INDEX +3, TYPE 2 FLUX = -1.4125 cm/hr
/
REFERENCE POINT 2,2,2 PRINT EVERY 1 STEPS
/
WINDOW 2,2,1 TO 2,2,100
/
MATRIX SWEEP IN Z DIRECTION P=1
SOLVE UNTIL TIME = 2.55 hrs IN STEPS OF .050 hrs
/
OUTPUT W,P,THETA in xz plane
/
END

```

THIS OUTPUT IS PRODUCED BY THE COMPUTATIONAL MODEL

----- P O R F L O - 3 D -----

FOR TRANSIENT OR STEADY STATE ANALYSIS
OF FLOW, HEAT AND MASS TRANSPORT
IN VARIABLY SATURATED POROUS OR FRACTURED MEDIA

DEVELOPED BY DR A.K. RUNCAL (ACRI, LOS ANGELES)
AND DR B. SAGAR (PNL, RICHLAND) UNDER CONTRACT FROM
WESTINGHOUSE HANFORD COMPANY, RICHLAND, WA

THIS COMPUTER CODE WAS DEVELOPED FOR USE BY
THE US DEPT. OF ENERGY AND ITS CONTRACTORS

FOR ENQUIRIES AND ASSISTANCE: CALL 213-398-0958 USA

OR 509-376-5897 USA

VERSION 1.00: DATED: 16 OCT 1988

DATE OF RUN: 1/24/1989 - TIME OF RUN: 16:56:54

RECORD OF INPUT DATA STREAM

- ** RECORD NO. 1 KEYWORD ***** TITLE CASE 3 - VERTICAL INFILTRATION WITH RAINFALL
- ** RECORD NO. 2 COMMENT ***** /
- ** RECORD NO. 3 KEYWORD ***** GRID 3 BY 3 BY 16
- ** RECORD NO. 4 COMMENT ***** /
- ** RECORD NO. 5 KEYWORD ***** SCREEN ECHO
- ** RECORD NO. 6 KEYWORD ***** Z MODE 3: min =-30, max 0
- ** RECORD NO. 7 COMMENT ***** /
- ** RECORD NO. 8 KEYWORD ***** ROCK DENSITY 1, POROSITY = 0.52
- ** RECORD NO. 9 KEYWORD ***** HYDRAULIC PROPS SS = 1.E-7, (KX,KY,KZ) --> 3*3.125
- ** RECORD NO. 10 KEYWORD ***** VISCOSITY GEOMETRIC MEAN OPTION
- ** RECORD NO. 11 COMMENT ***** /
- ** RECORD NO. 12 KEYWORD ***** UNSATURATED FLOW CHARACTERISTICS: COREY & BROOKS
- ** RECORD NO. 13 KEYWORD ***** CHARACTERISTIC: HREF=5.4, LAMDA=0.2
- ** RECORD NO. 14 KEYWORD ***** CONVERGENCE FOR P: MODE 2; VALUE=0.00001 MAX ITERATIONS = 20
- ** RECORD NO. 15 COMMENT ***** /
- ** RECORD NO. 16 KEYWORD ***** INITIAL P -130.54 everywhere (0*0) mode 1: gradx=0, grady=0, gradz=1
- ** RECORD NO. 17 COMMENT ***** /
- ** RECORD NO. 18 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX -1, TYPE 2

** RECORD NO. 19 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX +1, TYPE 2
** RECORD NO. 20 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX -2, TYPE 2
** RECORD NO. 21 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX +2, TYPE 2
** RECORD NO. 22 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX +3, TYPE 2 FLUX = -1.4125 cm/hr
** RECORD NO. 23 COMMENT ***** /
** RECORD NO. 24 KEYWORD ***** REFERENCE POINT 2,2,2 PRINT EVERY 1 STEPS
** RECORD NO. 25 COMMENT ***** /
** RECORD NO. 26 KEYWORD ***** WINDOW 2,2,1 TO 2,2,100
** RECORD NO. 27 COMMENT ***** /
** RECORD NO. 28 KEYWORD ***** MATRIX SWEEP IN Z DIRECTION P=1
** RECORD NO. 29 KEYWORD ***** SOLVE UNTIL TIME = 2.55 hrs IN STEPS OF .050 hrs
** RECORD NO. 30 COMMENT ***** /

CASE 3 - VERTICAL INFILTRATION WITH RAINFALL

GRID DIMENSIONS.....(IMAX,JMAX,KMAX) = 3 BY 3 BY 10
MAXIMUM NUMBER OF NODES IN EACH 3-D ARRAY. = 1000
NUMBER OF THREE DIMENSIONAL FIELD ARRAYS.. = 23
FIELD LENGTH ALLOCATED FOR 3-D ARRAYS..... = 143.8 Kbyte
FIELD LENGTH ACTUALLY USED FOR 3-D ARRAYS. = 12.9 Kbyte

X COORDINATE VALUES

=====

-0.5000 0.5000 1.5000

Y COORDINATE VALUES

=====

-0.5000 0.5000 1.5000

Z COORDINATE VALUES

=====

-30.0000 -28.0000 -26.0000 -24.0000 -22.0000 -20.0000 -18.0000 -16.0000
-14.0000 -12.0000 -10.0000 -8.0000 -6.0000 -4.0000 -2.0000 0.0000

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 1 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 2 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 3 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 4 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 5 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 6 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 7 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 8 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 9 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =10 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =11 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =12 =====

J=
3 1 1 1
2 1 1 1
1 1 1 1
I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =13 =====

J=
 3 1 1 1
 2 1 1 1
 1 1 1 1
 I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =14 =====

J=
 3 1 1 1
 2 1 1 1
 1 1 1 1
 I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =15 =====

J=
 3 1 1 1
 2 1 1 1
 1 1 1 1
 I= 1 2 3

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =16 =====

J=
 3 1 1 1
 2 1 1 1
 1 1 1 1
 I= 1 2 3

BOUNDING INDICES FOR ACTIVE ZONES

=====

ZONE#	LOWER BOUND	UPPER BOUND
1	(1, 1, 1)	(3, 3, 16)

 CASE 3 - VERTICAL INFILTRATION WITH RAINFALL

PROGRAM CONSTANTS, PARAMETERS AND REFERENCE VALUES

=====

CARTESIAN/RADIAL GEOMETRY INDEX	=	1
Y/Z DIR. PERIODIC BOUNDARY INDEX	=	0
DENSITY OPTION INDEX.....	=	0
HYDRAULIC CONDUCTIVITY INDEX ...	=	0
PROPERTY CALCULATION MODE	=	1
START TIME	=	0.000E+00
CURRENT VALUE OF MAX. TIME	=	2.550E+00
STARTING TIME STEP	=	5.000E-02

TIME STEP INCREMENT FACTOR = 1.000E+00
 MAXIMUM TIME STEP = 1.000E+30
 TOTAL VOLUME OF FLUID IN FIELD.. = 1.456E+01

HYDRAULIC PROPERTIES OF POROUS MEDIA

```

=====
ACTIVE   SPECIFIC   X-DIR.   Y-DIR.   Z-DIR.
ZONE #   STORATIVITY  HYDRAULIC K  HYDRAULIC K  HYDRAULIC K
    1     1.000E-07  3.125E+00  3.125E+00  3.125E+00
    
```

VALUES AT REFERENCE GRID NODE (2, 2, 2)

```

=====
U - X-DIR. VELOCITY COMPONENT = 0.000E+00
V - Y-DIR. VELOCITY COMPONENT = 0.000E+00
W - Z-DIR. VELOCITY COMPONENT = 0.000E+00
P - PRESSURE OR PRESSURE HEAD = -1.585E+02
THET- RELATIVE SATURATION LEVEL = 1.000E+00
POR - MATRIX EFFECTIVE POROSITY. = 5.200E-01
VOL - VOLUME OF GRID ELEMENTS... = 2.000E+00
    
```

DEPENDENT VARIABLE SPECIFICATIONS

```

=====
VARIABLE SYMBOL SOLVE OPTION INTEG. PROFILE # OF SWEEPS RELAX FACTOR
    1         P           1           1           1           1.00
    
```

MATRIX SWEEP DIRECTIONS: Z

STEP NO.	TIME	[-----REFERENCE VALUES AT NODE (2, 2, 2)-----]						[CONVERGENCE RATE / RESIDUALS]		
		U	V	W	P	T	C	PRESSURE	REF. VAR.	INDEX
0	0.00E+00	0.000E+00	0.000E+00	0.000E+00	-1.585E+02	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.0
1	5.00E-02	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	7.816E-04	7.816E-04	78.2
2	1.00E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	1.286E-04	1.286E-04	12.9
3	1.50E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	1.776E-05	1.776E-05	1.8
4	2.00E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	5.980E-06	5.980E-06	0.6
5	2.50E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	7.153E-06	7.153E-06	0.7
6	3.00E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	3.099E-06	3.099E-06	0.3
7	3.50E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	8.345E-06	8.345E-06	0.8
8	4.00E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	3.040E-06	3.040E-06	0.3
9	4.50E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	7.749E-06	7.749E-06	0.8
10	5.00E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	9.894E-06	9.894E-06	1.0
11	5.50E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	9.775E-06	9.775E-06	1.0
12	6.00E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	6.914E-06	6.914E-06	0.7
13	6.50E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	7.570E-06	7.570E-06	0.8
14	7.00E-01	0.000E+00	0.000E+00	-7.909E-04	-1.585E+02	0.000E+00	0.000E+00	8.881E-06	8.881E-06	0.9

-7.000E+00	13	-1.39E+00
-9.000E+00	12	-1.37E+00
-1.100E+01	11	-1.33E+00
-1.300E+01	10	-1.24E+00
-1.500E+01	9	-1.08E+00
-1.700E+01	8	-7.33E-01
-1.900E+01	7	-1.38E-01
-2.100E+01	6	-1.04E-02
-2.300E+01	5	-1.37E-03
-2.500E+01	4	-8.28E-04
-2.700E+01	3	-7.93E-04
-2.900E+01	2	-7.91E-04

I = 2
X = 5.00E-01

----*--*--* P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 52, TIME= 2.5500E+00 --*--*--*--*--*--*--*

Z =	K =	
0.000E+00	16	-7.36E+00
-2.000E+00	15	-9.39E+00
-4.000E+00	14	-1.14E+01
-6.000E+00	13	-1.36E+01
-8.000E+00	12	-1.58E+01
-1.000E+01	11	-1.82E+01
-1.200E+01	10	-2.10E+01
-1.400E+01	9	-2.49E+01
-1.600E+01	8	-3.22E+01
-1.800E+01	7	-6.20E+01
-2.000E+01	6	-1.30E+02
-2.200E+01	5	-1.51E+02
-2.400E+01	4	-1.54E+02
-2.600E+01	3	-1.57E+02
-2.800E+01	2	-1.59E+02
-3.000E+01	1	-1.61E+02

I = 2
X = 5.00E-01

----*--*--* THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 52, TIME= 2.5500E+00 --*--*--*--*--*--*--*

Z =	K =	
0.000E+00	16	9.40E-01
-2.000E+00	15	9.39E-01

-4.000E+00	14	9.38E-01
-6.000E+00	13	9.35E-01
-8.000E+00	12	9.30E-01
-1.000E+01	11	9.20E-01
-1.200E+01	10	9.02E-01
-1.400E+01	9	8.88E-01
-1.600E+01	8	8.83E-01
-1.800E+01	7	8.57E-01
-2.000E+01	6	5.47E-01
-2.200E+01	5	5.30E-01
-2.400E+01	4	5.29E-01
-2.600E+01	3	5.29E-01
-2.800E+01	2	5.29E-01
-3.000E+01	1	5.29E-01

I = 2
X = 5.00E-01

=====> UNIT 2 OPEN FOR I/O IN UNFORMATTED MODE; FILE NAME: [.ARCH]ARCHIVE

<---- START OF ARCHIVE READ/WRITE OPERATIONS ---->

CREATED BY PROGRAM : PORFLOW-3D - VERSION 1.00: DATED: 18 OCT 1988
DATA CREATED BY USER (ID) ... : WHC - JDD - DATE OF ARCHIVED RECORDS : 1/24/1989
TIME OF CREATION OF RECORDS . : 18:58:54
TITLE OF THE ARCHIVED DATA SET: CASE 3 - VERTICAL INFILTRATION WITH RAINFALL
SIMULATION TIME OF STORED DATA: 2.550E+00
STEP NUMBER AT WHICH GENERATED: 52
GRID DIMENSIONS OF STORED DATA: 3 BY 3 BY 16

----> WRITING VARIABLE: U - X-DIR. VELOCITY COMPONENT
----> WRITING VARIABLE: V - Y-DIR. VELOCITY COMPONENT
----> WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT
----> WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD
----> WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 1 WRITTEN TO ARCHIVES ---->

THIS OUTPUT IS PRODUCED BY THE COMPUTATIONAL MODEL

----- P O R F L O - 3 D -----

FOR TRANSIENT OR STEADY STATE ANALYSIS
OF FLOW, HEAT AND MASS TRANSPORT

IN VARIABLY SATURATED POROUS OR FRACTURED MEDIA

DEVELOPED BY DR A.K. RUNCHAL (ACRI, LOS ANGELES)
AND DR B. SAGAR (PNL, RICHLAND) UNDER CONTRACT FROM
WESTINGHOUSE HANFORD COMPANY, RICHLAND, WA

THIS COMPUTER CODE WAS DEVELOPED FOR USE BY
THE US DEPT. OF ENERGY AND ITS CONTRACTORS

FOR ENQUIRIES AND ASSISTANCE: CALL 213-398-0956 USA

OR 509-376-5897 USA

VERSION 1.00: DATED: 18 OCT 1988

DATE OF RUN: 1/24/1989 - TIME OF RUN: 18:59:23

ELAPSED TIME FOR THIS CASE : 2.48 MINUTES
TIME PER GRID NODE PER STEP: 19.90 MILLISECONDS
TIME PER NODE-STEP-EQUATION: 19.90 MILLISECONDS
1 EQUATIONS SOLVED AT 144 NODES FOR 52 STEPS.

RECORD OF INPUT DATA STREAM

=====

END-OF-FILE ENCOUNTERED IN READING INPUT DATA. KEYWORD SET TO QUIT.
=====

TITLE SHLOMO'S CASE 2 - VERTICAL INFILTRATION

/

GRID 24 IN X-DIR BY 3 IN Y-DIR BY 16 Z-DIR

/

SCREEN ECHO

/

/-----

/ MAKE GRID BY EXPANDING GEOMETRICALLY IN THE XZ PLANE

/-----

X MODE 2: RANGE 610 EXPAND BY 1.1

Y MODE 2: RANGE 100

Z MODE 3: MIN -122. cm MAX 0. EXPAND BY 0.9

/

/-----

/ MATERIAL PROPERTIES

/

/ SS: SPECIFIC STORAGE

/ KX: HYDRAULIC CONDUCTIVITY IN THE X DIRECTION

/ KY: HYDRAULIC CONDUCTIVITY IN THE Y DIRECTION

/ KZ: HYDRAULIC CONDUCTIVITY IN THE Z DIRECTION

/

/ The material is isotropic KX=KY=KZ

/-----

ROCK DENSITY 1, POROSITY = 0.348

HYDRAULIC PROPERTIES (SS)= 1.E-7, KX=556.4 KY=556.4, KZ=556.4 --> CM/DAY

VISCOSITY GEOMETRIC MEAN OPTION

/

/-----

UNSATURATED FLOW CHARACTERISTICS: TABLE OF VALUES

/-----

CHARACTERISTIC: RETENTION CURVE FOR ZONE 1: 53 CURVE POINTS

/

Se	Tension	Se: Rel. saturation
0.000000E+00	200.0000	
1.4906671E-03	196.9238	
2.3883670E-03	191.8755	
5.9289024E-03	184.5087	
9.0773413E-03	176.1117	
1.3174927E-02	167.3539	
1.5929889E-02	157.8496	
2.3897110E-02	136.9602	
3.2126632E-02	122.6126	
3.6445826E-02	116.6880	
4.0583938E-02	111.0548	
4.6040211E-02	105.1733	
5.2639848E-02	98.63003	
5.8485709E-02	92.91111	
6.2821142E-02	88.48029	
7.0769981E-02	83.32758	
7.7401511E-02	79.72044	
8.7075494E-02	75.44308	
9.6185446E-02	71.88699	
0.1092924	67.81497	

0.1222132	64.18084
0.1379908	60.31434
0.1532028	57.01459
0.1722248	53.53377
0.1927746	50.33596
0.2129471	47.47307
0.2298978	45.46078
0.2449269	43.73211
0.2641589	42.02840
0.2898741	39.70529
0.3106207	37.94973
0.3389995	36.06388
0.3713793	34.02272
0.4035723	32.31643
0.4340505	30.88774
0.4628179	29.49723
0.4980668	28.35894
0.5295029	27.19165
0.5641800	26.05148
0.6030505	24.98773
0.6438281	23.97512
0.6870034	22.98777
0.7248207	21.97500
0.7627330	21.24702
0.7928518	20.75170
0.8195214	20.28273
0.8498242	20.01911
0.8749799	19.70503
0.9008984	19.44229
0.9216713	19.20634
0.9502596	19.02034
0.9702700	18.78454
1.0000000	18.46953

/

CHARACTERISTIC: RELATIVE HYDRAULIC CONDUCTIVITY CURVE ZONE 1: 45 POINTS

/	So	K	So: Rel. Saturation
4.5862451E-02	9.9218077E-06		
5.0250437E-02	1.3347027E-05		
5.7839382E-02	1.8267483E-05		
6.2654935E-02	2.3792185E-05		
6.7481297E-02	3.1324485E-05		
7.3682845E-02	4.0800755E-05		
8.1088364E-02	5.4559989E-05		
8.7297864E-02	7.2171148E-05		
9.2939317E-02	9.1284339E-05		
0.1013517	1.2169755E-04		
0.1084172	1.5041286E-04		
0.1158098	1.8476255E-04		
0.1235487	2.3120297E-04		
0.1353367	3.2389455E-04		
0.1489308	4.5025381E-04		
0.1605368	6.2307407E-04		

0.1727580	8.4113551E-04
0.1834112	1.0740440E-03
0.1976358	1.4568017E-03
0.2126803	1.9337797E-03
0.2325100	2.8850051E-03
0.2513801	3.8147104E-03
0.2720189	4.8591187E-03
0.2932921	6.4320280E-03
0.3145333	8.8765090E-03
0.3382721	1.0945584E-02
0.3745098	1.6480954E-02
0.4099778	2.3764918E-02
0.4346914	3.0411992E-02
0.4849854	4.1218791E-02
0.4921043	5.3159828E-02
0.5284358	7.0982488E-02
0.5683907	8.9725994E-02
0.5861617	0.1074519
0.6265295	0.1399627
0.6709072	0.1840404
0.7097058	0.2285040
0.7687013	0.3148932
0.8078989	0.3984839
0.8479097	0.4877611
0.8887257	0.5991479
0.9241478	0.7079301
0.9517682	0.8032593
0.9787836	0.9043072
0.9983999	0.9868676

/

 CONVERGENCE CRITERIA FOR P: MODE 2; VALUE=0.001 MAX ITERATIONS = 20

/

 INITIAL P -30. EVERYWHERE FROM (1,1,1) TO (24,3,16)
 * MODE 1: GRADX=0, GRADY=0, GRADZ=1

```

/-----
BOUNDARY CONDITIONS FOR P: INDEX +1 (RIGHT BOUNDARY), TYPE 2
BOUNDARY CONDITIONS FOR P: INDEX -2 (FRONT BOUNDARY), TYPE 2
BOUNDARY CONDITIONS FOR P: INDEX +2 (BACK BOUNDARY), TYPE 2
BOUNDARY CONDITIONS FOR P: INDEX +3 (TOP BOUNDARY) , TYPE 2
*           WITH FLUX = -10.35 cm/DAY
BOUNDARY CONDITIONS FOR P: INDEX -3 (BOTTOM BOUNDARY), TYPE 2
/-----
/
REFERENCE POINT AT (2,2,9)
/
WINDOW FROM (1,2,1) TO (100,2,100) FOR OUTPUT
OUTPUT P NOW IN XZ PLANE
/
MATRIX SWEEP IN Z DIRECTION P=1
SOLVE UNTIL TIME = 0.01 DAYS IN STEP OF 0.001 DAY
OUTPUT U,W,P,THETA in xz plane ==> RIGHT NOW
SAVE NOW ON 'SHLOW012.PLT'
/
SOLVE UNTIL TIME = 1.00 DAYS IN STEP OF 0.0005 DAY INCREASE BY 1.1, MAX =0.05
OUTPUT NOW
SAVE NOW ON 'SHLOW012.PLT'
/
SOLVE UNTIL TIME = 5.00 DAYS IN STEP OF 0.05 DAY INCREASE BY 1.1, MAX =0.10
OUTPUT NOW
SAVE NOW ON 'SHLOW012.PLT'
/
/
END

```

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----- P O R F L O - 3 D -----

FOR TRANSIENT OR STEADY STATE ANALYSIS
OF FLOW, HEAT AND MASS TRANSPORT
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THIS COMPUTER CODE WAS DEVELOPED FOR USE BY
THE US DEPT. OF ENERGY AND ITS CONTRACTORS

FOR ENQUIRIES AND ASSISTANCE: CALL 213-398-0956 USA

OR 509-376-5897 USA

VERSION 1.00: DATED: 16 OCT 1988

DATE OF RUN: 1/24/1989 - TIME OF RUN: 16:59:24

RECORD OF INPUT DATA STREAM

- ** RECORD NO. 1 KEYWORD ***** TITLE SHLOMO'S CASE 2 - VERTICAL INFILTRATION
- ** RECORD NO. 2 COMMENT ***** /
- ** RECORD NO. 3 KEYWORD ***** GRID 24 IN X-DIR BY 3 IN Y-DIR BY 16 Z-DIR
- ** RECORD NO. 4 COMMENT ***** /
- ** RECORD NO. 5 KEYWORD ***** SCREEN ECHO
- ** RECORD NO. 6 COMMENT ***** /
- ** RECORD NO. 7 COMMENT ***** /-----
- ** RECORD NO. 8 COMMENT ***** / MAKE GRID BY EXPANDING GEOMETRICALLY IN THE XZ PLANE
- ** RECORD NO. 9 COMMENT ***** /-----
- ** RECORD NO. 10 KEYWORD ***** X MODE 2: RANGE 610 EXPAND BY 1.1
- ** RECORD NO. 11 KEYWORD ***** Y MODE 2: RANGE 100
- ** RECORD NO. 12 KEYWORD ***** Z MODE 3: MIN -122. cm MAX 0. EXPAND BY 0.9
- ** RECORD NO. 13 COMMENT ***** /
- ** RECORD NO. 14 COMMENT ***** /-----
- ** RECORD NO. 15 COMMENT ***** / MATERIAL PROPERTIES
- ** RECORD NO. 16 COMMENT ***** /
- ** RECORD NO. 17 COMMENT ***** / SS: SPECIFIC STORAGE
- ** RECORD NO. 18 COMMENT ***** / KX: HYDRAULIC CONDUCTIVITY IN THE X DIRECTION

WHC-EP-0041

```

** RECORD NO. 19 COMMENT ***** / KY: HYDRAULIC CONDUCTIVITY IN THE Y DIRECTION
** RECORD NO. 20 COMMENT ***** / KZ: HYDRAULIC CONDUCTIVITY IN THE Z DIRECTION
** RECORD NO. 21 COMMENT ***** /
** RECORD NO. 22 COMMENT ***** / The material is isotropic KX=KY=KZ
** RECORD NO. 23 COMMENT ***** /-----
** RECORD NO. 24 KEYWORD ***** ROCK DENSITY 1, POROSITY = 0.348
** RECORD NO. 25 KEYWORD ***** HYDRAULIC PROPERTIES (SS)= 1.E-7, KX=558.4 KY=558.4, KZ=558.4 --> CM/DAY
** RECORD NO. 26 KEYWORD ***** VISCOSITY GEOMETRIC MEAN OPTION
** RECORD NO. 27 COMMENT ***** /
** RECORD NO. 28 COMMENT ***** /-----
** RECORD NO. 29 KEYWORD ***** UNSATURATED FLOW CHARACTERISTICS: TABLE OF VALUES
** RECORD NO. 30 COMMENT ***** /-----
** RECORD NO. 31 KEYWORD ***** CHARACTERISTIC: RETENTION CURVE FOR ZONE 1: 53 CURVE POINTS
** RECORD NO. 32 COMMENT ***** / Se Tension Se: Rel. saturation
** RECORD NO. 33 CONTINUATION ** 0.000000E+00 200.0002
** RECORD NO. 34 CONTINUATION ** 1.4906671E-03 198.9238
** RECORD NO. 35 CONTINUATION ** 2.3883670E-03 191.8755
** RECORD NO. 36 CONTINUATION ** 5.9289024E-03 184.5007
** RECORD NO. 37 CONTINUATION ** 9.0773413E-03 176.1117
** RECORD NO. 38 CONTINUATION ** 1.3174927E-02 167.3539
** RECORD NO. 39 CONTINUATION ** 1.5929889E-02 157.8496
** RECORD NO. 40 CONTINUATION ** 2.3897110E-02 136.9602
** RECORD NO. 41 CONTINUATION ** 3.2126632E-02 122.8126
** RECORD NO. 42 CONTINUATION ** 3.6445826E-02 116.8880
** RECORD NO. 43 CONTINUATION ** 4.0583938E-02 111.8648
** RECORD NO. 44 CONTINUATION ** 4.8040211E-02 105.1733
** RECORD NO. 45 CONTINUATION ** 5.2839848E-02 98.63003
** RECORD NO. 46 CONTINUATION ** 5.8485709E-02 92.91111
** RECORD NO. 47 CONTINUATION ** 6.2821142E-02 88.48029
** RECORD NO. 48 CONTINUATION ** 7.0769981E-02 83.32758
** RECORD NO. 49 CONTINUATION ** 7.7401511E-02 79.72044
** RECORD NO. 50 CONTINUATION ** 8.7075494E-02 75.44308
** RECORD NO. 51 CONTINUATION ** 9.8185448E-02 71.88699
** RECORD NO. 52 CONTINUATION ** 0.1092924 67.81497
** RECORD NO. 53 CONTINUATION ** 0.1222132 64.18084
** RECORD NO. 54 CONTINUATION ** 0.1379908 60.31434
** RECORD NO. 55 CONTINUATION ** 0.1532028 57.01459
** RECORD NO. 56 CONTINUATION ** 0.1722248 53.53377
** RECORD NO. 57 CONTINUATION ** 0.1927746 50.33596
** RECORD NO. 58 CONTINUATION ** 0.2129471 47.47307
** RECORD NO. 59 CONTINUATION ** 0.2296978 45.48078
** RECORD NO. 60 CONTINUATION ** 0.2449269 43.73211
** RECORD NO. 61 CONTINUATION ** 0.2641589 42.02640
** RECORD NO. 62 CONTINUATION ** 0.2896741 39.70529
** RECORD NO. 63 CONTINUATION ** 0.3106207 37.94973
** RECORD NO. 64 CONTINUATION ** 0.3389995 36.06388
** RECORD NO. 65 CONTINUATION ** 0.3713793 34.02272
** RECORD NO. 66 CONTINUATION ** 0.4035723 32.31843
** RECORD NO. 67 CONTINUATION ** 0.4340505 30.68774
** RECORD NO. 68 CONTINUATION ** 0.4628179 29.49723
** RECORD NO. 69 CONTINUATION ** 0.4980668 28.35694
** RECORD NO. 70 CONTINUATION ** 0.5295029 27.19185

```

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** RECORD NO. 71 CONTINUATION ** 0.5641800      26.05148
** RECORD NO. 72 CONTINUATION ** 0.6030505      24.98773
** RECORD NO. 73 CONTINUATION ** 0.6438281      23.97512
** RECORD NO. 74 CONTINUATION ** 0.6870834      22.98777
** RECORD NO. 75 CONTINUATION ** 0.7246207      21.97580
** RECORD NO. 76 CONTINUATION ** 0.7627330      21.24702
** RECORD NO. 77 CONTINUATION ** 0.7926518      20.75170
** RECORD NO. 78 CONTINUATION ** 0.8195214      20.28273
** RECORD NO. 79 CONTINUATION ** 0.8498242      20.01911
** RECORD NO. 80 CONTINUATION ** 0.8749799      19.70503
** RECORD NO. 81 CONTINUATION ** 0.9008984      19.44229
** RECORD NO. 82 CONTINUATION ** 0.9216713      19.20634

```

```

=====
****WARNING: NO MORE THAN 100 NUMERIC VALUES MAY BE INPUT FOR A KEYWORD.
              DATA CONTAINED IN THE INPUT STRING GIVEN BELOW IGNORED.
              0.9216713      19.20634
=====

```

```

** RECORD NO. 83 CONTINUATION ** 0.9502596      19.02034
=====
MISSING KEYWORD. RECORD ABOVE IGNORED.

```

```

** RECORD NO. 84 CONTINUATION ** 0.9702700      18.78454
=====
MISSING KEYWORD. RECORD ABOVE IGNORED.

```

```

** RECORD NO. 85 CONTINUATION ** 1.0000000      18.48953
=====
MISSING KEYWORD. RECORD ABOVE IGNORED.

```

```

** RECORD NO. 86 COMMENT ***** /
** RECORD NO. 87 KEYWORD ***** CHARACTERISTIC: RELATIVE HYDRAULIC CONDUCTIVITY CURVE ZONE 1: 45 POINTS
** RECORD NO. 88 COMMENT ***** /      Se          K          Se: Rel. Saturation
** RECORD NO. 89 CONTINUATION ** 4.5882451E-02  9.9216077E-06
** RECORD NO. 90 CONTINUATION ** 5.0250437E-02  1.3347827E-05
** RECORD NO. 91 CONTINUATION ** 5.7839382E-02  1.8287483E-05
** RECORD NO. 92 CONTINUATION ** 6.2654935E-02  2.3792185E-05
** RECORD NO. 93 CONTINUATION ** 6.7461297E-02  3.1324485E-05
** RECORD NO. 94 CONTINUATION ** 7.3682845E-02  4.0000755E-05
** RECORD NO. 95 CONTINUATION ** 8.1088364E-02  5.4559989E-05
** RECORD NO. 96 CONTINUATION ** 8.7297864E-02  7.2171148E-05
** RECORD NO. 97 CONTINUATION ** 9.2939317E-02  9.1284339E-05
** RECORD NO. 98 CONTINUATION ** 0.1013517      1.2189755E-04
** RECORD NO. 99 CONTINUATION ** 0.1084172      1.5041286E-04
** RECORD NO.100 CONTINUATION ** 0.1158898      1.8476255E-04
** RECORD NO.101 CONTINUATION ** 0.1235487      2.3120297E-04
** RECORD NO.102 CONTINUATION ** 0.1353367      3.2389455E-04
** RECORD NO.103 CONTINUATION ** 0.1469308      4.5025381E-04
** RECORD NO.104 CONTINUATION ** 0.1605368      6.2307407E-04
** RECORD NO.105 CONTINUATION ** 0.1727560      8.4113551E-04
** RECORD NO.106 CONTINUATION ** 0.1834112      1.0740440E-03

```

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** RECORD NO.107 CONTINUATION ** 0.1976358      1.4568017E-03
** RECORD NO.108 CONTINUATION ** 0.2128803      1.9337797E-03
** RECORD NO.109 CONTINUATION ** 0.2325100      2.6850651E-03
** RECORD NO.110 CONTINUATION ** 0.2513601      3.6147104E-03
** RECORD NO.111 CONTINUATION ** 0.2720189      4.8591187E-03
** RECORD NO.112 CONTINUATION ** 0.2932921      6.4320280E-03
** RECORD NO.113 CONTINUATION ** 0.3145333      8.8765090E-03
** RECORD NO.114 CONTINUATION ** 0.3382721      1.0945584E-02
** RECORD NO.115 CONTINUATION ** 0.3745096      1.6480954E-02
** RECORD NO.116 CONTINUATION ** 0.4099776      2.3764918E-02
** RECORD NO.117 CONTINUATION ** 0.4346914      3.0411992E-02
** RECORD NO.118 CONTINUATION ** 0.4649854      4.1216791E-02
** RECORD NO.119 CONTINUATION ** 0.4921043      5.3159826E-02
** RECORD NO.120 CONTINUATION ** 0.5284358      7.0962466E-02
** RECORD NO.121 CONTINUATION ** 0.5603907      8.9725994E-02
** RECORD NO.122 CONTINUATION ** 0.5861617      0.1074519
** RECORD NO.123 CONTINUATION ** 0.6265295      0.1399627
** RECORD NO.124 CONTINUATION ** 0.6709072      0.1840404
** RECORD NO.125 CONTINUATION ** 0.7097058      0.2285040
** RECORD NO.126 CONTINUATION ** 0.7667013      0.3148932
** RECORD NO.127 CONTINUATION ** 0.8078989      0.3984839
** RECORD NO.128 CONTINUATION ** 0.8479097      0.4877611
** RECORD NO.129 CONTINUATION ** 0.8887257      0.5991479
** RECORD NO.130 CONTINUATION ** 0.9241478      0.7079301
** RECORD NO.131 CONTINUATION ** 0.9517682      0.8032593
** RECORD NO.132 CONTINUATION ** 0.9767836      0.9043072
** RECORD NO.133 CONTINUATION ** 0.9963999      0.9868676
** RECORD NO.134 COMMENT ***** /
** RECORD NO.135 COMMENT ***** /-----
** RECORD NO.136 KEYWORD ***** CONVERGENCE CRITERIA FOR P: MODE 2; VALUE=0.001  MAX ITERATIONS = 20
** RECORD NO.137 COMMENT ***** /-----
** RECORD NO.138 COMMENT ***** /
** RECORD NO.139 COMMENT ***** /-----
** RECORD NO.140 KEYWORD ***** INITIAL P -30. EVERYWHERE FROM (1,1,1) TO (24,3,16)
** RECORD NO.141 COMMENT ***** *      MODE 1: GRADX=0, GRADY=0, GRADZ=1
** RECORD NO.142 COMMENT ***** /-----
** RECORD NO.143 COMMENT ***** /
** RECORD NO.144 COMMENT ***** /-----
** RECORD NO.145 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX +1 (RIGHT BOUNDARY), TYPE 2
** RECORD NO.146 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX -2 (FRONT BOUNDARY), TYPE 2
** RECORD NO.147 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX +2 (BACK BOUNDARY), TYPE 2
** RECORD NO.148 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX +3 (TOP BOUNDARY) , TYPE 2
** RECORD NO.149 COMMENT ***** *      WITH FLUX = -10.35 cm/DAY
** RECORD NO.150 KEYWORD ***** BOUNDARY CONDITIONS FOR P: INDEX -3 (BOTTOM BOUNDARY), TYPE 2
** RECORD NO.151 COMMENT ***** /-----
** RECORD NO.152 COMMENT ***** /
** RECORD NO.153 KEYWORD ***** REFERENCE POINT AT (2,2,9)
** RECORD NO.154 COMMENT ***** /
** RECORD NO.155 KEYWORD ***** WINDOW FROM (1,2,1) TO (100,2,100) FOR OUTPUT
** RECORD NO.156 KEYWORD ***** OUTPUT P NOW IN XZ PLANE
** RECORD NO.157 COMMENT ***** /
** RECORD NO.158 KEYWORD ***** MATRIX SWEEP IN Z DIRECTION P=1

```

** RECORD NO.169 KEYWORD ***** SOLVE UNTIL TIME = 0.01 DAYS IN STEP OF 0.001 DAY

SHLOMO'S CASE 2 - VERTICAL INFILTRATION

GRID DIMENSIONS.....(IMAX,JMAX,KMAX) = 24 BY 3 BY 18
MAXIMUM NUMBER OF NODES IN EACH 3-D ARRAY. = 1800
NUMBER OF THREE DIMENSIONAL FIELD ARRAYS.. = 23
FIELD LENGTH ALLOCATED FOR 3-D ARRAYS..... = 143.8 Kbyte
FIELD LENGTH ACTUALLY USED FOR 3-D ARRAYS. = 103.5 Kbyte

X COORDINATE VALUES

=====

-4.49 4.49 13.48 23.37 34.25 46.21 59.37 73.84

89.77 107.28 126.55 147.74 171.06 196.70 224.91 255.94

290.07 327.02 368.92 414.35 464.33 519.30 579.77 640.23

Y COORDINATE VALUES

=====

-50.00 50.00 150.00

Z COORDINATE VALUES

=====

-122.0000-100.0421 -94.0842 -81.5221 -70.2162 -60.0400 -50.8831 -42.6411

-35.2233 -28.5472 -22.5388 -17.1312 -12.2644 -7.8843 -3.9421 0.0000

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 1 =====

J=

3 1
2 1
1
I= 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K = 2 =====

J=

3 1
2 1
1
I= 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

ZONE IDENTIFIERS FOR THE FLOW FIELD AT PLANE K =16 =====

J=
 3 1
 2 1
 1
 I= 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

BOUNDING INDICES FOR ACTIVE ZONES

=====

ZONE#	LOWER BOUND	UPPER BOUND
1	(1, 1, 1)	(24, 3, 16)

 SHLOMO'S CASE 2 - VERTICAL INFILTRATION

PROGRAM CONSTANTS, PARAMETERS AND REFERENCE VALUES

=====

CARTESIAN/RADIAL GEDMETRY INDEX = 1
 Y/Z DIR. PERIODIC BOUNDARY INDEX = 0
 DENSITY OPTION INDEX..... = 0
 HYDRAULIC CONDUCTIVITY INDEX ... = 0
 PROPERTY CALCULATION MODE = 1

START TIME = 0.000E+00
 CURRENT VALUE OF MAX. TIME = 1.000E-02
 STARTING TIME STEP = 1.000E-03
 TIME STEP INCREMENT FACTOR = 1.000E+00
 MAXIMUM TIME STEP = 1.000E+30
 TOTAL VOLUME OF FLUID IN FIELD.. = 2.400E+08

HYDRAULIC PROPERTIES OF POROUS MEDIA

=====

ACTIVE ZONE #	SPECIFIC STORATIVITY	X-DIR. HYDRAULIC K	Y-DIR. HYDRAULIC K	Z-DIR. HYDRAULIC K
1	1.000E-07	5.584E+02	5.584E+02	5.584E+02

VALUES AT REFERENCE GRID NODE (2, 2, 9)

=====

U - X-DIR. VELOCITY COMPONENT = 0.000E+00
 V - Y-DIR. VELOCITY COMPONENT = 0.000E+00
 W - Z-DIR. VELOCITY COMPONENT = 0.000E+00
 P - PRESSURE OR PRESSURE HEAD = -3.000E+01
 THET- RELATIVE SATURATION LEVEL = 1.000E+00
 POR - MATRIX EFFECTIVE POROSITY. = 3.480E-01
 VOL - VOLUME OF GRID ELEMENTS... = 6.334E+03

DEPENDENT VARIABLE SPECIFICATIONS

```
=====
VARIABLE SYMBOL SOLVE OPTION INTEG. PROFILE # OF SWEEPS RELAX FACTOR
      1      P           1           1           1           1.00
```

MATRIX SWEEP DIRECTIONS: Z

----*--*--* P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 0, TIME= 0.0000E+00 --*--*--*--*--*--*--*

```
Z =      K =
0.000E+00 18 -3.00E+01 -3.00E+01
-3.942E+00 15 -3.00E+01 -3.00E+01
-7.884E+00 14 -3.00E+01 -3.00E+01
-1.228E+01 13 -3.00E+01 -3.00E+01
-1.713E+01 12 -3.00E+01 -3.00E+01
-2.254E+01 11 -3.00E+01 -3.00E+01
-2.855E+01 10 -3.00E+01 -3.00E+01
-3.522E+01 9 -3.00E+01 -3.00E+01
-4.264E+01 8 -3.00E+01 -3.00E+01
-5.088E+01 7 -3.00E+01 -3.00E+01
-6.004E+01 6 -3.00E+01 -3.00E+01
-7.022E+01 5 -3.00E+01 -3.00E+01
-8.152E+01 4 -3.00E+01 -3.00E+01
-9.408E+01 3 -3.00E+01 -3.00E+01
-1.080E+02 2 -3.00E+01 -3.00E+01
-1.220E+02 1 -3.00E+01 -3.00E+01
```

```
I =      1      2      3      4      5      6      7      8      9      10     11
X = -4.49E+00  4.49E+00  1.35E+01  2.34E+01  3.42E+01  4.62E+01  5.94E+01  7.38E+01  8.98E+01  1.07E+02  1.27E+02
```

```
Z =      K =
0.000E+00 18 -3.00E+01 -3.00E+01
-3.942E+00 15 -3.00E+01 -3.00E+01
-7.884E+00 14 -3.00E+01 -3.00E+01
-1.228E+01 13 -3.00E+01 -3.00E+01
-1.713E+01 12 -3.00E+01 -3.00E+01
-2.254E+01 11 -3.00E+01 -3.00E+01
-2.855E+01 10 -3.00E+01 -3.00E+01
-3.522E+01 9 -3.00E+01 -3.00E+01
-4.264E+01 8 -3.00E+01 -3.00E+01
-5.088E+01 7 -3.00E+01 -3.00E+01
-6.004E+01 6 -3.00E+01 -3.00E+01
-7.022E+01 5 -3.00E+01 -3.00E+01
-8.152E+01 4 -3.00E+01 -3.00E+01
```

WHC-EP-0041

-9.488E+01 3 -3.00E+01
 -1.088E+02 2 -3.00E+01
 -1.220E+02 1 -3.00E+01 -3.00E+01

I = 12 13 14 15 16 17 18 19 20 21 22
 X = 1.48E+02 1.71E+02 1.97E+02 2.26E+02 2.56E+02 2.90E+02 3.28E+02 3.69E+02 4.14E+02 4.64E+02 5.19E+02

Z = K =
 0.000E+00 16 -3.00E+01 -3.00E+01
 -3.942E+00 15 -3.00E+01 -3.00E+01
 -7.884E+00 14 -3.00E+01 -3.00E+01
 -1.228E+01 13 -3.00E+01 -3.00E+01
 -1.713E+01 12 -3.00E+01 -3.00E+01
 -2.254E+01 11 -3.00E+01 -3.00E+01
 -2.855E+01 10 -3.00E+01 -3.00E+01
 -3.522E+01 9 -3.00E+01 -3.00E+01
 -4.264E+01 8 -3.00E+01 -3.00E+01
 -5.088E+01 7 -3.00E+01 -3.00E+01
 -6.004E+01 6 -3.00E+01 -3.00E+01
 -7.022E+01 5 -3.00E+01 -3.00E+01
 -8.152E+01 4 -3.00E+01 -3.00E+01
 -9.488E+01 3 -3.00E+01 -3.00E+01
 -1.088E+02 2 -3.00E+01 -3.00E+01
 -1.220E+02 1 -3.00E+01 -3.00E+01

I = 23 24
 X = 5.80E+02 6.40E+02

STEP NO.	TIME	[-----REFERENCE VALUES AT NODE (2, 2, 9)-----]						[CONVERGENCE RATE / RESIDUALS]		
		U	V	W	P	T	C	PRESSURE	REF. VAR.	INDEX
0	0.00E+00	0.000E+00	0.000E+00	0.000E+00	-3.000E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.0
1	1.00E-03	0.000E+00	0.000E+00	-2.861E-04	-3.000E+01	0.000E+00	0.000E+00	2.265E-06	2.265E-06	0.0
2	2.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	1.192E-06	1.192E-06	0.0
3	3.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
4	4.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
5	5.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	8.345E-07	8.345E-07	0.0
6	6.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
7	7.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
8	8.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
9	9.00E-03	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
10	1.00E-02	1.181E-04	0.000E+00	-1.431E-04	-3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0

** RECORD NO.160 KEYWORD ***** OUTPUT U,W,P,THETA in xz plane ==> RIGHT NOW

WHC-EP-0041

```

***--***--** U - X-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 10, TIME= 1.0000E-02 ***--***--***--***--***
Z = K =
0.000E+00 16 0.00E+00 1.87E-08 -1.81E-08 1.84E-08 -1.41E-08 -3.20E-09 2.18E-09 -8.61E-10 6.01E-10 -1.09E-09 4.97E-10
-3.942E+00 15 0.00E+00 1.87E-08 -1.81E-08 1.84E-08 -1.41E-08 -3.20E-09 2.18E-09 -8.61E-10 6.01E-10 -1.09E-09 4.97E-10
-7.884E+00 14 3.05E-08 -3.05E-08 -1.92E-08 2.03E-08 -8.16E-09 3.20E-09 7.27E-10 6.61E-10 -1.80E-09 -1.04E-08 3.97E-09
-1.228E+01 13 1.64E-08 -1.76E-08 1.06E-09 9.68E-10 -3.52E-09 2.40E-09 3.64E-09 -3.31E-09 6.01E-10 0.00E+00 -4.97E-10
-1.713E+01 12 2.34E-09 1.76E-08 -1.49E-08 -2.90E-09 8.80E-10 0.00E+00 7.27E-10 -1.32E-09 1.56E-08 -1.42E-08 -4.97E-10
-2.254E+01 11 -3.51E-09 -1.52E-08 1.60E-08 9.68E-10 -1.41E-08 1.60E-09 2.33E-08 -1.32E-08 9.02E-09 -1.26E-08 4.97E-09
-2.855E+01 10 2.34E-09 -3.51E-09 0.00E+00 3.87E-09 -5.28E-09 2.40E-09 -4.36E-09 -3.31E-09 -1.80E-09 -2.19E-09 2.98E-09
-3.522E+01 9 1.18E-04 1.18E-04 -1.07E-04 -2.93E-04 -2.68E-04 -2.42E-04 0.00E+00 -3.33E-04 -4.24E-04 1.10E-04 -1.00E-04
-4.264E+01 8 2.36E-04 -1.18E-04 0.00E+00 -2.93E-04 -3.55E-04 -2.42E-04 7.33E-05 -2.67E-04 -4.85E-04 1.65E-04 -5.01E-05
-5.088E+01 7 1.18E-04 0.00E+00 -1.07E-04 -2.93E-04 -1.77E-04 -1.61E-04 -7.33E-05 -3.33E-04 -2.42E-04 5.51E-05 -5.01E-05
-6.004E+01 6 1.18E-04 -1.18E-04 -1.07E-04 -2.93E-04 0.00E+00 -1.61E-04 -1.47E-04 -2.00E-04 -6.06E-05 -1.10E-04 -2.50E-04
-7.022E+01 5 0.00E+00 0.00E+00 -1.07E-04 -3.90E-04 0.00E+00 -2.42E-04 -7.33E-05 -1.33E-04 0.00E+00 -1.10E-04 -4.01E-04
-8.152E+01 4 2.36E-04 0.00E+00 -1.07E-04 -3.90E-04 -1.77E-04 -1.61E-04 -7.33E-05 -6.66E-05 -1.82E-04 -5.51E-05 -2.50E-04
-9.408E+01 3 0.00E+00 0.00E+00 -1.07E-04 -1.95E-04 -8.87E-05 -1.61E-04 -1.47E-04 -2.00E-04 -6.06E-05 -5.51E-05 -1.50E-04
-1.080E+02 2 0.00E+00 0.00E+00 -2.15E-04 -1.95E-04 -8.87E-05 -1.61E-04 -7.33E-05 -2.00E-04 -1.21E-04 -1.10E-04 -5.01E-05
-1.220E+02 1 0.00E+00 0.00E+00 -2.15E-04 -1.95E-04 -8.87E-05 -1.61E-04 -7.33E-05 -2.00E-04 -1.21E-04 -1.10E-04 -5.01E-05

I = 2 3 4 5 6 7 8 9 10 11 12
X = 0.00E+00 8.99E+00 1.84E+01 2.88E+01 4.02E+01 5.28E+01 6.66E+01 8.18E+01 9.85E+01 1.17E+02 1.37E+02

Z = K =
0.000E+00 16 0.00E+00 -4.11E-10 -4.11E-09 6.45E-09 -1.23E-09 -8.41E-10 0.00E+00 2.32E-10 -4.21E-10 3.83E-10 -3.48E-10
-3.942E+00 15 0.00E+00 -4.11E-10 -4.11E-09 6.45E-09 -1.23E-09 -8.41E-10 0.00E+00 2.32E-10 -4.21E-10 3.83E-10 -3.48E-10
-7.884E+00 14 8.58E-09 -3.28E-09 -3.36E-09 9.16E-09 -1.30E-08 6.17E-09 5.10E-10 3.48E-09 -2.74E-09 -9.58E-10 -6.97E-10
-1.228E+01 13 4.52E-10 -4.11E-10 -7.47E-10 1.36E-09 3.70E-09 0.00E+00 -3.31E-09 2.55E-09 -2.53E-09 4.21E-09 -4.18
-1.713E+01 12 4.52E-10 4.11E-10 0.00E+00 4.75E-09 -4.32E-09 3.93E-09 -3.42E-09 2.32E-09 -5.48E-09 2.87E-09 5.22
-2.254E+01 11 -7.23E-09 6.98E-09 -3.73E-10 -3.39E-10 3.08E-10 -6.45E-09 5.86E-09 -4.64E-10 2.11E-10 0.00E+00 -3.48E-10
-2.855E+01 10 4.52E-10 2.05E-09 -3.73E-09 -1.02E-09 -2.78E-09 -1.96E-09 -2.80E-09 -4.64E-10 -2.11E-10 -4.41E-09 2.09E-09
-3.522E+01 9 -1.37E-04 4.14E-05 -3.39E-04 -1.03E-04 -3.42E-04 -3.39E-04 -2.83E-04 -1.87E-04 -1.27E-04 -4.44E-04 2.63E-04
-4.264E+01 8 -3.19E-04 1.24E-04 -3.39E-04 -1.03E-04 -3.73E-04 -3.11E-04 -2.57E-04 -2.10E-04 -1.70E-04 -4.25E-04 2.81E-04
-5.088E+01 7 -3.19E-04 4.14E-05 -2.26E-04 -2.05E-04 -3.73E-04 -2.83E-04 -2.31E-04 -1.64E-04 -2.76E-04 -4.83E-04 3.16E-04
-6.004E+01 6 -2.73E-04 -4.14E-05 -1.88E-04 -1.71E-04 -2.80E-04 -3.96E-04 -1.28E-04 -1.87E-04 -3.19E-04 -5.79E-04 3.51E-04
-7.022E+01 5 -1.82E-04 -1.24E-04 -7.52E-05 -1.71E-04 -2.49E-04 -5.09E-04 -1.03E-04 -1.87E-04 -3.61E-04 -5.79E-04 3.51E-04
-8.152E+01 4 -2.28E-04 -8.28E-05 -1.50E-04 -1.71E-04 -3.73E-04 -3.96E-04 -1.80E-04 -1.17E-04 -4.25E-04 -6.18E-04 4.21E-04
-9.408E+01 3 -1.37E-04 -4.14E-05 -2.26E-04 -2.05E-04 -4.97E-04 -3.67E-04 -1.80E-04 -7.01E-05 -4.67E-04 -5.79E-04 3.86E-04
-1.080E+02 2 -4.55E-05 -8.28E-05 -1.50E-04 -2.39E-04 -4.66E-04 -5.09E-04 -7.71E-05 -1.40E-04 -4.46E-04 -5.60E-04 3.33E-04
-1.220E+02 1 -4.55E-05 -8.28E-05 -1.50E-04 -2.39E-04 -4.66E-04 -5.09E-04 -7.71E-05 -1.40E-04 -4.46E-04 -5.60E-04 3.33E-04

I = 13 14 15 16 17 18 19 20 21 22 23
X = 1.59E+02 1.84E+02 2.11E+02 2.40E+02 2.73E+02 3.09E+02 3.48E+02 3.92E+02 4.39E+02 4.92E+02 5.50E+02

Z = K =
0.000E+00 16 0.00E+00
-3.942E+00 15 0.00E+00
-7.884E+00 14 0.00E+00
-1.228E+01 13 0.00E+00
-1.713E+01 12 0.00E+00
-2.254E+01 11 0.00E+00
-2.855E+01 10 0.00E+00
-3.522E+01 9 0.00E+00

```


-1.713E+01	12	-3.00E+01											
-2.254E+01	11	-3.00E+01											
-2.855E+01	10	-3.00E+01											
-3.522E+01	9	-3.00E+01											
-4.264E+01	8	-3.00E+01											
-5.088E+01	7	-3.00E+01											
-6.004E+01	6	-3.00E+01											
-7.022E+01	5	-3.00E+01											
-8.152E+01	4	-3.00E+01											
-9.408E+01	3	-3.00E+01											
-1.080E+02	2	-3.00E+01											
-1.220E+02	1	-3.00E+01											

I =	12	13	14	15	16	17	18	19	20	21	22
X =	1.48E+02	1.71E+02	1.97E+02	2.25E+02	2.58E+02	2.90E+02	3.28E+02	3.69E+02	4.14E+02	4.64E+02	5.19E+02

Z =	K =		
0.000E+00	16	-3.00E+01	-3.00E+01
-3.942E+00	15	-3.00E+01	-3.00E+01
-7.884E+00	14	-3.00E+01	-3.00E+01
-1.228E+01	13	-3.00E+01	-3.00E+01
-1.713E+01	12	-3.00E+01	-3.00E+01
-2.254E+01	11	-3.00E+01	-3.00E+01
-2.855E+01	10	-3.00E+01	-3.00E+01
-3.522E+01	9	-3.00E+01	-3.00E+01
-4.264E+01	8	-3.00E+01	-3.00E+01
-5.088E+01	7	-3.00E+01	-3.00E+01
-6.004E+01	6	-3.00E+01	-3.00E+01
-7.022E+01	5	-3.00E+01	-3.00E+01
-8.152E+01	4	-3.00E+01	-3.00E+01
-9.408E+01	3	-3.00E+01	-3.00E+01
-1.080E+02	2	-3.00E+01	-3.00E+01
-1.220E+02	1	-3.00E+01	-3.00E+01

I =	23	24
X =	5.80E+02	6.40E+02

----*--*-- THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 10, TIME= 1.0000E-02 --*--*--*--*--*--*--*

Z =	K =												
0.000E+00	16	0.00E+00											
-3.942E+00	15	0.00E+00											
-7.884E+00	14	0.00E+00											
-1.228E+01	13	0.00E+00											
-1.713E+01	12	0.00E+00											

WHC-EP-0041

-2.254E+01	11	0.00E+00										
-2.855E+01	10	0.00E+00										
-3.522E+01	9	1.00E+00										
-4.264E+01	8	1.00E+00										
-5.088E+01	7	1.00E+00										
-6.004E+01	6	1.00E+00										
-7.022E+01	5	1.00E+00										
-8.152E+01	4	1.00E+00										
-9.408E+01	3	1.00E+00										
-1.080E+02	2	1.00E+00										
-1.220E+02	1	1.00E+00										

I =	1	2	3	4	5	6	7	8	9	10	11
X =	-4.49E+00	4.49E+00	1.35E+01	2.34E+01	3.42E+01	4.62E+01	5.94E+01	7.38E+01	8.98E+01	1.07E+02	1.27E+02

Z =	K =	0.00E+00										
-3.942E+00	15	0.00E+00										
-7.884E+00	14	0.00E+00										
-1.228E+01	13	0.00E+00										
-1.713E+01	12	0.00E+00										
-2.254E+01	11	0.00E+00										
-2.855E+01	10	0.00E+00										
-3.522E+01	9	1.00E+00										
-4.264E+01	8	1.00E+00										
-5.088E+01	7	1.00E+00										
-6.004E+01	6	1.00E+00										
-7.022E+01	5	1.00E+00										
-8.152E+01	4	1.00E+00										
-9.408E+01	3	1.00E+00										
-1.080E+02	2	1.00E+00										
-1.220E+02	1	1.00E+00										

I =	12	13	14	15	16	17	18	19	20	21	22
X =	1.48E+02	1.71E+02	1.97E+02	2.25E+02	2.56E+02	2.90E+02	3.28E+02	3.69E+02	4.14E+02	4.64E+02	5.19E+02

Z =	K =	0.00E+00	0.00E+00
-3.942E+00	15	0.00E+00	0.00E+00
-7.884E+00	14	0.00E+00	0.00E+00
-1.228E+01	13	0.00E+00	0.00E+00
-1.713E+01	12	0.00E+00	0.00E+00
-2.254E+01	11	0.00E+00	0.00E+00
-2.855E+01	10	0.00E+00	0.00E+00
-3.522E+01	9	1.00E+00	1.00E+00
-4.264E+01	8	1.00E+00	1.00E+00
-5.088E+01	7	1.00E+00	1.00E+00
-6.004E+01	6	1.00E+00	1.00E+00
-7.022E+01	5	1.00E+00	1.00E+00
-8.152E+01	4	1.00E+00	1.00E+00
-9.408E+01	3	1.00E+00	1.00E+00
-1.080E+02	2	1.00E+00	1.00E+00

-1.220E+02 1 1.00E+00 1.00E+00
 I = 23 24
 X = 5.80E+02 6.40E+02

```
*****
STEP          [-----REFERENCE VALUES AT NODE ( 2, 2, 9)-----] [CONVERGENCE RATE / RESIDUALS]
NO.    TIME      U        V        W        P        T        C        PRESSURE REF. VAR.    INDEX
10  1.00E-02  1.181E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  7.153E-07 7.153E-07  0.0
** RECORD NO.161 KEYWORD ***** SAVE NOW ON 'SHLOWM12.PLT'
** RECORD NO.162 COMMENT ***** /
```

=====> UNIT 2 OPEN FOR I/O IN UNFORMATTED MODE; FILE NAME: SHLOWM12.PLT

<---- START OF ARCHIVE READ/WRITE OPERATIONS ---->

CREATED BY PROGRAM : PORFLOW-3D - VERSION 1.00: DATED: 16 OCT 1988
 DATA CREATED BY USER (ID) ... : WHC - JDD - DATE OF ARCHIVED RECORDS : 1/24/1989
 TIME OF CREATION OF RECORDS . : 16:59:24
 TITLE OF THE ARCHIVED DATA SET: SHLOWM'S CASE 2 - VERTICAL INFILTRATION
 SIMULATION TIME OF STORED DATA: 1.000E-02
 STEP NUMBER AT WHICH GENERATED: 10
 GRID DIMENSIONS OF STORED DATA: 24 BY 3 BY 16

- > WRITING VARIABLE: U - X-DIR. VELOCITY COMPONENT
- > WRITING VARIABLE: V - Y-DIR. VELOCITY COMPONENT
- > WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT
- > WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD
- > WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 1 WRITTEN TO ARCHIVES ---->

```
10  1.00E-02  1.181E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  7.153E-07 7.153E-07  0.0
** RECORD NO.163 KEYWORD ***** SOLVE UNTIL TIME = 1.00 DAYS IN STEP OF 0.0005 DAY INCREASE BY 1.1, MAX =0.05
10  1.00E-02  1.181E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  7.153E-07 7.153E-07  0.0
11  1.05E-02  1.181E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.192E-06 1.192E-06  0.0
12  1.10E-02  2.361E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  1.550E-06 1.550E-06  0.0
13  1.17E-02  2.361E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
14  1.23E-02  -1.181E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.788E-06 1.788E-06  0.0
15  1.31E-02  1.181E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  2.027E-06 2.027E-06  0.0
16  1.39E-02  1.181E-04  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  9.537E-07 9.537E-07  0.0
17  1.47E-02  2.361E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
18  1.57E-02  -1.181E-04  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  8.345E-07 8.345E-07  0.0
19  1.68E-02  1.181E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
20  1.80E-02  0.000E+00  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
21  1.93E-02  -2.361E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.669E-06 1.669E-06  0.0
22  2.07E-02  0.000E+00  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.311E-06 1.311E-06  0.0
23  2.23E-02  -2.361E-04  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.073E-06 1.073E-06  0.0
```

24	2.40E-02	-1.181E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
25	2.59E-02	1.181E-04	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	2.027E-06	2.027E-06	0.0
26	2.80E-02	0.000E+00	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	1.311E-06	1.311E-06	0.0
27	3.03E-02	0.000E+00	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	1.669E-06	1.669E-06	0.0
28	3.28E-02	-2.361E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.192E-06	1.192E-06	0.0
29	3.56E-02	0.000E+00	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.431E-06	1.431E-06	0.0
30	3.86E-02	-1.181E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	8.941E-07	8.941E-07	0.0
31	4.20E-02	-3.542E-04	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	1.073E-06	1.073E-06	0.0
32	4.57E-02	-3.542E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	9.537E-07	9.537E-07	0.0
33	4.98E-02	-3.542E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.431E-06	1.431E-06	0.0
34	5.42E-02	-2.361E-04	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	1.550E-06	1.550E-06	0.0
35	5.92E-02	-2.361E-04	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
36	6.46E-02	-3.542E-04	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	2.503E-06	2.503E-06	0.0
37	7.05E-02	-5.904E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.073E-06	1.073E-06	0.0
38	7.71E-02	-4.723E-04	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
39	8.43E-02	-4.723E-04	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	8.345E-07	8.345E-07	0.0
40	9.22E-02	-4.723E-04	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
41	1.01E-01	-4.723E-04	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	1.311E-06	1.311E-06	0.0
42	1.11E-01	-4.723E-04	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	6.557E-07	6.557E-07	0.0
43	1.21E-01	-5.904E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	8.941E-07	8.941E-07	0.0
44	1.33E-01	-3.542E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.490E-06	1.490E-06	0.0
45	1.46E-01	-3.542E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.550E-06	1.550E-06	0.0
46	1.60E-01	-5.904E-04	0.000E+00	1.431E-04	3.000E+01	0.000E+00	0.000E+00	8.345E-07	8.345E-07	0.0
47	1.75E-01	-4.723E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.788E-06	1.788E-06	0.0
48	1.92E-01	-5.904E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	2.384E-06	2.384E-06	0.0
49	2.11E-01	-5.904E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.311E-06	1.311E-06	0.0
50	2.31E-01	-8.265E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.192E-06	1.192E-06	0.0
51	2.54E-01	-9.440E-04	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
52	2.79E-01	-7.084E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	8.345E-07	8.345E-07	0.0
53	3.06E-01	-7.084E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.550E-06	1.550E-06	0.0
54	3.36E-01	-7.084E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.192E-06	1.192E-06	0.0
55	3.69E-01	-7.084E-04	0.000E+00	0.000E+00	3.000E+01	0.000E+00	0.000E+00	1.013E-06	1.013E-06	0.0
56	4.06E-01	-8.265E-04	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	1.311E-06	1.311E-06	0.0
57	4.46E-01	-9.440E-04	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	8.345E-07	8.345E-07	0.0
58	4.90E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
59	5.39E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
60	5.89E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	8.345E-07	8.345E-07	0.0
61	6.39E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
62	6.89E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	7.153E-07	7.153E-07	0.0
63	7.39E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
64	7.89E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
65	8.39E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
66	8.89E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
67	9.39E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
68	9.89E-01	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	5.960E-07	5.960E-07	0.0
69	1.01E+00	-1.063E-03	0.000E+00	-1.431E-04	3.000E+01	0.000E+00	0.000E+00	1.431E-06	1.431E-06	0.0

** RECORD NO.164 KEYWORD ***** OUTPUT NOW

WHC-EP-0041

-4.264E+01 8 0.00E+00
 -6.088E+01 7 0.00E+00
 -8.004E+01 6 0.00E+00
 -7.022E+01 5 0.00E+00
 -8.152E+01 4 0.00E+00
 -9.408E+01 3 0.00E+00
 -1.080E+02 2 0.00E+00
 -1.220E+02 1 0.00E+00

I = 24
 X = 6.10E+02

----*--*--* W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 09, TIME= 1.0100E+00 *--*--*--*--*--*--*--*--*

Z =	K =	1	2	3	4	5	6	7	8	9	10	11
-1.971E+00	16	5.34E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
-5.913E+00	15	0.00E+00	1.07E-08	1.07E-08	-3.74E-08	2.67E-09	-1.34E-08	8.01E-09	-2.14E-08	-8.01E-09	-2.40E-08	2.67E-09
-1.007E+01	14	0.00E+00	-1.92E-08	-2.64E-08	-1.88E-08	4.81E-09	1.20E-08	-2.40E-09	-2.40E-09	0.00E+00	-2.40E-08	1.44E-08
-1.470E+01	13	0.00E+00	3.48E-08	8.65E-09	6.49E-09	1.51E-08	6.49E-09	4.33E-09	1.73E-08	3.25E-08	5.41E-08	2.16E-08
-1.984E+01	12	0.00E+00	3.89E-09	3.50E-08	1.38E-08	9.74E-09	0.00E+00	4.48E-08	2.53E-08	3.50E-08	7.20E-08	6.04E-08
-2.554E+01	11	0.00E+00	-5.28E-09	-5.28E-09	2.83E-08	5.08E-08	6.83E-08	7.89E-08	1.31E-07	1.40E-07	1.45E-07	1.63E-07
-3.189E+01	10	0.00E+00	1.00E-08	5.01E-07	-1.00E-08	1.00E-08	-5.01E-07	1.00E-08	0.00E+00	0.00E+00	0.00E+00	1.00E-08
-3.893E+01	9	0.00E+00	-1.43E-04	1.43E-04	0.00E+00	0.00E+00	1.43E-04	0.00E+00	-1.43E-04	-2.86E-04	1.43E-04	0.00E+00
-4.876E+01	8	0.00E+00	0.00E+00	0.00E+00	1.29E-04	0.00E+00	-3.86E-04	-3.86E-04	1.29E-04	3.86E-04	-5.15E-04	-3.86E-04
-5.546E+01	7	0.00E+00	-2.32E-04	0.00E+00	1.18E-04	0.00E+00	0.00E+00	0.00E+00	1.18E-04	-1.18E-04	-4.84E-04	-1.18E-04
-6.513E+01	6	0.00E+00	1.04E-04	0.00E+00	0.00E+00	1.04E-04	2.09E-04	2.09E-04	1.04E-04	-2.09E-04	0.00E+00	-3.11E-04
-7.587E+01	5	0.00E+00	0.00E+00	9.39E-05	9.39E-05	0.00E+00	9.39E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.81E-05
-8.780E+01	4	0.00E+00	8.45E-05	0.00E+00	1.89E-04	2.53E-04	1.89E-04	0.00E+00	-8.45E-05	8.45E-05	-1.89E-04	8.45E-05
-1.011E+02	3	0.00E+00	7.60E-05	-7.60E-05	1.52E-04	7.60E-05	7.60E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.60E-05
-1.150E+02	2	3.04E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

I = 1 2 3 4 5 6 7 8 9 10 11
 X = -4.49E+00 4.49E+00 1.35E+01 2.34E+01 3.42E+01 4.82E+01 5.94E+01 7.38E+01 8.98E+01 1.07E+02 1.27E+02

Z =	K =	1	2	3	4	5	6	7	8	9	10	11
-1.971E+00	16	0.00E+00										
-5.913E+00	15	4.27E-08	-1.07E-08	-1.07E-08	5.34E-09	1.60E-08	-2.67E-09	-2.14E-08	1.60E-08	-3.74E-08	1.34E-08	2.67E-09
-1.007E+01	14	-1.88E-08	4.81E-09	4.57E-08	3.13E-08	2.40E-09	1.44E-08	3.13E-08	3.61E-08	2.16E-08	5.05E-08	3.85E-08
-1.470E+01	13	-6.49E-09	4.33E-08	2.81E-08	5.19E-08	4.90E-08	7.14E-08	1.02E-07	9.09E-08	7.57E-08	1.04E-07	1.23E-07
-1.984E+01	12	9.15E-08	1.27E-07	1.25E-07	1.23E-07	1.82E-07	1.46E-07	1.82E-07	1.87E-07	2.20E-07	2.26E-07	2.36E-07
-2.554E+01	11	1.80E-07	1.95E-07	2.28E-07	2.77E-07	3.01E-07	3.14E-07	3.40E-07	3.82E-07	4.40E-07	4.70E-07	5.34E-07
-3.189E+01	10	-1.50E-08	-5.01E-07	1.00E-08	1.00E-08	0.00E+00	1.00E-08	5.01E-07	1.50E-08	1.00E-08	2.00E-08	2.00E-08
-3.893E+01	9	-2.86E-04	2.86E-04	-1.43E-04	1.43E-04	1.43E-04	1.43E-04	1.43E-04	-1.43E-04	0.00E+00	1.43E-04	0.00E+00
-4.876E+01	8	0.00E+00	-1.29E-04	-1.29E-04	-2.58E-04	-1.29E-04	1.29E-04	0.00E+00	2.58E-04	-3.86E-04	-1.29E-04	3.86E-04
-5.546E+01	7	2.32E-04	1.18E-04	2.32E-04	0.00E+00	-1.18E-04	-2.32E-04	2.32E-04	-1.18E-04	-2.32E-04	-2.32E-04	4.84E-04
-6.513E+01	6	2.09E-04	-1.04E-04	2.09E-04	-3.13E-04	-1.04E-04	-2.09E-04	2.09E-04	0.00E+00	0.00E+00	0.00E+00	1.04E-04
-7.587E+01	5	-2.82E-04	-1.88E-04	-3.75E-04	-9.39E-05	-9.39E-05	9.39E-05	0.00E+00	9.39E-05	0.00E+00	-9.39E-05	-9.39E-05
-8.780E+01	4	-2.53E-04	-2.53E-04	-4.22E-04	-5.07E-04	-1.89E-04	8.45E-05	-1.89E-04	1.89E-04	8.45E-05	-1.89E-04	-3.86E-04
-1.011E+02	3	0.00E+00	-7.60E-05	-7.60E-05	-3.04E-04	-3.04E-04	-1.52E-04	1.52E-04	0.00E+00	1.52E-04	-1.52E-04	-7.60E-05
-1.150E+02	2	0.00E+00										

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I = 12 13 14 15 16 17 18 19 20 21 22
 X = 1.48E+02 1.71E+02 1.97E+02 2.26E+02 2.56E+02 2.90E+02 3.28E+02 3.69E+02 4.14E+02 4.64E+02 5.19E+02

Z = K =
 -1.971E+00 16 0.00E+00 0.00E+00
 -5.913E+00 15 -8.01E-09 -8.01E-09
 -1.007E+01 14 1.20E-08 1.20E-08
 -1.470E+01 13 9.30E-08 9.30E-08
 -1.984E+01 12 2.45E-07 2.45E-07
 -2.554E+01 11 5.10E-07 5.10E-07
 -3.189E+01 10 1.50E-06 1.50E-06
 -3.893E+01 9 0.00E+00 0.00E+00
 -4.678E+01 8 5.15E-04 5.15E-04
 -5.548E+01 7 3.48E-04 3.48E-04
 -6.513E+01 6 4.17E-04 4.17E-04
 -7.587E+01 5 0.00E+00 0.00E+00
 -8.780E+01 4 -8.45E-05 -8.45E-05
 -1.011E+02 3 0.00E+00 0.00E+00
 -1.150E+02 2 0.00E+00 0.00E+00

I = 23 24
 X = 5.80E+02 6.40E+02

----*--*--* P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 09, TIME= 1.0100E+00 --*--*--*--*--*--*--*

Z = K =
 0.000E+00 18 -3.00E+01
 -3.942E+00 15 -3.00E+01
 -7.884E+00 14 -3.00E+01
 -1.226E+01 13 -3.00E+01
 -1.713E+01 12 -3.00E+01
 -2.254E+01 11 -3.00E+01
 -2.855E+01 10 -3.00E+01
 -3.522E+01 9 -3.00E+01
 -4.264E+01 8 -3.00E+01
 -5.088E+01 7 -3.00E+01
 -6.004E+01 6 -3.00E+01
 -7.022E+01 5 -3.00E+01
 -8.152E+01 4 -3.00E+01
 -9.408E+01 3 -3.00E+01
 -1.080E+02 2 -3.00E+01
 -1.220E+02 1 -3.00E+01 -3.00E+01

I = 1 2 3 4 5 6 7 8 9 10 11
 X = -4.49E+00 4.49E+00 1.35E+01 2.34E+01 3.42E+01 4.62E+01 5.94E+01 7.38E+01 8.98E+01 1.07E+02 1.27E+02

Z = K =
 0.000E+00 16 -3.00E+01
 -3.942E+00 15 -3.00E+01
 -7.884E+00 14 -3.00E+01
 -1.226E+01 13 -3.00E+01 -3.00E+01

-1.713E+01	12	-3.00E+01	-3.00									
-2.254E+01	11	-3.00E+01	-3.00									
-2.855E+01	10	-3.00E+01										
-3.522E+01	9	-3.00E+01										
-4.284E+01	8	-3.00E+01										
-5.088E+01	7	-3.00E+01										
-6.004E+01	6	-3.00E+01										
-7.022E+01	5	-3.00E+01										
-8.152E+01	4	-3.00E+01										
-9.408E+01	3	-3.00E+01										
-1.080E+02	2	-3.00E+01										
-1.220E+02	1	-3.00E+01										

I = 12 13 14 15 16 17 18 19 20 21 22
X = 1.48E+02 1.71E+02 1.97E+02 2.25E+02 2.58E+02 2.90E+02 3.28E+02 3.89E+02 4.14E+02 4.64E+02 5.19E+02

Z = K =
0.000E+00 16 -3.00E+01 -3.00E+01
-3.942E+00 15 -3.00E+01 -3.00E+01
-7.884E+00 14 -3.00E+01 -3.00E+01
-1.228E+01 13 -3.00E+01 -3.00E+01
-1.713E+01 12 -3.00E+01 -3.00E+01
-2.254E+01 11 -3.00E+01 -3.00E+01
-2.855E+01 10 -3.00E+01 -3.00E+01
-3.522E+01 9 -3.00E+01 -3.00E+01
-4.284E+01 8 -3.00E+01 -3.00E+01
-5.088E+01 7 -3.00E+01 -3.00E+01
-6.004E+01 6 -3.00E+01 -3.00E+01
-7.022E+01 5 -3.00E+01 -3.00E+01
-8.152E+01 4 -3.00E+01 -3.00E+01
-9.408E+01 3 -3.00E+01 -3.00E+01
-1.080E+02 2 -3.00E+01 -3.00E+01
-1.220E+02 1 -3.00E+01 -3.00E+01

I = 23 24
X = 5.80E+02 6.40E+02

--*-*-* THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 69, TIME= 1.0100E+00 -*-*-*-*-*

Z = K =
0.000E+00 16 0.00E+00
-3.942E+00 15 0.00E+00
-7.884E+00 14 0.00E+00
-1.228E+01 13 0.00E+00
-1.713E+01 12 0.00E+00 0.00E+00

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-2.254E+01	11	0.00E+00										
-2.855E+01	10	0.00E+00										
-3.522E+01	9	1.00E+00										
-4.264E+01	8	1.00E+00										
-5.088E+01	7	1.00E+00										
-6.004E+01	6	1.00E+00										
-7.022E+01	5	1.00E+00										
-8.152E+01	4	1.00E+00										
-9.408E+01	3	1.00E+00										
-1.080E+02	2	1.00E+00										
-1.220E+02	1	1.00E+00										

I =	1	2	3	4	5	6	7	8	9	10	11
X =	-4.49E+00	4.49E+00	1.35E+01	2.34E+01	3.42E+01	4.62E+01	5.94E+01	7.38E+01	8.98E+01	1.07E+02	1.27E+02

Z =	K =	0.00E+00										
-3.942E+00	15	0.00E+00										
-7.884E+00	14	0.00E+00										
-1.228E+01	13	0.00E+00										
-1.713E+01	12	0.00E+00										
-2.254E+01	11	0.00E+00										
-2.855E+01	10	0.00E+00										
-3.522E+01	9	1.00E+00										
-4.264E+01	8	1.00E+00										
-5.088E+01	7	1.00E+00										
-6.004E+01	6	1.00E+00										
-7.022E+01	5	1.00E+00										
-8.152E+01	4	1.00E+00										
-9.408E+01	3	1.00E+00										
-1.080E+02	2	1.00E+00										
-1.220E+02	1	1.00E+00										

I =	12	13	14	15	16	17	18	19	20	21	22
X =	1.48E+02	1.71E+02	1.97E+02	2.25E+02	2.56E+02	2.90E+02	3.28E+02	3.69E+02	4.14E+02	4.64E+02	5.19E+02

Z =	K =	0.00E+00	0.00E+00
-3.942E+00	15	0.00E+00	0.00E+00
-7.884E+00	14	0.00E+00	0.00E+00
-1.228E+01	13	0.00E+00	0.00E+00
-1.713E+01	12	0.00E+00	0.00E+00
-2.254E+01	11	0.00E+00	0.00E+00
-2.855E+01	10	0.00E+00	0.00E+00
-3.522E+01	9	1.00E+00	1.00E+00
-4.264E+01	8	1.00E+00	1.00E+00
-5.088E+01	7	1.00E+00	1.00E+00
-6.004E+01	6	1.00E+00	1.00E+00
-7.022E+01	5	1.00E+00	1.00E+00
-8.152E+01	4	1.00E+00	1.00E+00
-9.408E+01	3	1.00E+00	1.00E+00
-1.080E+02	2	1.00E+00	1.00E+00

-1.220E+02 1 1.00E+00 1.00E+00

I = 23 24
X = 5.80E+02 6.40E+02

```
*****
STEP          [-----REFERENCE VALUES AT NODE ( 2, 2, 9)-----] [CONVERGENCE RATE / RESIDUALS]
NO.    TIME      U          V          W          P          T          C          PRESSURE REF. VAR.    INDEX

 89  1.01E+00  -1.063E-03  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
** RECORD NO.165 KEYWORD ***** SAVE NOW ON 'SHLOWO12.PLT'
** RECORD NO.166 COMMENT ***** /
```

<---- START OF ARCHIVE READ/WRITE OPERATIONS ---->

CREATED BY PROGRAM : PORFLOW-3D - VERSION 1.00: DATED: 18 OCT 1988
 DATA CREATED BY USER (ID) ... : WHC - JDD - DATE OF ARCHIVED RECORDS : 1/24/1989
 TIME OF CREATION OF RECORDS . : 18:59:24
 TITLE OF THE ARCHIVED DATA SET: SHLOWO'S CASE 2 - VERTICAL INFILTRATION
 SIMULATION TIME OF STORED DATA: 1.010E+00
 STEP NUMBER AT WHICH GENERATED: 89
 GRID DIMENSIONS OF STORED DATA: 24 BY 3 BY 18

- > WRITING VARIABLE: U - X-DIR. VELOCITY COMPONENT
- > WRITING VARIABLE: V - Y-DIR. VELOCITY COMPONENT
- > WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT
- > WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD
- > WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 2 WRITTEN TO ARCHIVES ---->

```
 89  1.01E+00  -1.063E-03  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
** RECORD NO.167 KEYWORD ***** SOLVE UNTIL TIME = 5.00 DAYS IN STEP OF 0.05 DAY INCREASE BY 1.1, MAX =0.10
 89  1.01E+00  -1.063E-03  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
 90  1.06E+00  -1.063E-03  0.000E+00 -1.431E-04 -3.000E+01  0.000E+00  0.000E+00  8.345E-07 8.345E-07  0.0
 91  1.11E+00  -0.265E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  8.345E-07 8.345E-07  0.0
 92  1.18E+00  -0.265E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  8.345E-07 8.345E-07  0.0
 93  1.24E+00  -0.265E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  2.027E-06 2.027E-06  0.0
 94  1.32E+00  -0.265E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  1.431E-06 1.431E-06  0.0
 95  1.40E+00  -0.265E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  1.073E-06 1.073E-06  0.0
 96  1.48E+00  -0.265E-04  0.000E+00  0.000E+00 -3.000E+01  0.000E+00  0.000E+00  8.941E-07 8.941E-07  0.0
 97  1.58E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.788E-06 1.788E-06  0.0
 98  1.68E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  1.192E-06 1.192E-06  0.0
 99  1.78E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  9.537E-07 9.537E-07  0.0
100  1.88E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  8.345E-07 8.345E-07  0.0
101  1.98E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  5.960E-07 5.960E-07  0.0
102  2.08E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  5.960E-07 5.960E-07  0.0
103  2.18E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  5.364E-07 5.364E-07  0.0
104  2.28E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  4.768E-07 4.768E-07  0.0
105  2.38E+00  -1.181E-03  0.000E+00  1.431E-04 -3.000E+01  0.000E+00  0.000E+00  4.172E-07 4.172E-07  0.0
```

86	2.48E+00	-1.299E-03	0.000E+00	0.000E+00	-3.000E-01	0.000E+00	0.000E+00	5.364E-07	5.364E-07	0.0
87	2.58E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	4.172E-07	4.172E-07	0.0
88	2.68E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	4.172E-07	4.172E-07	0.0
89	2.78E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
90	2.88E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	4.172E-07	4.172E-07	0.0
91	2.98E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
92	3.08E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
93	3.18E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	4.172E-07	4.172E-07	0.0
94	3.28E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	4.172E-07	4.172E-07	0.0
95	3.38E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	5.364E-07	5.364E-07	0.0
96	3.48E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
97	3.58E+00	-1.299E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
98	3.68E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
99	3.78E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
100	3.88E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
101	3.98E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
102	4.08E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
103	4.18E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
104	4.28E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
105	4.38E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
106	4.48E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
107	4.58E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
108	4.68E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
109	4.78E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
110	4.88E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
111	4.98E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
112	5.08E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
113	5.18E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
114	5.28E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
115	5.38E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
116	5.48E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	3.576E-07	3.576E-07	0.0
117	5.58E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
118	5.68E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
119	5.78E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.980E-07	2.980E-07	0.0
120	5.88E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
121	5.98E+00	-1.417E-03	0.000E+00	1.431E-04	-3.000E-01	0.000E+00	0.000E+00	2.384E-07	2.384E-07	0.0
122	6.01E+00	-1.535E-03	0.000E+00	0.000E+00	-3.000E-01	0.000E+00	0.000E+00	1.550E-06	1.550E-06	0.0

** RECORD NO.168 KEYWORD ***** OUTPUT NOW

---- U - X-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 122, TIME= 6.0100E+00 ***--***--***--***--

Z = K =

0.000E+00	16	-5.86E-09	8.20E-09	-1.17E-08	1.84E-08	-7.92E-09	0.00E+00	-1.80E-08	-1.59E-08	-2.83E-08	-1.09E-09	2.43E-08
-3.942E+00	15	-1.05E-08	8.20E-09	-1.17E-08	1.84E-08	-7.92E-09	0.00E+00	-1.80E-08	-1.59E-08	-2.83E-08	-1.09E-09	2.43E-08
-7.884E+00	14	-1.41E-08	1.29E-08	-8.52E-09	1.84E-08	-1.14E-08	-8.00E-10	-1.82E-08	-1.52E-08	-1.80E-08	-1.09E-08	2.19E-08
-1.228E+01	13	-7.03E-09	3.51E-09	-1.06E-09	8.71E-09	-9.68E-09	0.00E+00	-2.47E-08	-1.72E-08	-6.01E-09	-1.42E-08	1.04E-08
-1.713E+01	12	-1.64E-08	-3.51E-09	1.17E-08	-6.78E-09	0.00E+00	-4.80E-09	-2.91E-08	-1.28E-08	0.00E+00	-1.58E-08	4.97E-10
-2.254E+01	11	-2.11E-08	4.89E-09	-5.32E-09	-9.68E-09	-7.04E-09	-8.40E-09	-2.55E-08	-1.85E-08	2.40E-09	-1.58E-08	-4.47E-09

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I = 24
X = 8.10E+02

---- W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 122, TIME= 8.0100E+00 ***--***--***--***--

Z =	K =	1	2	3	4	5	6	7	8	9	10	11
-1.971E+00	18	-1.07E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
-5.913E+00	15	0.00E+00	8.01E-09	-2.87E-09	-1.07E-08	-1.07E-08	0.00E+00	2.67E-09	1.07E-08	8.01E-09	-3.74E-08	1.07E-08
-1.007E+01	14	0.00E+00	-1.44E-08	4.81E-09	-1.20E-08	1.20E-08	7.21E-09	4.81E-09	2.64E-08	3.37E-08	-1.44E-08	0.00E+00
-1.470E+01	13	0.00E+00	1.73E-08	3.03E-08	4.33E-09	3.09E-08	1.51E-08	2.81E-08	4.11E-08	2.60E-08	4.33E-09	1.08E-08
-1.984E+01	12	0.00E+00	7.79E-09	-5.84E-09	2.53E-08	3.12E-08	4.67E-08	5.08E-08	4.09E-08	5.28E-08	4.48E-08	4.48E-08
-2.554E+01	11	0.00E+00	-1.23E-08	1.93E-08	4.03E-08	4.56E-08	6.83E-08	8.59E-08	5.43E-08	5.43E-08	1.05E-07	1.03E-07
-3.189E+01	10	0.00E+00	1.00E-08	5.01E-07	-5.01E-07	1.00E-08	-1.00E-08	5.01E-07	0.00E+00	-1.00E-08	1.00E-08	5.01E-07
-3.893E+01	9	0.00E+00	0.00E+00	1.43E-04	0.00E+00	-1.43E-04	0.00E+00	2.86E-04	0.00E+00	-1.43E-04	0.00E+00	1.43E-04
-4.876E+01	8	0.00E+00	0.00E+00	0.00E+00	-1.29E-04	1.29E-04	-2.58E-04	-5.16E-04	1.29E-04	1.29E-04	-5.16E-04	-3.86E-04
-5.546E+01	7	0.00E+00	-1.16E-04	-1.16E-04	0.00E+00	-1.16E-04	2.32E-04	-1.16E-04	0.00E+00	0.00E+00	-3.48E-04	-4.84E-04
-6.513E+01	6	0.00E+00	1.04E-04	0.00E+00	1.04E-04	1.04E-04	1.04E-04	3.13E-04	0.00E+00	-2.09E-04	1.04E-04	-4.17E-04
-7.587E+01	5	0.00E+00	0.00E+00	1.88E-04	0.00E+00	0.00E+00	1.88E-04	9.39E-05	1.88E-04	1.88E-04	0.00E+00	-9.39E-05
-8.780E+01	4	0.00E+00	0.00E+00	-1.89E-04	8.45E-05	2.53E-04	0.00E+00	0.00E+00	1.89E-04	2.53E-04	8.45E-05	1.89E-04
-1.011E+02	3	0.00E+00	1.52E-04	0.00E+00	1.52E-04	0.00E+00	1.52E-04	7.60E-05	7.60E-05	7.60E-05	7.60E-05	7.60E-05
-1.150E+02	2	5.32E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

I = 1 2 3 4 5 6 7 8 9 10 11
X = -4.49E+00 4.49E+00 1.35E+01 2.34E+01 3.42E+01 4.62E+01 5.94E+01 7.38E+01 8.98E+01 1.07E+02 1.27E+02

Z =	K =	12	13	14	15	16	17	18	19	20	21	22
-1.971E+00	18	0.00E+00										
-5.913E+00	15	2.40E-08	8.01E-09	1.07E-08	-8.01E-09	1.00E-08	4.81E-08	8.01E-09	3.21E-08	2.94E-08	2.14E-08	2.94E-08
-1.007E+01	14	5.53E-08	3.37E-08	2.16E-08	1.44E-08	5.53E-08	4.09E-08	5.77E-08	4.33E-08	5.53E-08	5.05E-08	4.57E-08
-1.470E+01	13	5.41E-08	6.27E-08	7.36E-08	4.98E-08	6.27E-08	7.36E-08	9.52E-08	8.65E-08	8.66E-08	8.44E-08	1.02E-07
-1.984E+01	12	6.43E-08	7.79E-08	8.37E-08	8.98E-08	8.37E-08	1.25E-07	1.27E-07	1.03E-07	8.76E-08	8.76E-08	1.19E-07
-2.554E+01	11	1.21E-07	1.12E-07	8.59E-08	1.16E-07	1.33E-07	1.75E-07	1.63E-07	1.21E-07	1.31E-07	1.33E-07	1.23E-07
-3.189E+01	10	-5.01E-07	-5.01E-07	1.00E-08	5.01E-07	-5.01E-07	0.00E+00	5.01E-07	1.50E-08	1.00E-08	1.00E-08	1.00E-08
-3.893E+01	9	-4.29E-04	1.43E-04	0.00E+00	1.43E-04	1.43E-04	1.43E-04	1.43E-04	1.43E-04	-1.43E-04	1.43E-04	0.00E+00
-4.876E+01	8	-1.29E-04	0.00E+00	1.29E-04	-2.58E-04	-1.29E-04	1.29E-04	0.00E+00	0.00E+00	-2.58E-04	2.58E-04	5.15E-04
-5.546E+01	7	2.32E-04	-2.32E-04	1.16E-04	-1.16E-04	-1.16E-04	-2.32E-04	1.16E-04	-1.16E-04	0.00E+00	1.16E-04	4.84E-04
-6.513E+01	6	1.04E-04	0.00E+00	3.13E-04	-2.09E-04	-1.04E-04	-3.13E-04	2.09E-04	0.00E+00	2.09E-04	1.04E-04	1.04E-04
-7.587E+01	5	-3.75E-04	-2.82E-04	-1.88E-04	0.00E+00	-1.88E-04	-1.88E-04	-1.88E-04	9.39E-05	0.00E+00	1.88E-04	0.00E+00
-8.780E+01	4	-1.89E-04	-2.53E-04	-2.53E-04	-2.53E-04	-8.45E-05	0.00E+00	0.00E+00	2.53E-04	8.45E-05	-8.45E-05	-2.53E-04
-1.011E+02	3	0.00E+00	0.00E+00	-7.60E-05	-7.60E-05	-1.52E-04	-2.28E-04	2.28E-04	0.00E+00	7.60E-05	-7.60E-05	-1.52E-04
-1.150E+02	2	0.00E+00										

I = 12 13 14 15 16 17 18 19 20 21 22
X = 1.48E+02 1.71E+02 1.97E+02 2.25E+02 2.56E+02 2.90E+02 3.28E+02 3.69E+02 4.14E+02 4.64E+02 5.19E+02

Z =	K =	1	2
-1.971E+00	18	0.00E+00	0.00E+00
-5.913E+00	15	3.47E-08	3.47E-08
-1.007E+01	14	8.89E-08	8.89E-08
-1.470E+01	13	6.87E-08	6.87E-08
-1.984E+01	12	1.46E-07	1.46E-07

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-1.080E+02 2 1.00E+00 1.00
 -1.220E+02 1 1.00E+00 1.00

I = 1 2 3 4 5 6 7 8 9 10 11
 X = -4.49E+00 4.49E+00 1.35E+01 2.34E+01 3.42E+01 4.62E+01 5.94E+01 7.38E+01 8.98E+01 1.07E+02 1.27E+02

Z = K =
 0.000E+00 16 0.00E+00
 -3.942E+00 15 0.00E+00
 -7.884E+00 14 0.00E+00
 -1.220E+01 13 0.00E+00
 -1.713E+01 12 0.00E+00
 -2.254E+01 11 0.00E+00
 -2.855E+01 10 0.00E+00
 -3.522E+01 9 1.00E+00
 -4.264E+01 8 1.00E+00
 -5.088E+01 7 1.00E+00
 -6.004E+01 6 1.00E+00
 -7.022E+01 5 1.00E+00
 -8.152E+01 4 1.00E+00
 -9.488E+01 3 1.00E+00
 -1.080E+02 2 1.00E+00
 -1.220E+02 1 1.00E+00 1.00E+00

I = 12 13 14 15 16 17 18 19 20 21 22
 X = 1.48E+02 1.71E+02 1.97E+02 2.25E+02 2.58E+02 2.90E+02 3.28E+02 3.89E+02 4.14E+02 4.64E+02 5.19E+02

Z = K =
 0.000E+00 16 0.00E+00 0.00E+00
 -3.942E+00 15 0.00E+00 0.00E+00
 -7.884E+00 14 0.00E+00 0.00E+00
 -1.220E+01 13 0.00E+00 0.00E+00
 -1.713E+01 12 0.00E+00 0.00E+00
 -2.254E+01 11 0.00E+00 0.00E+00
 -2.855E+01 10 0.00E+00 0.00E+00
 -3.522E+01 9 1.00E+00 1.00E+00
 -4.264E+01 8 1.00E+00 1.00E+00
 -5.088E+01 7 1.00E+00 1.00E+00
 -6.004E+01 6 1.00E+00 1.00E+00
 -7.022E+01 5 1.00E+00 1.00E+00
 -8.152E+01 4 1.00E+00 1.00E+00
 -9.488E+01 3 1.00E+00 1.00E+00
 -1.080E+02 2 1.00E+00 1.00E+00
 -1.220E+02 1 1.00E+00 1.00E+00

I = 23 24
 X = 5.80E+02 6.40E+02

WHC-EP-0041

-1.080E+02 2 -1.77E-03 -1.30E-03 -1.93E-03 -1.56E-03 -1.89E-03 -1.45E-03 -1.47E-03 -1.40E-03 -1.27E-03 -1.27E-03 -9.01
 -1.220E+02 1 -9.45E-04 -1.30E-03 -1.93E-03 -1.56E-03 -1.89E-03 -1.45E-03 -1.47E-03 -1.40E-03 -1.27E-03 -1.27E-03 -9.01

I = 2 3 4 5 6 7 8 9 10 11 12
 X = 0.00E+00 8.99E+00 1.84E+01 2.88E+01 4.02E+01 5.28E+01 6.66E+01 8.18E+01 9.85E+01 1.17E+02 1.37E+02

Z = K =
 0.000E+00 16 -1.26E-08 -8.62E-09 -1.01E-08 6.45E-09 1.11E-08 -4.21E-09 -1.35E-08 -5.58E-09 -5.06E-09 -3.06E-09 9.93E-09
 -3.942E+00 15 -1.26E-08 -8.62E-09 -1.01E-08 6.45E-09 1.11E-08 -4.21E-09 -1.35E-08 -5.58E-09 -5.06E-09 -3.06E-09 9.93E-09
 -7.884E+00 14 -9.94E-09 -9.03E-09 -7.47E-09 3.39E-09 7.40E-09 0.00E+00 -1.58E-08 -5.33E-09 -4.42E-09 -3.64E-09 9.58E-09
 -1.226E+01 13 -5.87E-09 -6.98E-09 -6.35E-09 -2.38E-09 9.25E-09 -1.96E-09 -1.43E-08 -6.49E-09 -4.00E-09 -3.26E-09 6.44E-09
 -1.713E+01 12 -7.68E-09 -9.03E-09 -2.24E-09 -4.41E-09 7.71E-09 -4.77E-09 -1.33E-08 -3.71E-09 -8.32E-09 -4.79E-09 7.49E-09
 -2.254E+01 11 -1.08E-08 -1.03E-08 -3.36E-09 -3.39E-09 1.23E-09 -5.05E-09 -1.02E-08 -1.85E-09 -6.32E-09 -7.85E-09 5.05E-09
 -2.855E+01 10 -8.58E-08 -4.11E-09 -9.70E-09 -6.79E-09 -6.17E-09 -3.06E-09 -4.08E-09 -3.24E-09 -6.53E-09 -6.70E-09 3.31E-09
 -3.522E+01 9 -8.58E-04 -5.38E-04 -9.41E-04 -6.16E-04 -6.53E-04 -3.39E-04 -4.63E-04 -3.04E-04 -6.58E-04 -6.78E-04 3.33E-04
 -4.264E+01 8 -1.05E-03 -4.97E-04 -9.78E-04 -6.16E-04 -6.53E-04 -3.39E-04 -4.63E-04 -2.57E-04 -7.01E-04 -6.56E-04 3.33E-04
 -5.088E+01 7 -1.09E-03 -5.38E-04 -8.65E-04 -6.50E-04 -7.15E-04 -3.11E-04 -4.63E-04 -2.10E-04 -7.66E-04 -6.95E-04 3.51E-04
 -6.004E+01 6 -9.10E-04 -6.62E-04 -7.90E-04 -6.50E-04 -6.84E-04 -3.98E-04 -4.11E-04 -2.34E-04 -8.07E-04 -7.53E-04 3.09E-04
 -7.022E+01 5 -8.65E-04 -7.86E-04 -6.02E-04 -6.84E-04 -6.22E-04 -5.37E-04 -3.60E-04 -2.80E-04 -7.86E-04 -7.53E-04 3.33E-04
 -8.152E+01 4 -9.10E-04 -8.28E-04 -6.77E-04 -6.16E-04 -6.22E-04 -5.37E-04 -4.37E-04 -2.57E-04 -8.28E-04 -7.14E-04 3.33E-04
 -9.408E+01 3 -8.65E-04 -8.28E-04 -6.77E-04 -6.84E-04 -6.53E-04 -5.37E-04 -5.14E-04 -2.10E-04 -7.86E-04 -6.78E-04 2.83E-04
 -1.080E+02 2 -8.65E-04 -7.86E-04 -6.77E-04 -6.50E-04 -6.22E-04 -7.07E-04 -4.37E-04 -2.34E-04 -7.43E-04 -6.56E-04 2.48E-04
 -1.220E+02 1 -8.65E-04 -7.86E-04 -6.77E-04 -6.50E-04 -6.22E-04 -7.07E-04 -4.37E-04 -2.34E-04 -7.43E-04 -6.56E-04 2.48E-04

I = 13 14 15 16 17 18 19 20 21 22 23
 X = 1.59E+02 1.84E+02 2.11E+02 2.40E+02 2.73E+02 3.09E+02 3.48E+02 3.92E+02 4.39E+02 4.92E+02 5.50E+02

Z = K =
 0.000E+00 16 0.00E+00
 -3.942E+00 15 0.00E+00
 -7.884E+00 14 0.00E+00
 -1.226E+01 13 0.00E+00
 -1.713E+01 12 0.00E+00
 -2.254E+01 11 0.00E+00
 -2.855E+01 10 0.00E+00
 -3.522E+01 9 0.00E+00
 -4.264E+01 8 0.00E+00
 -5.088E+01 7 0.00E+00
 -6.004E+01 6 0.00E+00
 -7.022E+01 5 0.00E+00
 -8.152E+01 4 0.00E+00
 -9.408E+01 3 0.00E+00
 -1.080E+02 2 0.00E+00
 -1.220E+02 1 0.00E+00

I = 24
 X = 6.10E+02

WHC-EP-0041

----*--*-- W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 122, TIME= 6.0100E+00 --*--*--*--*--*--*--

Z =	K =	1	2	3	4	5	6	7	8	9	10	11
-1.971E+00	16	-1.07E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
-5.913E+00	15	0.00E+00	8.01E-09	-2.67E-09	-1.07E-08	-1.07E-08	0.00E+00	2.67E-09	1.07E-08	8.01E-09	-3.74E-08	1.07E-08
-1.007E+01	14	0.00E+00	-1.44E-08	4.81E-09	-1.20E-08	1.20E-08	7.21E-09	4.81E-09	2.64E-08	3.37E-08	-1.44E-08	0.00E+00
-1.470E+01	13	0.00E+00	1.73E-08	3.03E-08	4.33E-09	3.89E-08	1.51E-08	2.81E-08	4.11E-08	2.60E-08	4.33E-09	1.00E-08
-1.984E+01	12	0.00E+00	7.79E-09	-5.84E-09	2.53E-08	3.12E-08	4.67E-08	5.06E-08	4.09E-08	5.28E-08	4.48E-08	4.48E-08
-2.554E+01	11	0.00E+00	-1.23E-08	1.93E-08	4.03E-08	4.56E-08	6.83E-08	8.59E-08	5.43E-08	5.43E-08	1.05E-07	1.03E-07
-3.189E+01	10	0.00E+00	1.00E-08	5.01E-07	-5.01E-07	1.00E-08	-1.00E-08	5.01E-07	0.00E+00	-1.00E-08	1.00E-08	5.01E-07
-3.893E+01	9	0.00E+00	0.00E+00	1.43E-04	0.00E+00	-1.43E-04	0.00E+00	2.86E-04	0.00E+00	-1.43E-04	0.00E+00	1.43E-04
-4.676E+01	8	0.00E+00	0.00E+00	0.00E+00	-1.29E-04	1.29E-04	-2.58E-04	-5.15E-04	1.29E-04	1.29E-04	-5.15E-04	-3.86E-04
-5.546E+01	7	0.00E+00	-1.16E-04	-1.16E-04	0.00E+00	-1.16E-04	2.32E-04	-1.16E-04	0.00E+00	0.00E+00	-3.48E-04	-4.64E-04
-6.513E+01	6	0.00E+00	1.04E-04	0.00E+00	1.04E-04	1.04E-04	1.04E-04	3.13E-04	0.00E+00	-2.09E-04	1.04E-04	-4.17E-04
-7.587E+01	5	0.00E+00	0.00E+00	1.88E-04	0.00E+00	0.00E+00	1.88E-04	9.39E-05	1.88E-04	1.88E-04	0.00E+00	-9.39E-05
-8.780E+01	4	0.00E+00	0.00E+00	-1.69E-04	8.45E-05	2.53E-04	0.00E+00	0.00E+00	1.69E-04	2.53E-04	8.45E-05	1.69E-04
-1.011E+02	3	0.00E+00	1.52E-04	0.00E+00	1.52E-04	0.00E+00	1.52E-04	7.60E-05	7.60E-05	7.60E-05	7.60E-05	7.60E-05
-1.150E+02	2	5.32E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

I =	1	2	3	4	5	6	7	8	9	10	11
X =	-4.49E+00	4.49E+00	1.35E+01	2.34E+01	3.42E+01	4.62E+01	5.94E+01	7.38E+01	8.98E+01	1.07E+02	1.27E+02

Z =	K =	12	13	14	15	16	17	18	19	20	21	22
-1.971E+00	16	0.00E+00										
-5.913E+00	15	2.40E-08	8.01E-09	1.07E-08	-8.01E-09	1.60E-08	4.81E-08	8.01E-09	3.21E-08	2.94E-08	2.14E-08	2.94E-08
-1.007E+01	14	5.53E-08	3.37E-08	2.16E-08	1.44E-08	5.53E-08	4.09E-08	5.77E-08	4.33E-08	5.53E-08	5.05E-08	4.57E-08
-1.470E+01	13	5.41E-08	6.27E-08	7.36E-08	4.98E-08	6.27E-08	7.36E-08	9.52E-08	8.65E-08	8.06E-08	8.44E-08	1.02E-07
-1.984E+01	12	6.43E-08	7.79E-08	8.37E-08	8.96E-08	8.37E-08	1.25E-07	1.27E-07	1.03E-07	8.76E-08	8.76E-08	1.19E-07
-2.554E+01	11	1.21E-07	1.12E-07	8.59E-08	1.16E-07	1.33E-07	1.75E-07	1.63E-07	1.21E-07	1.31E-07	1.33E-07	1.23E-07
-3.189E+01	10	-5.01E-07	-5.01E-07	1.00E-06	5.01E-07	-5.01E-07	0.00E+00	5.01E-07	1.50E-06	1.00E-06	1.00E-06	1.00E-06
-3.893E+01	9	-4.29E-04	1.43E-04	0.00E+00	1.43E-04	1.43E-04	1.43E-04	1.43E-04	1.43E-04	-1.43E-04	1.43E-04	0.00E+00
-4.676E+01	8	-1.29E-04	0.00E+00	1.29E-04	-2.58E-04	-1.29E-04	1.29E-04	0.00E+00	0.00E+00	-2.58E-04	2.58E-04	5.15E-04
-5.546E+01	7	2.32E-04	-2.32E-04	1.16E-04	-1.16E-04	-1.16E-04	-2.32E-04	1.16E-04	-1.16E-04	0.00E+00	1.16E-04	4.64E-04
-6.513E+01	6	1.04E-04	0.00E+00	3.13E-04	-2.09E-04	-1.04E-04	-3.13E-04	2.09E-04	0.00E+00	2.09E-04	1.04E-04	1.04E-04
-7.587E+01	5	-3.75E-04	-2.82E-04	-1.88E-04	0.00E+00	-1.88E-04	-1.88E-04	-1.88E-04	9.39E-05	0.00E+00	1.88E-04	0.00E+00
-8.780E+01	4	-1.69E-04	-2.53E-04	-2.53E-04	-2.53E-04	-8.45E-05	0.00E+00	0.00E+00	2.53E-04	8.45E-05	-8.45E-05	-2.53E-04
-1.011E+02	3	0.00E+00	0.00E+00	-7.60E-05	-7.60E-05	-1.52E-04	-2.28E-04	2.28E-04	0.00E+00	7.60E-05	-7.60E-05	-1.52E-04
-1.150E+02	2	0.00E+00										

I =	12	13	14	15	16	17	18	19	20	21	22
X =	1.48E+02	1.71E+02	1.97E+02	2.25E+02	2.56E+02	2.90E+02	3.28E+02	3.69E+02	4.14E+02	4.64E+02	5.19E+02

Z =	K =	12	13
-1.971E+00	16	0.00E+00	0.00E+00
-5.913E+00	15	3.47E-08	3.47E-08
-1.007E+01	14	8.89E-08	8.89E-08
-1.470E+01	13	8.87E-08	8.87E-08
-1.984E+01	12	1.46E-07	1.46E-07
-2.554E+01	11	1.40E-07	1.40E-07
-3.189E+01	10	1.00E-06	1.00E-06
-3.893E+01	9	0.00E+00	0.00E+00
-4.676E+01	8	3.86E-04	3.86E-04
-5.546E+01	7	3.48E-04	3.48E-04

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X = 1.48E+02 1.71E+02 1.97E+02 2.25E+02 2.56E+02 2.90E+02 3.28E+02 3.69E+02 4.14E+02 4.64E+02 5.19E+02

Z = K =

0.000E+00	16	-3.00E+01	-3.00E+01
-3.942E+00	15	-3.00E+01	-3.00E+01
-7.884E+00	14	-3.00E+01	-3.00E+01
-1.228E+01	13	-3.00E+01	-3.00E+01
-1.713E+01	12	-3.00E+01	-3.00E+01
-2.254E+01	11	-3.00E+01	-3.00E+01
-2.855E+01	10	-3.00E+01	-3.00E+01
-3.522E+01	9	-3.00E+01	-3.00E+01
-4.264E+01	8	-3.00E+01	-3.00E+01
-5.088E+01	7	-3.00E+01	-3.00E+01
-6.004E+01	6	-3.00E+01	-3.00E+01
-7.022E+01	5	-3.00E+01	-3.00E+01
-8.152E+01	4	-3.00E+01	-3.00E+01
-9.408E+01	3	-3.00E+01	-3.00E+01
-1.080E+02	2	-3.00E+01	-3.00E+01
-1.220E+02	1	-3.00E+01	-3.00E+01

I = 23 24
X = 5.80E+02 6.40E+02

--*-*-*-- THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 122, TIME= 6.0100E+00 --*-*-*-*-*--*-*-*-*--

Z = K =

0.000E+00	16	0.00E+00																					
-3.942E+00	15	0.00E+00																					
-7.884E+00	14	0.00E+00																					
-1.228E+01	13	0.00E+00																					
-1.713E+01	12	0.00E+00																					
-2.254E+01	11	0.00E+00																					
-2.855E+01	10	0.00E+00																					
-3.522E+01	9	1.00E+00																					
-4.264E+01	8	1.00E+00																					
-5.088E+01	7	1.00E+00																					
-6.004E+01	6	1.00E+00																					
-7.022E+01	5	1.00E+00																					
-8.152E+01	4	1.00E+00																					
-9.408E+01	3	1.00E+00																					
-1.080E+02	2	1.00E+00																					
-1.220E+02	1	1.00E+00																					

I = 1 2 3 4 5 6 7 8 9 10 11
X = -4.49E+00 4.49E+00 1.35E+01 2.34E+01 3.42E+01 4.62E+01 5.94E+01 7.38E+01 8.98E+01 1.07E+02 1.27E+02

Z =	K =													
0.000E+00	16	0.00E+00												
-3.942E+00	15	0.00E+00												
-7.884E+00	14	0.00E+00												
-1.228E+01	13	0.00E+00												
-1.713E+01	12	0.00E+00												
-2.254E+01	11	0.00E+00												
-2.855E+01	10	0.00E+00												
-3.522E+01	9	1.00E+00												
-4.284E+01	8	1.00E+00												
-5.088E+01	7	1.00E+00												
-6.004E+01	6	1.00E+00												
-7.022E+01	5	1.00E+00												
-8.152E+01	4	1.00E+00												
-9.408E+01	3	1.00E+00												
-1.080E+02	2	1.00E+00												
-1.220E+02	1	1.00E+00												

I = 12 13 14 15 16 17 18 19 20 21 22
X = 1.40E+02 1.71E+02 1.97E+02 2.25E+02 2.58E+02 2.90E+02 3.28E+02 3.89E+02 4.14E+02 4.84E+02 5.19E+02

Z =	K =		
0.000E+00	16	0.00E+00	0.00E+00
-3.942E+00	15	0.00E+00	0.00E+00
-7.884E+00	14	0.00E+00	0.00E+00
-1.228E+01	13	0.00E+00	0.00E+00
-1.713E+01	12	0.00E+00	0.00E+00
-2.254E+01	11	0.00E+00	0.00E+00
-2.855E+01	10	0.00E+00	0.00E+00
-3.522E+01	9	1.00E+00	1.00E+00
-4.284E+01	8	1.00E+00	1.00E+00
-5.088E+01	7	1.00E+00	1.00E+00
-6.004E+01	6	1.00E+00	1.00E+00
-7.022E+01	5	1.00E+00	1.00E+00
-8.152E+01	4	1.00E+00	1.00E+00
-9.408E+01	3	1.00E+00	1.00E+00
-1.080E+02	2	1.00E+00	1.00E+00
-1.220E+02	1	1.00E+00	1.00E+00

I = 23 24
X = 5.80E+02 6.40E+02

<---- START OF ARCHIVE READ/WRITE OPERATIONS ---->

CREATED BY PROGRAM : PORFLOW-3D - VERSION 1.00: DATED: 18 OCT 1988
DATA CREATED BY USER (ID) ... : WHC - JDD - DATE OF ARCHIVED RECORDS : 1/24/1989
TIME OF CREATION OF RECORDS . : 18:59:24

TITLE OF THE ARCHIVED DATA SET: SHLOMO'S CASE 2 - VERTICAL INFILTRATION
SIMULATION TIME OF STORED DATA: 6.010E+00
STEP NUMBER AT WHICH GENERATED: 122
GRID DIMENSIONS OF STORED DATA: 24 BY 3 BY 16

----> WRITING VARIABLE: U - X-DIR. VELOCITY COMPONENT
----> WRITING VARIABLE: V - Y-DIR. VELOCITY COMPONENT
----> WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT
----> WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD
----> WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 4 WRITTEN TO ARCHIVES ---->

THIS OUTPUT IS PRODUCED BY THE COMPUTATIONAL MODEL

----- P O R F L O - 3 D -----

FOR TRANSIENT OR STEADY STATE ANALYSIS
OF FLOW, HEAT AND MASS TRANSPORT
IN VARIABLY SATURATED POROUS OR FRACTURED MEDIA

DEVELOPED BY DR A.K. RUNCHAL (ACRI, LOS ANGELES)
AND DR B. SAGAR (PNL, RICHLAND) UNDER CONTRACT FROM
WESTINGHOUSE HANFORD COMPANY, RICHLAND, WA

THIS COMPUTER CODE WAS DEVELOPED FOR USE BY
THE US DEPT. OF ENERGY AND ITS CONTRACTORS

FOR ENQUIRIES AND ASSISTANCE: CALL 213-398-0956 USA

OR 509-376-5897 USA

VERSION 1.00: DATED: 16 OCT 1988

DATE OF RUN: 1/24/1989 - TIME OF RUN: 17:03:13

ELAPSED TIME FOR THIS CASE : 3.82 MINUTES
TIME PER GRID NODE PER STEP: 1.63 MILLISECONDS
TIME PER NODE-STEP-EQUATION: 1.63 MILLISECONDS
1 EQUATIONS SOLVED AT 1152 NODES FOR 122 STEPS.

RECORD OF INPUT DATA STREAM

WHC-EP-0041

=====
END-OF-FILE ENCOUNTERED IN READING INPUT DATA. KEYWORD SET TO QUIT.
=====

WHC-EP-0041

APPENDIX C

ERROR MESSAGES OF PORFLO-3

ERROR MESSAGES OF PORFLO-3

PORFLO-3 provides considerable, but not complete, checking of data input to ensure that the data specified by the user meet certain basic conditions of validity. When a discrepancy is detected, the program stops execution and a diagnostic message with an error number is printed. The error numbers and their meanings are described in Table C-1.

Table C-1. Error Messages of PORFLO-3.
(sheet 1 of 3)

Error number	Error description
111	Number of x-direction nodes (IMAX) specified by the GRID command exceeds the LX parameter or is less than the minimum permissible value of 3.
112	Number of y-direction nodes (JMAX) specified by the GRID command exceeds the LY parameter or is less than the minimum permissible value of 3.
113	Number of z-direction nodes (KMAX) specified by the GRID command exceeds the LZ parameter or is less than the minimum permissible value of 3.
114	The product of IMAX, JMAX, and KMAX of the GRID command exceeds the LMAX parameter or is less than the minimum permissible value of 27.
118	The number of internal field nodes exceeds the LFLD parameter; in most installations, no more than 100 numerical values may be specified.
121	Grid generation index of the X, Y, or Z command is not one of the allowable values of 1, 2, and 3.
141	The zone designation index of the ZONE command is less than unity or greater than the value of the LZN parameter.
211	The x-coordinate values specified by the X command are not increasing in a monotonic fashion as required.
212	The y-coordinate values specified by the Y command are not increasing in a monotonic fashion as required.
213	The z-coordinate values specified by the Z command are not increasing in a monotonic fashion as required.

Table C-1. Error Messages of PORFLO-3
(sheet 2 of 3)

Error number	Error description
251	The time step specified for simulations of the SOLVE command is smaller than 1 E-20 or larger than 1 E+20.
311	The number of tabulated values specified by the immediately preceding command exceeds the corresponding dimension parameter (LSR for the SOURCE command and LUS for the CHARACTERISTIC command).
321	The zone number specified by the immediately preceding command was not previously defined by a ZONE command.
411	The density of solid material specified by the ROCK or SOIL command is less than zero.
412	The effective porosity specified by the ROCK or SOIL command is less than zero.
413	The total porosity specified by the ROCK or SOIL command is less than zero.
414	The connective porosity specified by the ROCK or SOIL command is less than zero.
511	The specific storativity specified by the HYDRAULIC command is less than zero.
512	The x-directional hydraulic conductivity specified by the HYDRAULIC command is less than zero.
513	The y-directional hydraulic conductivity specified by the HYDRAULIC command is less than zero.
514	The z-directional hydraulic conductivity specified by the HYDRAULIC command is less than zero.
521	The specific heat specified by the THERMAL command is less than zero.
522	The thermal conductivity specified by the THERMAL command is less than zero.
523	The longitudinal dispersivity specified by the THERMAL command is less than zero.

Table C-1. Error Messages of PORFLO-3
(sheet 3 of 3)

Error number	Error description
524	The transverse dispersivity specified by the THERmal command is less than zero.
531	The distribution or retardation coefficient specified by the TRANsport command is less than zero.
532	The molecular diffusivity specified by the TRANsport command is less than zero.
533	The longitudinal dispersivity specified by the TRANsport command is less than zero.
534	The transverse dispersivity specified by the TRANsport command is less than zero.
651	The reference air-entry pressure, h^* , of Equations 6.42-1 and 6.42-6 that is specified by the CHARacteristic command is less than zero.
652	The soil characteristic exponent, 'a', of Equations 6.42-1 and 6.42-6 that is specified by the CHARacteristic command is less than zero.
710	The dependent variable character string specified by the SOURce command is not one of C, P, or T, as required.
711	The total number of active source zones specified by the SOURce commands exceeds the LSZ parameter.
712	The zone number specified by the SOURce command was not previously defined by a ZONE command.

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