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PORMC: A Model for Monte Carlo Simulation of Fluid Flow, Heat, and Mass Transport in Variably Saturated Geologic Media

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CREDITS

This report on the theory and use of the PORMC computer code was written by Dr. Budhi Sagar under contract to Pacific Northwest Laboratory, Richland, Washington. Dr. Sagar was assisted in this effort by Jeff Smyth of Pacific Northwest Laboratory. Even though he was not involved directly in the development and documentation of PORMC, neither the code nor this report would exist without the contribution from Dr. Aki Runchal, Analytic and Computational Research, Inc., Los Angeles, California. Dr. Runchal is the senior author of the PORFLO-3 software package from which the PORMC code is derived. This report has freely borrowed from two previously issued Westinghouse Hanford Company documents on the PORFLO-3 code, which Dr. Runchal co-authored.

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Help was received from several individuals during model development and documentation. Suggestions from Signe Wurstner and Will Nichols motivated many useful changes in the model and associated computer program described in this report. Paul Eslinger provided a number of subroutines related to sampling of random variables. Signe Wurstner and Jeff Smyth developed the input data for the example problem included in the report. Jeff Smyth and Mike Connelly helped debug the initial version of the computer program. Dave Langford helped develop the subroutine on travel time. This report benefitted from review by Will Nichols, Signe Wurstner, and Jerry Davis. Material was freely borrowed from two earlier documents on PORFLO-3, of which Aki Runchal is a senior author. The contributions of all these individuals are sincerely and gratefully acknowledged.

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PORMC: A MODEL FOR MONTE CARLO SIMULATION OF
FLUID FLOW, HEAT, AND MASS TRANSPORT IN
VARIABLY SATURATED GEOLOGIC MEDIA

THEORY AND USER'S MANUAL

ABSTRACT

*This computer program was developed in support of environmental restoration activities being conducted at the Hanford Site to comply with the Resource Conservation and Recovery Act of 1976 and its 1984 amendum; the Comprehensive Environmental Response, Compensation, and Liability Act as amended in 1986; and the Hanford Federal Facility Agreement and Consent Order (Ecology et al. 1990).** The results of analyses made using the computer program will be used in remedial investigations to study the possible nature and extent of contamination and in feasibility studies to analyze the environmental consequences associated with alternative remediation methods.

This document provides details of the theory and instructions for use of the PORMC computer program.

The PORMC computer program is based on a mathematical formulation of the processes of fluid flow, heat transfer, and mass transport in variably saturated geologic media. The geologic media may be heterogeneous and anisotropic and may contain linear and planar features such as boreholes and fractures. The program can be used to analyze three-dimensional problems involving partially and fully saturated media with various types of fluid,

*Ecology, EPA, and DOE, 1990, Hanford Federal Facility Agreement and Consent Order, Washington State Department of Ecology, U.S. Environmental Protection Agency, and U.S. Department of Energy, Olympia, Washington.

heat, and mass sources limited to the analysis of a single fluid. PORMC employs a Monte Carlo approach to treat uncertainties in soil (rock) properties and source terms.

The theory of PORMC is described in Chapter 2. It includes a derivation of the governing equations, a description of the numerical solution method, and the application of the Monte Carlo method to incorporate parametric uncertainties. The governing equations are derived in their integral form, which is suitable for use with the nodal point integration method of discretization. Both the direct and the iterative solution methods are used to solve the matrix of algebraic equations, the nonlinearity in the flow equation being handled through the Picard method. Assumptions are stated to make obvious the limitations on the applicability of the model incorporated in PORMC.

The modular structure of the PORMC computer code is described in Chapter 3. Details of the input instructions for PORMC are provided in Chapter 4. PORMC uses the same free-format command language as PORFLO-3. An illustration of PORMC use on a realistic problem is given in Appendix B.

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
(sheet 1 of 4)

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	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
\underline{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
\vec{J}_c	Species diffusional flux	$M L^{-2} t^{-1}$	kg/(m ² ·s)	lbm/(ft ² ·s)
\vec{J}_D	Species dispersive flux	$M L^{-2} t^{-1}$	kg/(m ² ·s)	lbm/(ft ² ·s)
\underline{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)
kd	Sorption coefficient	$M^{-1} L^3$	m ³ /kg	ft ³ /lbm
\underline{K}	Hydraulic conductivity tensor	$L t^{-1}$	m/s	ft/s
w	Rate of injection of fluid	$M L^{-3} t^{-1}$	kg/(m ³ ·s)	lbm/(ft ³ ·s)
wv	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	--	--	--

MATHEMATICAL NOTATION
(sheet 2 of 4)

Symbol	Meaning	Dimensions	SI units ^a	FPS units ^b
N	Normal coordinate	L	m	ft
p	Thermodynamic pressure	M L ⁻¹ t ⁻²	N/m ²	lbf/ft ²
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
S _T	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

MATHEMATICAL NOTATION
(sheet 3 of 4)

Greek symbol	Meaning	Dimensions	SI units ^a	FPS units ^b
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
θ	Volumetric moisture content	--	--	--
∂	Partial derivative	--	--	--
$\vec{\nabla}$	Gradient operator	--	--	--
q	Soil-water potential	L	m	ft
λ	Radioactive decay coefficient	t^{-1}	s^{-1}	s^{-1}
η	Porosity	--	--	--

MATHEMATICAL NOTATION
(sheet 4 of 4)

Superscripts and subscripts	Meaning
e	Equivalent or effective value of a soil matrix property
m	Pertaining to rock (soil) matrix
p	Pertaining to planer (fractures) or linear (boreholes) features
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
≈	Tensor or matrix
*	Pertaining to a reference state of the system
→	Vector

^aSI = International System of Units (metric).

^bFPS = Foot-Pound-Second (or English) Units.

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THEORY AND USER'S MANUAL

1.0 OVERVIEW AND INTRODUCTION

1.1 PURPOSE AND HISTORY OF PORMC DEVELOPMENT

The PORMC computer code is designed for analyzing problems of fluid flow, heat transfer, and mass transport in variably saturated geologic media when some of the problem variables are uncertain and described through probability distributions. This computer program has been developed in support of environmental remediation activities being conducted at the Hanford Site (Washington State) to comply with the *Resource Conservation and Recovery Act of 1976* (RCRA) and its 1984 amendments; the *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* (CERCLA) as amended in 1986; and the *Hanford Federal Facility Agreement and Consent Order* (Ecology et al. 1990). Specifically, this computer program may be used to analyze the nature and extent of contaminants and the feasibility of alternate remediation measures through estimation of environmental impacts.

The spatial variability of vadose zone properties is widely recognized (Jury 1985, Jury et al. 1987). This variability affects the distribution and migration of moisture and contaminants in the vadose zone. However, there is a lack of consensus on methods for quantifying the effect of the variability on estimation of moisture content and contaminant concentrations. These methods range from assuming conservative values of parameters for use in deterministic models to obtaining statistical descriptions for use in stochastic models.

The PORMC computer code can be used to study problems related to disposal of low- and medium-level nuclear waste and other hazardous chemical wastes in shallow geologic environments. Several regulations may apply to such disposal: the *National Interim Primary Drinking Water Regulations* (40 CFR 141); *Licensing Requirements for Land Disposal of Radioactive Waste* (10 CFR 61); *Environmental Protection, Safety, and Health Protection Programs for DOE Operations*, DOE Order 5480.1A (DOE 1981); *Radioactive Waste Management*, DOE Order 5820.2 (DOE 1984); RCRA, and its 1984 amendments; CERCLA; and the *Superfund Amendments and Reauthorization Act of 1986* (SARA). All of these regulations have some type of quantitative limit on contaminant releases that is stated in terms of either concentration or dose.

The design of a waste disposal system and the estimation of contaminant releases for a selected design compared to these limits usually will be based on a mathematical model that requires the values of the vadose zone properties as input. Because these properties are spatially variable and only a limited number of field-measured values can be obtained (because field testing is usually destructive and expensive), there is always some uncertainty as to the conceptual model and the distribution of these properties. In assessing the

safety of (or risk from) a disposal system in the presence of data uncertainties, an important question often arises regarding the confidence in one's estimate. It is in response to this question that the need arises to consider conservative designs and estimates or, alternatively, to turn to statistical analysis. Currently, there does not appear to be an explicit statement requiring probabilistic estimates in the regulations. However, recent trends seems to favor probabilistic treatment of the performance assessment problem. The PORMC computer code was developed in response to this need.

The PORMC Version 1.0 is derived from the PORFLO-3¹ Version 1.0 enhanced¹ software package (Runchal and Sagar 1989, Sagar and Runchal 1990). The latter is designed to perform the corresponding deterministic calculations. In the absence of all uncertainties (i.e., when all input quantities are deterministic), PORMC Version 1.0 performs the same functions as PORFLO-3 Version 1.0 enhanced. The current and earlier versions of the PORFLO (Runchal et al. 1985, Kline et al. 1983, Eyler and Budden 1984, Runchal and Sagar 1989, Sagar and Runchal 1990) software were developed by Analytic and Computational Research, Inc. under contract to Rockwell Hanford Operations and its successor, Westinghouse Hanford Company (Westinghouse Hanford), the current operating contractor of the Hanford Site for the U.S. Department of Energy (DOE). On October 26, 1989, the DOE granted a request by ACRI that title to the copyright of PORFLO-3 be waived to allow ACRI to claim the right to all versions of PORFLO-3 developed with DOE support. However, the U.S. Government retains a paid-up, nonexclusive, irrevocable worldwide license for use of PORFLO-3 and its derivatives by the government. This license includes rights to develop derivatives of PORFLO-3. Under the Hanford Site Performance Assessment Program funded by Westinghouse Hanford, PORMC was developed during 1988 to 1990 at the Pacific Northwest Laboratory. The PORMC computer code may be regarded as a derivative of PORFLO-3.

1.2 OBJECTIVE AND ORGANIZATION OF THE REPORT

The objective of this report is to detail the theory of PORMC and to provide detailed instructions for designing input data. The theory of PORMC may be classified into two parts: (1) the deterministic governing differential equations and methods for their numerical solution, and (2) stochastic description of uncertain quantities and their incorporation into governing equations. The governing differential equations and methods for their numerical solution are common to PORMC and PORFLO-3. These are described in detail in the PORFLO-3 theory document (Sagar and Runchal 1990). For the sake of completeness, it is also incorporated in this report in a slightly modified form. The stochastic aspects are, however, unique to PORMC.

This document is organized as follows: Chapter 1.0 presents a brief description of the Hanford Site and an overview of the main features of PORMC. The theory of the model on which the computer code is based is provided in

¹PORFLO-3 Version 1.0 enhanced is copyrighted by Analytic and Computational Research, Incorporated, subject to the Limited Government License.

Chapter 2.0. Discussion on the structure of PORMC and a summary of the input and output options is given in Chapter 3.0. Chapter 4.0 provides a detailed description of all commands for creating an input data set.

Because most features (except those that require a stochastic description) are common to PORMC and PORFLO-3, major portions of the report are taken from the two earlier documents on PORFLO-3 (Runchal and Sagar 1989, Sagar and Runchal 1990).

1.3 BRIEF DESCRIPTION OF THE HANFORD SITE

1.3.1 Environmental Aspects

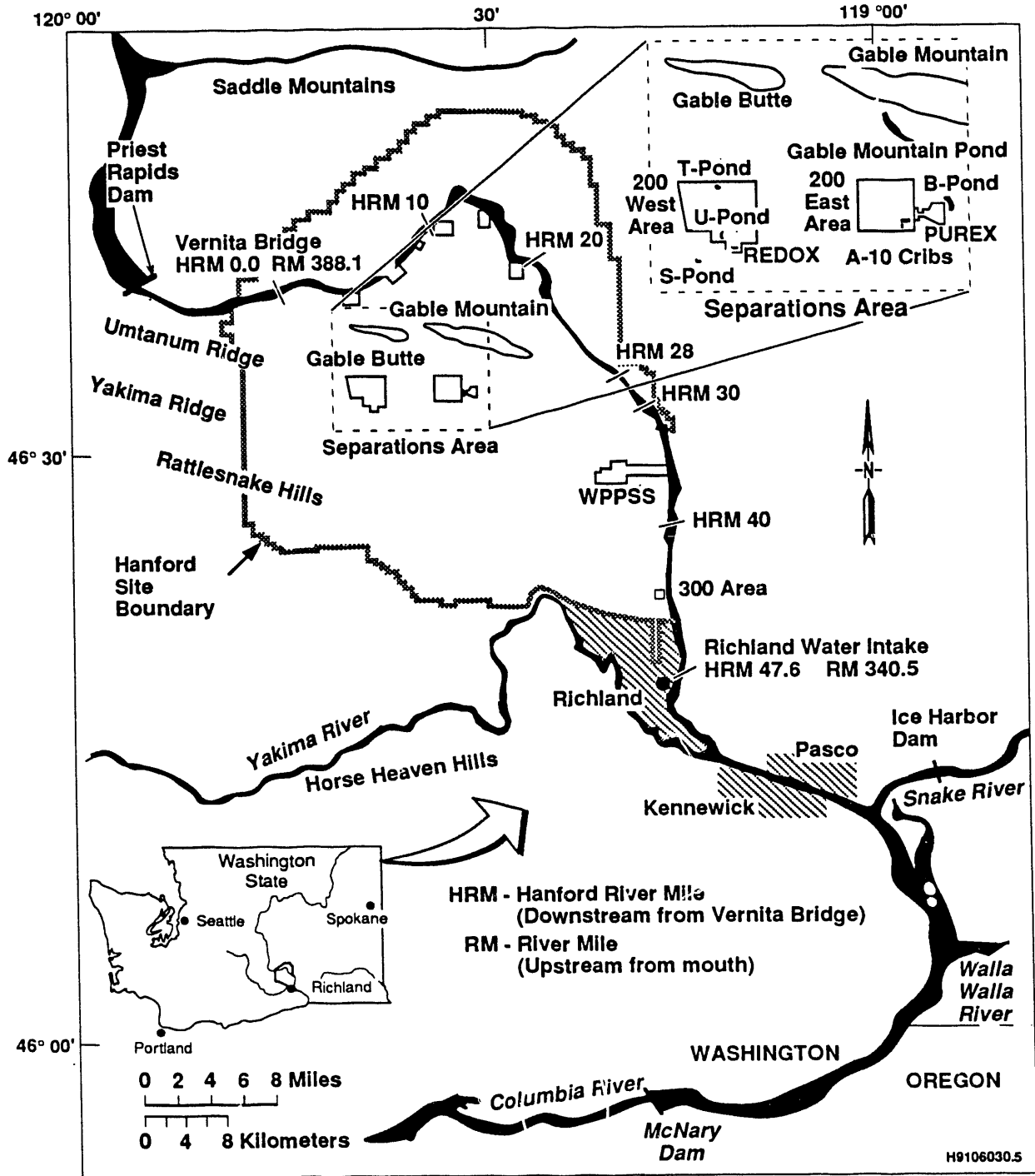
The Hanford Site, located in south-central Washington, has been dedicated to nuclear research and defense materials production, nuclear materials processing, and storage and disposal of nuclear and chemical process wastes since the early 1940's. During this time, the chemical processing of spent nuclear fuel for recovery of plutonium, uranium, and neptunium has produced the world's largest identified inventory of defense-related wastes. This waste contains fission products, relatively small quantities of actinides, and process chemicals. Some of the waste products originally were stored below the surface as liquids contained in 149 single-shell, steel-lined concrete tanks. Other liquid wastes with low-level radioactivity were disposed of to the soil column by ponds, cribs, trenches, and french drains. In addition, radioactively contaminated solids, such as equipment, paper, and clothing, have been buried in soil-covered trenches.

Leakage of a single-shell tank was first detected in 1956 (see Smoot and Sagar 1990 for analysis of a tank-leak problem using PORFLO-3). Starting in the early 1960's, work was initiated to convert the single-shell tank wastes to a stable, semisolid form consisting of salt cake and sludge that contains residual liquids trapped in the pore space of the solids. Transfer of free liquids from the single-shell tanks to underground double-shell tanks is part of an ongoing program of waste stabilization. Final disposal of the low-level fraction of the double-shell tank waste will be as grout monoliths enclosed in buried concrete vaults.

Figure 1-1 shows the location of the Hanford Site. Most of the Hanford Site occupies a terrace of the Columbia River (COE 1970). The elevation of the terrace increases gradually from about 112 m above mean sea level at Richland, Washington, to about 270 m in the northwest, and decreases to about 150 m in the northern part of the Hanford Site. The so-called Hanford Reach of the Columbia River, extending downstream from Priest Rapids Dam at River Mile 397 to the backwaters of McNary Dam, is free flowing. The flow of the Columbia River in the Hanford Reach is regulated by releases from Priest Rapids Dam.

The Hanford Site has a semiarid climate, with approximately 15 cm of annual precipitation and sparse vegetation. A fraction of the annual precipitation enters the vadose zone at the ground surface as natural recharge. The actual recharge depends on meteorologic conditions, soil properties, and vegetation, and may vary both spatially and temporally.

Figure 1-1. Location of the Hanford Site.



The UNSAT-H model (Fayer et al. 1986) has been developed to estimate recharge specific to the Hanford Site, using environmental data such as precipitation, temperature, and relative humidity.

Water balance data have been collected at selected locations on the Hanford Site during the past 10 yr (Gee et al. 1988). These data indicate that coarse-textured soils (i.e., soils that contain 90% or more sand-size or larger particles) that are sparsely vegetated or are covered with shallow-rooted grasses (e.g., cheatgrass or native bluegrass) are susceptible to drainage that is a significant proportion of precipitation, especially in winter. Drainage measurements in 1988, from 12 bare-surface lysimeters in the 300 Area of the Hanford Site, ranged from 3.1 to 5.6 cm/yr from precipitation of 12.5 cm/yr (Gee et al. 1988). In contrast, no drainage was measured at another lysimeter at the same location that was covered by deep-rooted (greater than 1 m) vegetation (e.g., tumble mustard).

In addition to the surface recharge at the scale of the Pasco Basin, natural recharge also occurs along the periphery of the basin from precipitation and ephemeral streams. Past waste disposal activities at the Hanford Site have contributed locally to recharge. Recharge from irrigated farming occurs east and north of the Columbia River and in the synclinal valleys west of the Hanford Site (Gephart et al. 1979). Upward leakage from confined intrabasalt aquifers to the overlying unconfined aquifer also is thought to occur within the northern and western sections of the Hanford Site. Groundwater discharge is principally into the Columbia River.

1.3.2 Vadose Zone Hydrogeology

The sediments overlying the basalts of the Hanford Site (suprabasalt sediments) were derived from a variety of sources. However, the fluvial-lacustrine Ringold Formation and glaciofluvial Hanford formation dominate (Bjornstad 1985). A brief description of these formations follows.

1.3.2.1 Ringold Formation. The Ringold Formation overlies the Elephant Mountain Member of the Saddle Mountains Basalt (Figure 1-2) and ranges in thickness from about 110 to 215 m. Based on texture, grain size, and stratigraphic position, the Ringold Formation has been divided into four units: basal, lower, middle, and upper.

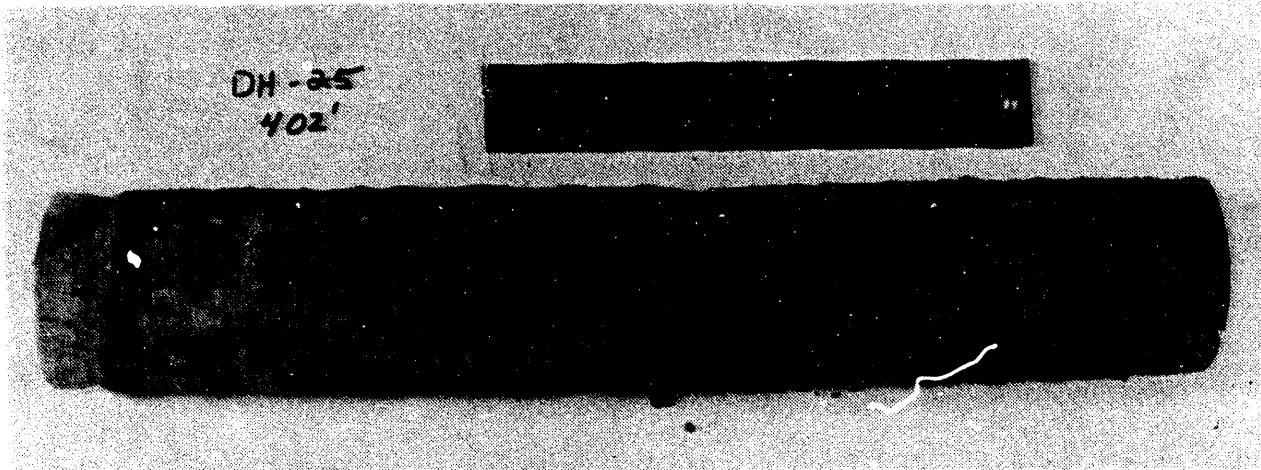
The basal Ringold unit, up to 60 m thick, has been divided into two subunits. The coarse-grained subunit is primarily gravelly sand, although lenses of sandy gravel and cross-bedded sand occur locally. Overlying the coarse-grained subunit is the fine-grained subunit, which is a conformable sequence of ripple-laminated micaceous muds and sands. This subunit includes and is capped by a well-developed paleosol sequence (Bjornstad 1985). This interval consists of a massive, bioturbated, olive-colored, clay-rich alluvial horizon. Subhorizontal stringers of light-colored pedogenic calcium carbonate occur toward the base of the paleosol (Figure 1-3). A 2- to 5-cm layer of tephra lies at or near the top of the paleosol sequence.

Figure 1-2. Typical Stratigraphic Units at the Hanford Site.

Period	Epoch	Group	Subgroup	Formation	K-Ar Age Years x 10 ⁶	Member (Formal and Informal)	Sediment Stratigraphy or Basalt Flows															
							Loess	Sand Dunes	Alluvium and Alluvial Fans	Land Slides	Talus	Colluvium										
QUATERNARY	Holocene	Columbia River Basalt Group	Yakima Basalt Subgroup	Hanford		Surficial Units																
														Pleistocene	Ringold	Touchet beds	Pasco gravels	Plio-Pleistocene unit	fanglomerate			
	upper Ringold																					
	middle Ringold																					
	lower Ringold																					
	basal Ringold																					
	TERTIARY														Miocene	Yakima Basalt Subgroup	Wanapum Basalt	Saddle Mountains Basalt	8.5	Ice Harbor Member	basalt of Goose Island	Ellensburg Formation
																					basalt of Martindale	
																					basalt of Basin City	
														Levey interbed								
basalt of Ward Gap																						
basalt of Elephant Mountain																						
10.5	Elephant Mountain Member	Rattlesnake Ridge interbed																				
		basalt of Pomona																				
12.0	Pomona Member	Selah interbed																				
		basalt of Gable Mountain																				
13.5	Esquatzel Member	Cold Creek interbed																				
		basalt of Huntzinger																				
14.5	Asotin Member	basalt of Lapwai																				
		basalt of Wahluke																				
14.5	Wilbur Creek Member	basalt of Sillusi																				
		basalt of Umatilla																				
14.5	Umatilla Member	Mabton interbed																				
		basalt of Lolo																				
14.5	Priest Rapids Member	basalt of Rosalia																				
		Quincy interbed																				
14.5	Roza Member	basalt of Roza																				
		Squaw Creek interbed																				
15.6	Frenchman Springs Member	basalt of Lyons Ferry																				
		basalt of Sentraal Gap																				
15.6	Sentinel Bluffs Unit	basalt of Sand Hollow																				
		basalt of Silver Falls																				
15.6	Sentinel Bluffs Unit	basalt of Ginkgo																				
		basalt of Palouse Falls																				
15.6	Sentinel Bluffs Unit	Vantage interbed																				
		basalt of Museum																				
15.6	Sentinel Bluffs Unit	basalt of Rocky Coulee																				
		basalt of Levering																				
15.6	Sentinel Bluffs Unit	basalt of Cohasset																				
		basalt of Birkett																				
15.6	Sentinel Bluffs Unit	basalt of McCoy Canyon																				
		basalt of Umtanum																				
16.5	Umtanum Unit	basalt of Benson Ranch																				
		Slack Canyon Unit																				
16.5	Slack Canyon Unit																					
		Ortley Unit																				
16.5	Grouse Creek Unit																					
		Wapshilla Ridge Unit																				
16.5	Grouse Creek Unit																					
		Mt. Horrible Unit																				
16.5	China Creek Unit																					
		Teepee Butte Unit																				
16.5	China Creek Unit																					
		Buckhorn Springs Unit																				
17.5	Rock Creek Unit																					
		American Bar Unit																				

*The Grande Ronde Basalt consists of at least 120 major basalt flows. Only a few flows have been named. N₂, R₂, N₁ and R₁ are magnetostratigraphic units.

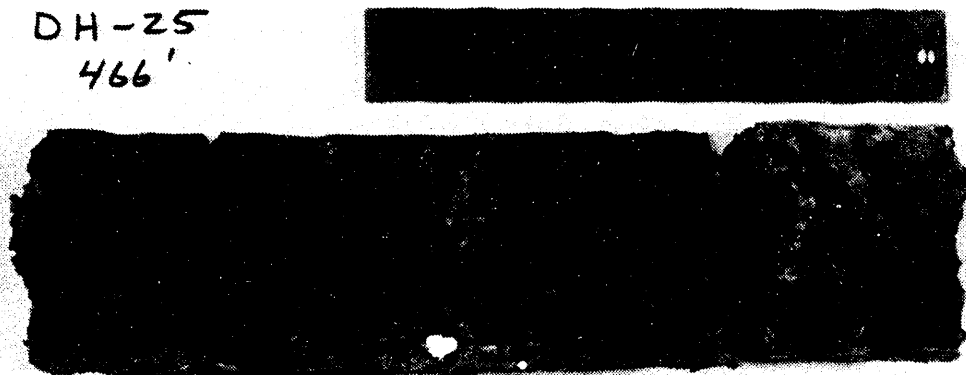
Figure 1-3. Core from a Segment of the Basal Ringold Paleosol Sequence. Light-colored subhorizontal layers are pedogenic calcium carbonate within illustrated clay.



Silt and clay of the lower Ringold unit, up to 16 m thick, overlie the basal Ringold unit. Sedimentary structures within the lower Ringold range from thin, rhythmic laminations at the base to generally more massive, irregular, and subhorizontal laminations upward. Occasionally, an interval of pale yellow to gray, even-laminated mud exists in the uppermost lower Ringold unit.

The middle Ringold unit is composed of stream gravel (Routson and Fecht 1979) and is the thickest of the suprabasalt units. These gravels consist mostly of quartzite, with lesser amounts of volcanic and plutonic clasts (Figure 1-4). The uniform, clast-supported texture of the middle Ringold unit is locally interrupted by thin zones of current-laminated sand and mud.

Figure 1-4. Core from Middle Ringold Unit that Consists of Semiconsolidated, Bimodal, Clast-Supported Conglomerate.



The upper Ringold unit consists of alternately bedded and laminated arkosic sand and mud that are representative of a low-energy fluvial and lacustrine environment. Its thickness varies considerably because of erosion by post-Ringold fluvial incision and cataclysmic flooding.

1.3.2.2 Hanford Formation. Varying in thickness from 5 m to 65 m, Pleistocene cataclysmic flood deposits of the Hanford formation also have a wide range of grain size. The two recognized units of the Hanford formation are the Pasco gravels and the Touchet beds.

The Pasco gravels are composed of basaltic, massive-to-laminated coarse sand, and/or large-scale, foreset-bedded gravel. They are mainly restricted to the Pleistocene flood bars and terraces that developed along high-energy flood channelways. The Touchet beds are a rhythmically bedded and fine-grained flood facies deposited away from main flood channelways in slack-water or backflooded areas during flooding (Waitt 1980). At many locations of the Hanford Site, Holocene surficial deposits of dune and sheet sand, alluvium, loess, and colluvium overlie the Hanford formation. The thickness of these deposits is a few meters.

1.3.3 Saturated Zone Hydrogeology

The principal geologic feature of the saturated zone of the Hanford Site is the layered nature of the Columbia River basalt flows; most conceptual models of the Hanford Site include this layered aspect. The other geologic features of hydrologic interest are the cooling joints and fractures and the intraflow structures that exist within individual basalt flows. The Columbia River Basalt Group is formally divided into five formations, from oldest to youngest: Imnaha Basalt, Picture George Basalt, Grande Ronde Basalt, Wanapum Basalt, and Saddle Mountains Basalt. Only the last three occur at the Hanford Site. A brief description of these three formations follows.

1.3.3.1 Grande Ronde Basalt. The Grande Ronde Basalt is geographically the most extensive and voluminous formation within the Columbia River Basalt Group. More than 50 flows of Grande Ronde Basalt underlie the Pasco Basin; however, relatively little is known about the hydrology of the lower 80% to 90% of the Grande Ronde Basalt. Flows of the Grande Ronde Basalt erupted from fissures and vents throughout the eastern half of the Columbia Plateau. These basalt flows are typically aphyric, although a few flows scattered throughout the section contain sparse to abundant plagioclase phenocrysts.

Aquifers of the Grande Ronde Basalt are confined to semiconfined (with some vertical leakage). The aquifers are regionally recharged along the margins of the Columbia Plateau where the flows crop out or are near the ground surface. Portions of the Columbia River and Snake River drainage systems intersect outcrops of the Grande Ronde Basalt; hence, direct recharge or discharge of its confined aquifers can occur at these locations.

1.3.3.2 Wanapum Basalt. The Wanapum Basalt consists of up to 26 flows that erupted from vents and fissures some 14.5 to 15.6 million years ago. This formation is the most extensively exposed of the Columbia Plateau. On the basis of chemistry, paleomagnetic polarity, lithology, and stratigraphic relationships (Swanson et al. 1979), the Wanapum Basalt formation has been

formally divided into five members: Eckler Mountain, Frenchman Springs, Roza, Priest Rapids, and Onaway. Its contact with the overlying Saddle Mountains Basalt is generally conformable, although local angular and erosional unconformities are known to exist.

Aquifers of the Wanapum Basalt are confined to semiconfined. Recharge to this formation is thought to occur (1) from precipitation where the Wanapum Basalt is not overlain by thick, younger basalts, (2) from leakage from adjoining formations, and (3) from surface and groundwater inflows from lands adjoining the Columbia Plateau. Within the Pasco Basin, recharge also occurs along the anticlinal ridges that bound the north and west parts of the basin. Intrabasin transfer and vertical leakage from adjacent formations also are believed to contribute to recharge and discharge of the Wanapum Basalt.

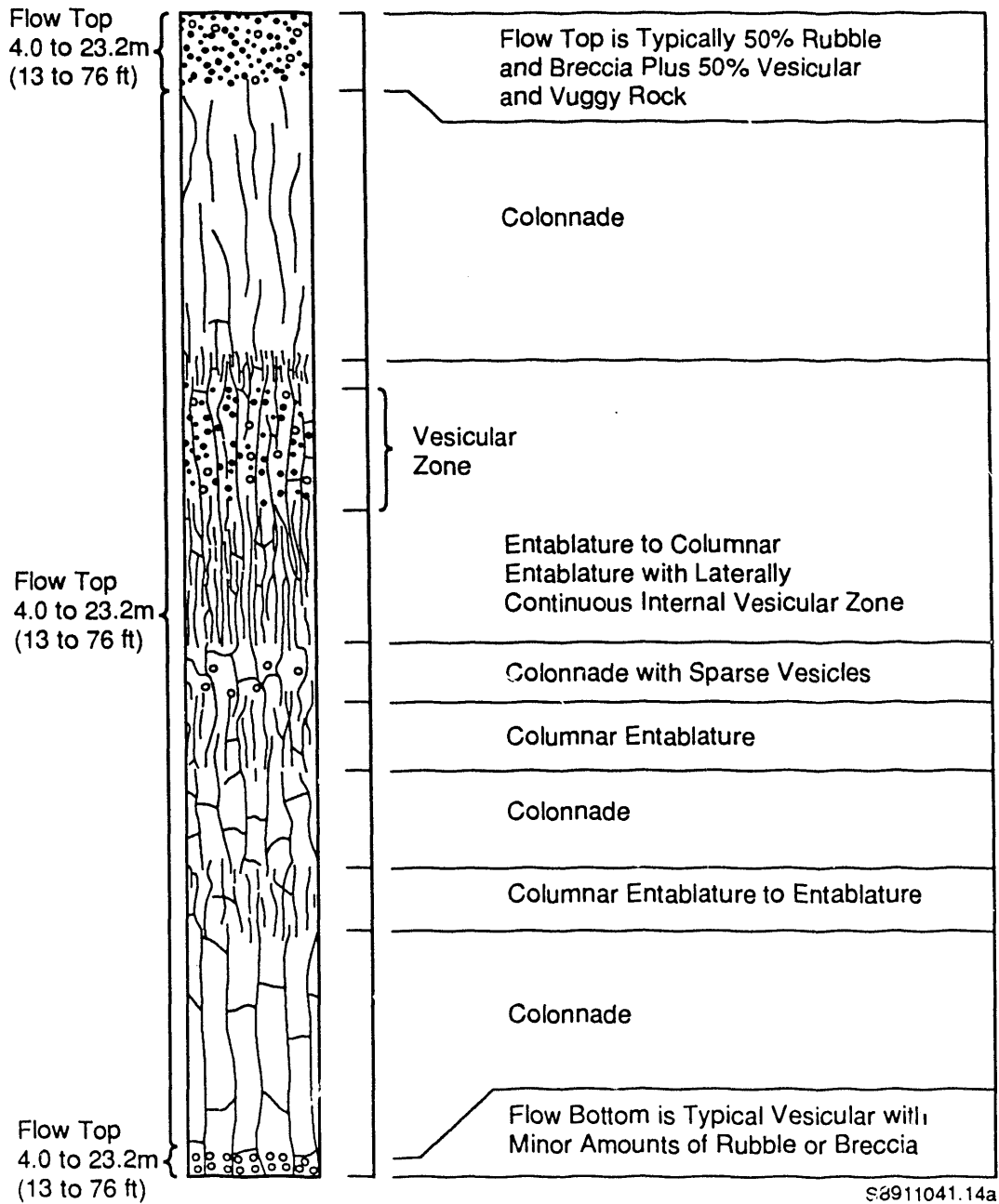
1.3.3.3 Saddle Mountains Basalt. The Saddle Mountains Basalt is the youngest formation (14.5 to 6 million years) of the Columbia River Basalt Group. It consists of 14 chemically diverse members. Up to 25% of the thickness between the top and bottom of this formation is composed of thick sedimentary interbeds of the Ellensburg Formation or equivalent sediments. The maximum thickness of the Saddle Mountains Basalt within the Pasco Basin is approximately 290 m.

Lateral groundwater movement through flows of the Saddle Mountains Basalt occurs in a semiconfined system. Recharge and discharge of this system are thought to occur locally. Recharge occurs at the periphery of the Pasco Basin, along anticlinal ridges, and from the overlying and underlying aquifers. Significant recharge is also derived from irrigation of the Columbia Basin Project in the eastern and the northeastern portions of the Pasco Basin (Gephart et al. 1979). Discharge is primarily to the Columbia River.

1.3.3.4 Intraflow Structures. Intraflow structures are primary, internal features that originated during the emplacement and consolidation of each basalt flow. These structures result from variation in cooling rates, degassing, thermal contraction, and interaction with surface water. Intraflow structures have groundwater flow properties that differ from those of the basalt formations as a whole. Consequently, the objectives of specific simulations may require that their hydrologic characteristics be included as distinct zones in the model.

Intraflow structures of a typical basalt flow are described according to their position in the flow: (1) flow top, (2) flow bottom, and (3) flow interior. Figure 1-5 depicts the various types of intraflow structures. The flow top is the chilled upper crust of the flow. It may consist of vesicular to scoriaceous basalt or it may be rubbly and brecciated. Flow top thicknesses are typically about 10% of the flow but may vary greatly. The flow bottom is predominantly a thin, glassy zone a few centimeters thick. The thickest flow bottoms observed in the Columbia River Basalt Group (as much as 30% of a flow) are associated with pillow-palagonite zones. Within the interior of a basalt flow, the predominant intraflow structures are zones characterized by patterns of cooling joints. These are commonly referred to as colonnade and entablature.

Figure 1-5. Typical Intraflow Structures of the Cohasset Flow.



1.3.3.5 Cooling Joints and Tectonic Fractures. Cooling joints in the Columbia River Basalt Group result from tensional stress in response to the contraction of solidified portions of a flow as it cools at temperatures below the solidus (Spry 1962). As primary features, cooling joints are distinct from secondary tectonic fractures such as faults, shear zones, and joint sets. Tectonic fractures are typically closely spaced, are located in parallel or subparallel zones, and are sometimes associated with clay minerals and breccia. Fractures resulting from tectonic forces are believed to be significantly less prevalent than those resulting from primary cooling. At the Hanford Site, field studies of the primary cooling joints and fractures of the deep basalt flows have been made to collect data on width and infilling characteristics (Lindberg 1986). Data on approximately 3,200 randomly selected primary cooling joints have been compiled from core samples. These data indicate that most fractures are completely filled by secondary minerals; in fact, only 19 of 3,200 were found to be even partially open. These observations suggest that very few discrete features need to be considered in simulating the groundwater system of the Hanford Site.

Nevertheless, some localized zones with discrete, unfilled, and extensively interconnected fractures are suspected to exist. Most of these zones may be associated with fracturing and faulting resulting from tectonic forces.

1.3.4 Factors Affecting Flow and Transport at the Hanford Site

The interior of Columbia River Basalt flows typically is very dense, with relatively low specific storage and hydraulic conductivity (DOE 1988), and low porosity (Leonhart et al. 1985). The entablature, which is generally below the flow top, is characterized by joint patterns that vary in orientation from nearly random to well-defined fanning columns. In contrast, the colonnade is composed of relatively uniform, vertically oriented, hexagonal columns (Long and WCC 1984). Because of its higher hydraulic conductivity, the basalt flow top generally forms the main pathway for groundwater movement. The amount of such detail included in a numerical simulation depends on the purpose of simulation; but for most large-scale simulations, the flow interiors and flow tops can be treated as distinct layers. For purposes of defining simulation problems on a regional scale, the combination of many flows into one composite layer would probably be appropriate.

Beneath the waste disposal areas of the Hanford Site, the basalt flows generally dip gently (less than a few degrees). Therefore, the choice of one axis of the model coordinate system as vertical and the other two as horizontal should be adequate to represent groundwater flow anisotropy. However, it is possible to explicitly consider the dip in modeling.

The geology of the basalt flows beneath the Hanford Site indicates that their compressibility is small. The value of specific storage in the basalts varies between 10^{-4} and 10^{-7} . Consequently, the neglect of rock deformation will not cause appreciable error in the groundwater flow simulations.

Laboratory measurements of heat transfer parameters such as bulk density, specific heat, and thermal conductivity have been obtained from block tests and tests on intact core samples from various basalt flows from beneath the

Hanford Site (Sublette 1983). These data indicate that the average values for different basalt flows are very similar, suggesting that there are no significant differences in thermal properties across a dense flow interior and that the average values are generally independent of horizontal location within a basalt flow. In addition, available data indicate that the thermal properties of the basalts are relatively weak functions of temperature. These considerations suggest that a relatively simple conceptual model for heat transfer is adequate.

Groundwater velocities in deep basalts with natural hydraulic gradients have been estimated to be small. This is primarily because of the small in situ hydraulic gradients and small hydraulic conductivities (Clifton 1986). Consequently, assumption of local thermal equilibrium between the geologic media and fluid is tenable, and the rate of convective heat transfer is relatively small. In terms of numerical significance, the buoyancy term of PORMC is probably the term of most importance in coupling fluid flow and heat transfer. Next in importance is the change in hydraulic conductivity caused by changes in the fluid density and viscosity because of thermal variations. The transient source term for the fluid is of comparatively minor significance.

The buoyancy term has been found to be significant for the simulation of fluid migration in the saturated zone of the Hanford Site. The vertical hydraulic gradients of the Hanford Site in areas free of manmade heat sources are known to be small (on the order of 10^{-3} to 10^{-4}). However, local (close to the thermal source) thermal buoyancy can create hydraulic gradients of up to two orders of magnitude greater than that of thermally undisturbed sites.

1.4 MAIN FEATURES OF PORMC VERSION 1.0

PORMC Version 1.0 (the version number will hereafter be omitted) is written in American National Standard Fortran 77 and is essentially independent of any specific computer hardware. Subroutines in PORMC 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 PORMC code is very flexible; several options are available to the user. By choosing appropriate combinations of these options, a wide range of problems can be solved. Methods for choosing and executing these options are discussed in subsequent chapters. The following sections of this chapter give an overview of the main features of PORMC.

1.4.1 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.

1.4.2 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.

1.4.3 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.

1.4.4 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.

1.4.5 Coupling of Equations

There are three main equations in PORMC, 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; 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).

1.4.6 Boundary Conditions

Varied types of boundary conditions can be specified in PORMC. 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. A seepage boundary condition for flow in the vadose zone is also included.

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, these equations can be solved in grids that are smaller than the total domain. 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.

1.4.7 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 PORMC is based on integrating the approximating functions for each grid element.

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, Gaussian Elimination, and conjugate gradients.

1.4.8 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-PORMC 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.

1.4.9 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 PORMC. 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, PORMC 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.

1.4.10 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 PORMC 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 manmade 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, because of 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 PORMC. The choice of this option will reduce the required grid sizes and computational time, but will only approximate the solutions in proximity to the features.

1.4.11 Pore Structure

The user can define up to three types of porosities in PORMC. The smallest type 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 not to contribute to fluid flow, but 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.

1.4.12 Sources and Sinks

Several options are provided in PORMC 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 can be constant or can vary with time. For mass, the sources can be limited by their inventory, solubility, or both.

1.4.13 Stochastic Parameters

Twenty-three of the input quantities in PORMC can be stochastic. These include the hydraulic, thermal, and mass transport properties of the solid matrix as well as the source terms. The stochastic variables may be cross-correlated. A limited number of variables may also be spatially autocorrelated.

1.4.14 Format-Free Input

The input to PORMC 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 PORMC 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 4.0 describes in detail all the keywords of the input and their associated alphanumeric data. Details of the preprocessor FREEFORM are provided in Appendix A (Runchal 1987).

1.5 SUMMARY

Several user-selected options in PORMC 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 PORMC, 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.

2.0 THEORETICAL BASIS OF PORMC

Three governing equations provide the mathematical basis for PORMC. The three dependent (or state) variables are (1) fluid pressure (or hydraulic head), (2) temperature, and (3) solute concentration. Application of the classic principles of the conservation of mass, momentum, and energy lead to these equations. To account for spatial and temporal uncertainty, many of the equation parameters are allowed to vary randomly. This introduces the stochastic aspects to PORMC, which also will be discussed in the following section.

In addition to the three governing equations, several auxiliary equations, including the equation of state and the constitutive equations, are used to complete the set of equations. The theoretical basis of these equations is well known and is described in detail by several texts (e.g., Bear 1972). The specific form of the equations employed in PORMC is described briefly in the following sections.

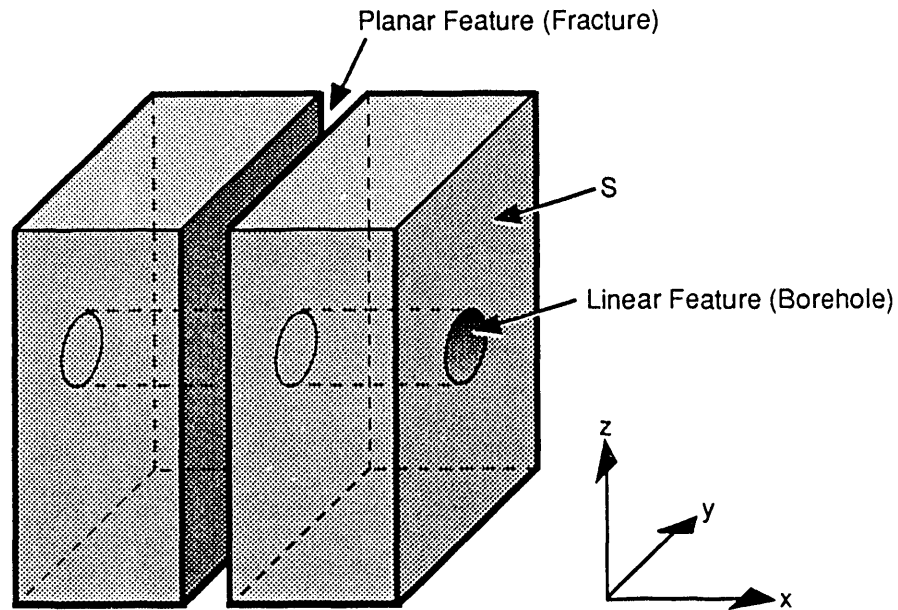
2.1 EQUATION FOR FLUID FLOW

2.1.1 The Equation of Continuity

Consider a control volume, V , bounded by a control surface, S , as shown in Figure 2-1. For deriving the equations, the control volume can be of any shape; the rectangular parallelepiped is used (Figure 2-1) because this is also the shape of the discrete elements (see Section 2.8.2) used for numerical solution in PORMC. The control volume is filled with rock or soil of uniform properties. The control volume may also contain a number of planar (e.g., fractures and clastic dikes) or linear features (e.g., boreholes). The volume of the rock (or soil) matrix in V is V_m . $V_p = V - V_m$ is the volume of planar and linear features. $V_p = 0$ in the absence of planar and linear features. Throughout this chapter, the subscripts m and p refer to rock matrix and planar (and linear) features.

The rock (or soil) and the planar and linear features are conceived as having three types of pores. The first type is interconnected and permits fluid flow. These pores constitute the effective (or flow) porosity, n_e , of the geologic media. The second type does not participate in fluid flow but is nevertheless filled with liquid and participates in heat and mass diffusion. The sum of the effective porosity and the porosity provided by these pores is termed diffusive porosity, n_d . The third type of pores is isolated from other pores and participates neither in fluid flow nor in heat and mass diffusion. These pores, however, conduct heat. The sum of the effective porosity, diffusive porosity, and the porosity provided by these isolated pores is termed total porosity, n_t . The effective porosity, n_e , in the control volume is assumed to be partitioned between liquid water and air. For conditions in which all of the n_e is filled with liquid water, the medium becomes fully saturated with liquid. ($n_d - n_e$) is assumed to be the residual water. The solids, liquid, and air (when present) are assumed to exist as continuous phases in the control volume.

Figure 2-1. Control Volume With Planar and Linear Features.



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The statement of mass conservation for the control volume may be stated as

$$\partial_t M = w - q_f, \quad (2.1-1)$$

where, at any time,

M = the total mass of liquid in V

q_f = the rate of fluid migration out of V across S

w = the rate of mass injection into V , across S .

The expression for M can be written as follows:

$$M = \int_{V_m} \theta_m \rho \, dV + \sum_i \int_{V_{p_i}} \theta_{p_i} \rho \, dV \quad (2.1-2)$$

where θ is the volumetric liquid content and ρ is the liquid density. The summation in Equation 2.1-2 is over the planar and linear features. It is

assumed that no mass interchange between the liquid and other phases (e.g., vapor) occurs. The expression for q_f is

$$q_f = \int_{S_m} \rho \vec{V}_m \cdot \vec{s}_m dS + \sum_i \int_{S_{p_i}} \rho \vec{V}_{p_i} \cdot \vec{s}_{p_i} dS \quad (2.1-3)$$

where \vec{V} is the apparent velocity vector of the fluid and \vec{s} is an outward unit normal to the surface, S . Note that the velocity in Equation 2.1-3 is not the real (pore) fluid velocity because flow is assumed to occur through the entire surface, S , irrespective of whether a specific point on it is occupied by a solid particle or a pore. In the following section this velocity is to be identified as the Darcy velocity. It is also apparent that only those fractures that intersect the bounding surface of the control volume appear in Equation 2.1-3.

Using Equations 2.1-1 to 2.1-3, it is possible to write the mass conservation equation in traditional differential form. However, for use in PORMC, the differential form presents no advantage, and the equations in the integral form are used. That is, the continuity equation of PORMC is

$$\int_{V_m} \partial_t [\theta_m \rho] dV + \sum_i \int_{V_{p_i}} \partial_t [\theta_{p_i} \rho] dV = - \int_{S_m} \rho \vec{V}_m \cdot \vec{s} dS - \sum_i \int \rho \vec{V}_{p_i} \cdot \vec{s}_{p_i} dS + w. \quad (2.1-4)$$

A similar continuity equation can also be written for the gas phase. However, in PORMC the gas phase is assumed to be at atmospheric pressure and passive, and therefore its motion is not considered.

The right side in Equation 2.1-4 contains the time derivatives of the volumetric moisture contained in the rock matrix and the planar features. The transformation of this term is explained in the following equations. (Because the transformation is the same for the rock matrix and the planar features, the subscripts are omitted.)

$$\partial_t(\theta \rho) = \theta \partial_t(\rho) + \rho \partial_t(\theta). \quad (2.1-5)$$

The fluid density, ρ , is, in general, a function of pressure (p) and temperature (T); i.e.,

$$\rho = \rho(p, T) \quad (2.1-6a)$$

and, therefore,

$$\partial_t(\rho) = \partial_p(\rho)|_T \partial_t(p) + \partial_T(\rho)|_p \partial_t(T). \quad (2.1-6b)$$

Defining fluid compressibilities as

$$\beta_p = (1/\rho) \partial_p(\rho)|_T \quad (2.1-7a)$$

and the fluid thermal expansion coefficient as

$$\beta_T = -(1/\rho) \partial_T(\rho)|_p, \quad (2.1-7b)$$

Equation 2.1-6b becomes

$$\partial_t(\rho) = \left[\beta_p \partial_t(p) - \beta_T \partial_t(T) \right] \rho. \quad (2.1-8a)$$

Instead of the thermodynamic pressure, p , a pseudo hydraulic head, P , is used as the dependent variable in PORMC. P is defined as

$$P = (p/\rho^*g) + z - z^* \quad (2.1-9a)$$

or

$$P = -\Psi + z - z^* \quad (2.1-9b)$$

where

ρ^* = the reference fluid density at a reference temperature and pressure

z^* = an arbitrarily defined datum from which z is measured

g = the gravitational acceleration.

Although a datum may be arbitrarily selected, it is most convenient to assign it to the water table, ground surface, or mean sea level elevation. Although z^* may be assigned any numerical value, it is usually convenient to give it a value of zero by locating the origin of the coordinate axes at the datum.

The new variable, P (units of length), is a normalized pressure that is equivalent to hydraulic head defined with respect to the reference density ρ^* . However, P is not a true potential function because potential would be defined with respect to the local fluid density. The thermodynamic liquid pressure, p , is negative (less than atmospheric pressure, which is taken to be zero) in

partially saturated media and is positive in fully saturated media. For partially saturated systems, soil-moisture tension, Ψ , is defined as indicated in Equation 2.1-9b. Soil-moisture tension is defined only when saturation, σ , is less than 1. Note that it is not physically possible for saturation to be negative.

In terms of P, Equation 2.1-8a becomes

$$\partial_t(\rho) = [\beta_p \rho^* g \partial_t(P) - \beta_T \partial_t(T)] \rho. \quad (2.1-8b)$$

The volumetric moisture content, θ , in Equation 2.1-5 is a product of diffusive porosity (n_D) and σ . For saturated media, $\sigma = 1$ (constant) and n_D is a much stronger function of p than it is of T. For unsaturated media, n_D remains constant and σ varies. Consequently, for saturated media, neglecting temperature effects on n_D , the variation of θ may be written as

$$\partial_t(\theta) = \partial_t(n_D) = \partial_p(n_D) \partial_t(p) \quad (2.1-10a)$$

and for unsaturated media

$$\partial_t(\theta) = n_D \partial_p(\sigma) \partial_t(p). \quad (2.1-10b)$$

Defining porous media compressibility as

$$\alpha_p = \partial_p(n_D) \quad (2.1-11)$$

Equation 2.1-10a becomes, in terms of P,

$$\partial_t(\theta) = \alpha_p \rho^* g \partial_t(P) \quad (2.1-12a)$$

while Equation 2.1-10b, in terms of P, takes the form

$$\partial_t(\theta) = n_D \partial_p(\sigma) \partial_t(P). \quad (2.1-12b)$$

Substituting Equations 2.1-8b and 2.1-12a into Equation 2.1-5,

$$\begin{aligned} \partial_t (\theta \rho) &= (\alpha_p + \eta_b \beta_p) \rho g \rho^* \partial_t(P) \\ &\quad - \eta_b \rho \beta_T \partial_t(T) \text{ if } \sigma = 1, \end{aligned} \quad (2.1-13a)$$

and for $\sigma < 1$, using Equation 2.1-12b,

$$\partial_t(\theta \rho) = \eta_b \partial_p(\sigma) \rho \partial_t(P) - \theta \rho \beta_T \partial_t(T), \quad \sigma < 1. \quad (2.1-13b)$$

On the right-hand side of Equations 2.1-13a and -13b, the first term is a 'storage' term; the second term depends on time variation of temperature and couples the pressure equation to the temperature equation. For fully saturated media ($\sigma = 1$), the coefficient of specific storage is defined as

$$S_s = (\alpha_p + \eta_b \beta_p) \rho^* g. \quad (2.1-14a)$$

The units of S_s are (1/L) where L denotes length dimension (e.g., feet or meters). For partially saturated media ($\sigma < 1$), the coefficient of specific storage is taken to be

$$S_s = \eta_b \partial_p(\sigma). \quad (2.1-14b)$$

Commonly, S_s for unsaturated media is written in terms of Ψ , which is

$$S_s = -\partial_\Psi(\theta), \quad \sigma < 1 \text{ (unsaturated)}. \quad (2.1-14c)$$

For unsaturated media, the $\Psi - \theta$ relationship is known as the soil (or rock) characteristic curve and is experimentally determined. For saturated media, either the liquid and soil or rock compressibilities can be specified (from which the coefficient of specific storage can be estimated) or the coefficient of specific storage can be directly specified. The second option, that of specifying S_s , is adopted in PORMC. The reason for specifying S_s (rather than compressibilities) for saturated media is that this parameter is usually directly estimated from analysis of pumping-test data. In terms of S_s , the time derivative in Equation 2.1-5 becomes

$$\partial_t(\theta \rho) = \rho S_s \partial_t(P) - \theta \rho \beta \partial_t(T). \quad (2.1-15)$$

Just like the pressure, P, within a control volume, the temperature, T, in the rock matrix and the planar features also are assumed to be the same.

2.1.2 Darcy's Law for Flow Dynamics

The velocity vector, \vec{V} , in Equation 2.1-4 must be obtained from dynamic considerations. Applications of the principle of conservation of momentum leads to the Navier Stokes equations (Bear 1972). For laminar flow with low velocities through porous media, the much simpler Darcy's equation is employed. Darcy's equation, which originated from experimental observations, has subsequently been derived from basic principles by assuming that the inertial forces are negligible (Hassanizadeh 1986a, 1986b). This equation is

$$\vec{V} = -(\underline{k}_s k_r / \mu) \{ \vec{\nabla} p + \rho \vec{g} \} \quad (2.1-16a)$$

where

\underline{k}_s = the saturated intrinsic permeability tensor

k_r = the (scaler) relative permeability

μ = the fluid dynamic viscosity

p = the thermodynamic pressure

\vec{g} = the gravitational vector in the adopted coordinate system

z = the coordinate in the vertical direction.

The x and y coordinates are assumed to be in the horizontal plane. If the z -axis is taken to be vertical, $g_x = g_y = 0$, and $g_z = g = 9.81 \text{ m/s}^2$. In terms of P , Equation 2.1-16a becomes

$$\vec{V} = -(\underline{k}_s k_r \rho^* g / \mu) \{ \vec{\nabla} p + (\rho / \rho^*) (\vec{g} / g) - \vec{\nabla} z \}. \quad (2.1-16b)$$

In Equations 2.1-16a and -16b, \underline{k}_s is a property of the porous medium. For anisotropic media, \underline{k}_s is a tensor of the second order. For the equations in PORMC, it is assumed that the coordinate directions coincide with the principal directions of \underline{k}_s , so that all the off-diagonal components of the \underline{k}_s tensor are zero. On the other hand, k_r is a scaler and is unity for fully saturated media. For partially saturated media, $0 \leq k_r \leq 1$. The estimation of k_r will be discussed in Section 2.7.3. Equation 2.1-16b applies to the estimation of velocity in both the rock matrix and the planar features.

The limits of applicability of the Darcy flow equation for saturated flow have been explored by several investigators (Bear 1972, Cheng 1978). These researchers generally believe that Equations 2.1-16a and -16b are applicable

without appreciable error for flows with a Reynold's number of less than 10, where the Reynold's number is based on a representative grain size of the equivalent porous medium.

2.1.3 Governing Equation for Hydraulic Head

The governing equation in terms of P is obtained by substituting Equations 2.1-15 and 2.1-16b in Equation 2.1-4. This equation is

$$\begin{aligned}
 & \int_{V_n} R S_{s_n} \partial_t [P] dV + \sum_i \int_{V_{p_i}} R S_{s_{p_i}} \partial_t [P] dV \\
 & = \int_{S_n} R \xi \underline{k}_m k_r [\vec{\nabla}P + R \zeta - \vec{\nabla}z] dS + \sum_i \int_{S_{p_i}} R \\
 & \quad \xi \underline{k}_{p_i} k_r [\vec{\nabla}P + R \zeta - \vec{\nabla}z] dS \\
 & + \int_{V_n} w_V dV + \int_V w_{m_r} dV + \sum_i \int_{V_{p_i}} w_{p_r_i} dV
 \end{aligned} \tag{2.1-17}$$

where

$$R = \rho/\rho^* \tag{2.1-18a}$$

$$\underline{k}_m = (\underline{k}_m \rho^* g/\mu^*) \tag{2.1-18b}$$

$$\underline{k}_p = (\underline{k}_p \rho^* g/\mu^*) \tag{2.1-18c}$$

$$\xi = \mu^*/\mu \tag{2.1-18d}$$

$$\zeta = \vec{g}/g \tag{2.1-18e}$$

$$w_V = m/\rho^* \tag{2.1-18f}$$

$$w_m = \theta_m R \beta_T \partial_t(T) \quad (2.1-18g)$$

$$w_{p_r} = \theta_p R \beta_T \partial_t(T). \quad (2.1-18h)$$

Note that even though the pressure and the temperature are assumed to be the same in the planar feature and the rock matrix within a control volume, the mass and energy fluxes through them are different.

2.1.4 Equations for Velocity Components

The equations for the Darcy velocity are now written as

$$U = -K_x [\partial_x P + g_x] \quad (2.1-19a)$$

$$V = -K_y [\partial_y P + g_y] \quad (2.1-19b)$$

$$W = -K_z [\partial_z P + g_z - 1] \quad (2.1-19c)$$

where K_x , K_y , and K_z are the principal components of the hydraulic conductivity tensor, \underline{k} , in the x, y, and z directions, respectively.

The average fluid velocity in the pores (i.e., the pore velocity) is obtained by dividing the Darcy velocity by the effective porosity, n_E . The effective (or flow) porosity, n_E , is different from the total porosity, n_T , in that n_E is based on only those pores that are interconnected and through which fluid flow occurs. These velocity components are given by

$$u = U / n_E \quad (2.1-20a)$$

$$v = V / n_E \quad (2.1-20b)$$

$$w = W / n_E. \quad (2.1-20c)$$

2.2 EQUATION FOR HEAT TRANSFER

2.2.1 Conservation of Thermal Energy

From the Second Law of Thermodynamics, it follows that the rate of increase of the total energy of a system in a control volume, \mathcal{V} , must be equal to the rate of energy generation inside \mathcal{V} minus the rate at which energy flows

out the boundary, S (Figure 2-1), minus the rate at which work is done by the control volume on the surroundings.

Generally, the total energy of a system consists of (1) the internal energy resulting from molecular motion, (2) the kinetic energy, (3) the potential energy, and (4) other energy forms such as electromagnetic, nuclear, and chemical.

Compared to the internal energy of the system, the changes in the kinetic and potential energy are negligible because the solid component of the fluid-solid matrix is nearly stationary, the fluid moves relatively slowly, and the gravitational (potential) force is time-independent and constant for all practical purposes (Bird et al. 1966, p. 314). The other forms of energy mentioned previously also are assumed to be negligible. Consequently, the rate of change of energy of the system, E , is given by

$$E = \partial_t \int_{V_m} \rho_e e_e dV + \sum_i \partial_t \int_{V_{p_i}} \rho_{e_{p_i}} e_{e_{p_i}} dV \quad (2.2-1)$$

where

ρ_e = the effective mass density (i.e., composite density of the solid-fluid matrix)

e_e = the internal energy per unit mass of the fluid-solid matrix

m and p = the rock matrix and the planar (or linear) features, respectively.

The rate at which energy leaves the control volume is given by

$$Q_T = \int_{S_m} (\rho \vec{V}_m e_m + \vec{q}_{T_m} + \vec{q}_{D_m}) \cdot \vec{s}_m dS + \sum_i \int_{S_{p_i}} (\rho \vec{V}_{p_i} e_{p_i} + \vec{q}_{T_{p_i}} + \vec{q}_{D_{p_i}}) \cdot \vec{s}_{p_i} dS \quad (2.2-2)$$

where

ρ = the density

e = the internal energy of the fluid per unit volume

\vec{q}_T = the energy flux resulting from thermal conduction

\vec{q}_D = the energy flux resulting from mechanical dispersion (Bear 1972, p. 644).

Other forms of energy exchange, such as those resulting from radiation and the Dufour effect, are assumed to be negligible.

With S_T as the rate of energy generation per unit volume of the system, the total energy generated in the control volume is given by

$$E_T = \int_V S_T dV. \quad (2.2-3)$$

The work done by the system on the surroundings is composed of external work and internal work because of the normal (pressure) and shear (viscous) forces in the fluid. In PORMC, the former is assumed to be included in the S_T term and the latter is considered to be negligible because of the relatively low velocity of the fluid (an alternative argument leads to the same conclusion in Bird et al. 1960, p. 314).

The equation expressing energy conservation for the control volume, V , is obtained by combining Equations 2.2-1 through 2.1-3 as

$$\begin{aligned} & \partial_t \int_V \rho_{e_m} e_{e_m} dV + \sum_i \partial_t \int_{V_{p_i}} \rho_{e_{p_i}} e_{e_{p_i}} dV \\ & + \int_{S_m} (\rho \vec{V}_m e + \vec{q}_{T_m} + \vec{q}_{D_m}) \\ & \bullet \vec{s}_m dS + \sum_i \int_{S_{p_i}} (\rho \vec{V}_{p_i} e_{p_i} \\ & + \vec{q}_{T_{p_i}} + \vec{q}_{D_{p_i}}) \\ & \bullet \vec{s}_{p_i} dS + \int_V S_T dV = 0. \end{aligned} \quad (2.2-4)$$

2.2.2 Governing Equation for Temperature

The following relations are applicable to both the rock matrix and the planar features. For convenience of writing, subscripts (m and p) are omitted from these equations. Assuming that the fluid and solid are in thermal equilibrium, the internal energy of the fluid-solid matrix is given by

$$\rho_e e_e = \rho_e c_e T. \quad (2.2-5)$$

The volumetric specific heat ($\rho_e c_e$) of the composite solid-liquid matrix depends on the amount of liquid (the specific heat of gas is neglected) present in the matrix; i.e.,

$$\rho_e c_e = \eta_T \rho c_f + (1-\eta_T) \rho_s c_s \quad (2.2-6a)$$

where η_T is defined as

$$\eta_T = n_T - n_D + \theta. \quad (2.2-6b)$$

In writing Equation 2.2-6b, it is assumed that the pore space defined by $(n_T - n_E)$ is filled with liquid. Although some of this liquid is immobile, it stores heat and participates in heat conduction. In saturated media, $\theta = n_D$ and the total porosity participates in heat conduction. In Equation 2.2-6a, ρ_s and c_s are, respectively, the density and specific heat of the solid matrix, and c_f is the specific heat of the pore liquid.

From Fourier's Law, the heat conduction term is written as

$$\vec{q}_T = -k_e \vec{\nabla} T \quad (2.2-7)$$

where the effective thermal conductivity of the fluid-solid matrix, k_e , is given by

$$k_e = \eta_T k_f + (1-\eta_T) k_s \quad (2.2-8)$$

with k_f and k_s as the coefficients of thermal conductivity for the fluid and the solid, respectively.

The mechanical dispersion (Bear 1972, p. 646) term is written as

$$\vec{q}_D = -\rho c_f \eta_D \underline{D} \vec{\nabla} T \quad (2.2-9)$$

where \underline{D} is a second-order tensor of mechanical dispersion, the nature of which is discussed in Section 2.7.4. Assuming that mechanical dispersion occurs only in the flowing fluid, η_D is defined as

$$\eta_D = \theta - (n_T - n_E). \quad (2.2-10)$$

Substitution of Equations 2.2-5, 2.2-7, and 2.2-9 into Equation 2.2-4, with the assumption that $\rho_e c_e$ is independent of time, leads to the governing equation for temperature

$$\begin{aligned}
 & \partial_t \int_{V_m} \rho_e c_e dV + \sum_i \partial_t \int_{V_{p_i}} \rho_{e_{p_i}} c_{e_{p_i}} dV \\
 & + \int_{S_m} [\rho \vec{V}_m \zeta T \\
 & - (k_e + \rho c_f \eta_{D_m} D_m) \vec{\nabla} T] \\
 & \bullet \vec{s}_m dS + \sum_i \int_{S_{p_i}} [\rho \vec{V}_{p_i} \zeta T \\
 & - (k_{e_{p_i}} + \rho c_f \eta_{D_{p_i}} D_{p_i}) \vec{\nabla} T] \\
 & \bullet \vec{s}_{p_i} dS + \int_V S_T dV = 0.
 \end{aligned} \tag{2.2-11}$$

2.3 EQUATION FOR MASS TRANSFER

2.3.1 Conservation of Chemical Species

The derivation of an equation for conservation of chemical species parallels that for the conservation of heat. From the principle of mass conservation, it follows that the rate of change of the mass of a chemical species in a control volume, V , must be equal to the sum of the rate at which the species is added through the boundary, S , of the control volume and the rate of species generation inside the volume (Figure 2-1) minus the rate at which the species is consumed through chemical reaction or radioactive decay.

The rate of change of mass of a species in control volume, V , is given by

$$\partial_t M_c = \partial_t \left[\int_{V_m} C_{e_m} dV \right] + \partial_t \sum_i \left[\int_{V_{p_i}} C_{e_{p_i}} dV \right] \tag{2.3-1}$$

where C_e is the mass density (or concentration) of the chemical species.

The rate at which the species leaves the control volume is given by

$$\begin{aligned} \vec{J}_c = & - \int_{S_m} (\vec{V}_m C_m + \vec{J}_c + \vec{J}_d) \cdot \vec{s}_m dS \\ & - \sum_i \int_{S_{p_i}} (\vec{V}_{p_i} C_{p_i} + \vec{J}_{c_{p_i}} + \vec{J}_{d_{p_i}}) \cdot \vec{s}_{p_i} dS \end{aligned} \quad (2.3-2)$$

where

C = the mass of the species in fluid per unit volume of fluid

\vec{J}_c = the species flux as a result of diffusion

\vec{J}_d = the flux as a result of dispersion (Bear 1972, p. 643).

Other forms of species exchange, such as those due to the Soret effect, are assumed to be negligible in PORMC.

With S_c as the rate of mass species generation due to direct injection and chemical reaction per unit volume of the system, the rate of increase of the species in the control volume is

$$E_c = \int_V S_c dV. \quad (2.3-3)$$

With R_c as the rate of reaction or decay, the rate of disappearance of the chemical species because of either radioactive decay or an Arrhenious-type chemical reaction in the fluid-solid matrix is given by

$$e_c = - \int_V R_c C_e dV. \quad (2.3-4)$$

Combining Equations 2.3-1 through 2.3-4 results in the governing equation for the conservation of chemical species:

$$\begin{aligned}
 \partial_t \left[\int_{V_m} C_{e_m} dV \right] + \partial_t \sum_i \left[\int_{V_{p_i}} C_{e_{p_i}} dV \right] = \\
 - \int_{S_m} (\vec{V}_m C_{e_m} + \vec{J}_{c^+} + \vec{J}_d) \cdot \vec{s}_m dS \\
 - \sum_i \int_{S_{p_i}} (\vec{V}_{p_i} C_{e_{p_i}} + \vec{J}_{c_{p_i}} \\
 + \vec{J}_{d_{p_i}}) \cdot \vec{s}_{p_i} dS + \int_V S_c dV \\
 - \int_V R_c C_e dV.
 \end{aligned}
 \tag{2.3-5}$$

2.3.2 Governing Equation for Species Concentration

The quantity C_e in Equation 2.3-5 depends on the way in which a chemical species is partitioned between the solid matrix and the fluid. This is true of the rock matrix as well as the planar features. For convenience in the following equations, the subscripts m and p are not used. Denoting by C and C_s the concentrations in the fluid and solid, respectively, C_e may be written as

$$C_e = \theta C + (1-\eta_T) C_s
 \tag{2.3-6}$$

assuming that no chemical species is contained in the isolated pores ($n_T - n_D$) (i.e., the processes of convection, diffusion, and dispersion do not exchange mass in these pores). Consequently, the liquid in these pores participates only in heat conduction.

In PORMC, adsorption-desorption processes are considered to be responsible for the partitioning of a radionuclide or chemical mass between the fluid and the solid phases. In general, descriptions of the sorption process may be grouped into two classes, local equilibrium models and disequilibrium models. For either class, sorption occurs at the interface between the liquid film and solid surface. The disequilibrium models assume that there is a time-dependent mass exchange between the immobile and mobile liquids and also between these liquids and the solid phase (Goltz and Roberts 1988).

The more complex of these models assumes a specific geometry for the immobile region (Sudicky and Frind 1982). Mass is then diffused from the immobile to the mobile region. The disequilibrium models result in one concentration equation for the mobile regions and one for the immobile regions, and require extra parameters to characterize the processes.

The local equilibrium models assume that the solid and liquid phases are in continuously reversible equilibrium; i.e., any change in the concentration in the liquid is accompanied by an instantaneous, corresponding change in the concentration in the solid phase. In addition, the concentration in the mobile and the immobile regions is assumed to be the same. In the simplest of these models included in PORMC, the solid surface available for sorption is assumed to be inversely proportional to the density of solids. In addition, this model assumes that the sorption process is described by a linear Freundlich isotherm such that for saturated media

$$C_s = \rho_s k_d C \quad (2.3-7a)$$

where k_d is variously called the distribution, sorption, or partition coefficient (Freeze and Cherry 1979, p. 403). Equation 2.3-7a implicitly assumes that the adsorption reaction is fully reversible (i.e., as the concentration, C , in the solution decreases, the mass adsorbed by the solids is released back into the solution).

One additional assumption regarding the extent of a wetted surface for conditions of variable saturation is required before Equation 2.3-7a can be used for unsaturated media. One assumption that could be made is that the fluid will wet all of the available solid surface, regardless of liquid saturation. With this assumption, which appears to be appropriate for higher saturations, Equation 2.3-7a requires no modification. On the other hand, especially at lower saturations, an assumption could be made that some of the pores are dry and, therefore, that the solid surface available for sorption is proportional to saturation. With such an assumption, Equation 2.3-7a is modified to

$$C_s = \sigma \rho_s k_d C. \quad (2.3-7b)$$

Substitution of Equation 2.3-7a into Equation 2.3-6 leads to

$$C_e = \theta C + (1-\eta_T) \rho_s k_d C \quad (2.3-8)$$

which can be written as

$$C_e = \theta C \left[1 + \frac{(1-\eta_T)\rho_s k_d}{\theta} \right]. \quad (2.3-9a)$$

On the other hand, substitution of Equation 2.3-7b into Equation 2.3-6 leads to

$$C_e = \theta C \left[1 + \frac{(1-\eta_T)\rho_s k_d}{\eta_D} \right]. \quad (2.3-9b)$$

The quantity enclosed by the brackets in Equations 2.3-9a and -9b is termed the retardation coefficient, R_D . In terms of R_D , Equations 2.3-9a and -9b become

$$C_e = \theta R_D C. \quad (2.3-10)$$

In moving fluid, R_D depicts the ratio between the migration velocity of the fluid and the migration velocity of the radionuclide or chemical species. In general, it is analogous to the heat capacity in the heat transfer equation or to specific storage in the flow equation. It represents the capacity of the medium to store the chemical species. In the present version of PORMC, R_D is given in terms of the definition provided by Equation 2.3-9b. This definition is used because at higher saturations $\theta \rightarrow n_D$, and at lower saturations Equation 2.3-9b may be more appropriate.

From Fick's Law, the diffusion flux term is written as

$$\vec{j}^C = -\theta D_M \vec{\nabla} C \quad (2.3-11)$$

where D_M is the molecular diffusivity of species in the fluid. In saturated media, $\theta = n_D$ and the entire diffusive porosity participates in mass exchange through molecular diffusion.

The mechanical dispersion term is written as (Bear 1972, p. 646)

$$\vec{j}^D = -\eta_D \underline{\underline{D}} \vec{\nabla} C \quad (2.3-12)$$

where $\underline{\underline{D}}$ is a second-order tensor of fluid dispersion that is discussed in Section 2.7.4.

Substitution of Equations 2.3-6 through 2.3-12 in Equation 2.3-5 leads to the species concentration equation

$$\begin{aligned}
 \partial_t \left[\int_{V_m} \theta_m R_{D_m} C \, dV \right] + \partial_t \sum_i \left[\int_{V_{p_i}} \theta_{p_i} R_{D_{p_i}} C \, dV \right] = \\
 - \int_{S_m} \left[\vec{V}_m C + \left(\theta_m D_M + \eta_{D_m} D_m \right) \vec{\nabla} C \right] \cdot \vec{s}_m \, dS \\
 - \sum_i \int_{S_{p_i}} \left[\vec{V}_{p_i} C + \left(\theta_{p_i} D_{p_i} + \eta_{D_{p_i}} D_{p_i} \right) \vec{\nabla} C \right] \\
 \cdot \vec{s}_{p_i} \, dS + \int_V S_C \, dV - \int_{V_m} \theta_m R_{D_m} R_C C \, dV \\
 - \sum_i \int_{V_{p_i}} \theta_{p_i} R_{D_{p_i}} R_C C \, dV.
 \end{aligned} \tag{2.3-13}$$

2.4 COMMENTS ON INCLUSION OF FRACTURES AND BOREHOLES

Governing equations in terms of P, T, and C presented in Sections 2.1 to 2.3 explicitly consider the presence of features such as fractures and boreholes. The derivation in Sections 2.1 to 2.3 is contingent on the basic assumption that the values of pressure, temperature, and concentration in a fracture and the surrounding rock matrix within a control volume are the same. Implications of this assumption are (1) the control volume is suitably small and (2) the fractures and the rock matrix within a control volume attain equilibrium in a period much shorter than the time of interest. Obviously, this approach will not provide a correct picture of the fracture-matrix interaction at a scale smaller than that of the control volume.

Another obvious method of considering flow and transport through fractures (a method requiring no additional assumptions and therefore probably the most correct) would be to explicitly consider fractures as defining zones that are distinct from the adjoining rock (or soil) matrix. Such a method has been used by various researchers for small-scale problems in which only one or two fractures are involved (e.g., Wang and Narasimhan 1985). Significantly larger numbers of fractures would tax the memory capability of even the largest computer. This method has the advantage that pressures, temperatures, and concentrations have values in the fractures that are distinct from those in the rock, thus permitting a continuous exchange of fluid, energy, and species between the fractures and the adjacent medium.

A third method of incorporating fractures (or other such features) is to treat them as part of a composite media and not distinguish between the fractures and the rock. This method requires that the flow and transport properties of the composite media be specified. This method is preferred for conditions in which numerous randomly distributed fractures exist. In such cases, field testing usually would provide values of parameters for the composite media. In any case, testing of each specific fracture would not be practical.

A fourth method for incorporating fractures in flow and transport models, although not available in PORMC, is to assume a dual porosity (rock matrix and fracture) and solve the separate but coupled equations. The coupling term in this formulation is the source/sink created by the interaction between the fractures and rock matrix at the control volume scale. This method is not available because the two separate equations used in the dual-porosity formulation are not consistent with the formulation of PORMC.

In all the methods previously discussed, both the fractures and the boreholes are considered to be filled with porous material; consequently, the flow is assumed to be Darcian. This assumption is not considered to be a limitation of the code, because even for open fractures, a Darcian flow equation is commonly invoked in which a surrogate hydraulic conductivity is specified based on the "cubic law" or a variant (Snow 1969, Sagar and Runchal 1982). The open boreholes or other manmade excavations usually act as internal boundary conditions with fixed heads and can be treated as such. For example, an open tunnel or shaft would be at atmospheric pressure, while an open borehole filled with water would be at hydrostatic pressure.

2.5 THE COUPLING TERMS

The pressure and the temperature equations are coupled to each other through the fluid properties and the velocity components. The matrix properties, specific storage coefficient, and hydraulic conductivities are functions of fluid density and viscosity (Section 2.1.1). The latter, in turn, are functions of the temperature (the dependence of these on pressure is neglected in PORMC; Section 2.7.1). The buoyancy term arises in response to differences in fluid densities created by the temperature field. This term accounts for the natural convection caused by the thermal field.

Another coupling comes from the fluid expansion term on the right side of Equation 2.1-17. This term contains a product of the fluid thermal expansion coefficient and the time-rate-of-change of temperature. In terms of relative magnitudes, the most important of these coupling effects usually arises from the buoyancy term. The fluid expansion term is usually the smallest for most hydrologic problems; it becomes important only if there is a rapid change in the temperature field. The pressure equation determines the velocity components which, in turn, provide the convective flux of the temperature equation. Strong coupling usually occurs between the pressure and temperature equations for most nonisothermal flow fields.

There is only a one-way coupling between the concentration equation and the pressure equation; that is, although the pressure field affects the concentrations through the velocity field, the reverse is not true. Having neglected the Dufour and Sorret effects, there is no direct coupling between the temperature and concentration equations. However, an indirect coupling between these two equations exists because of the dependence of the convective velocity on the buoyancy.

As stated earlier, the temperature and the concentration equations are coupled to the pressure equation through the convective velocities. The strength of this coupling depends on the magnitudes of the velocities. The ratio of the convective to dispersive transport of heat and species is known

as the Peclet number. The solution of the temperature and concentration equations depends largely on the values of the Peclet number. In the absence of convective transport, the equations are fully parabolic. When transport by dispersion and diffusion is negligible compared to that resulting from convection, the equations become hyperbolic. As will be seen in Chapter 4.0, the Peclet number plays a crucial role in proper discretization of these equations.

2.6 GENERAL FORM OF THE GOVERNING EQUATIONS

Each of the three governing Equations 2.1-17, 2.2-11, and 2.3-13 of PORMC represents the transport of a certain property (fluid, heat, or species) and has a similar mathematical structure. When reduced to their differential form, all three are second-order, coupled, parabolic equations. The general form of these equations can be written as

$$\begin{aligned}
 & \partial_t \int_V \alpha_m F \, dV + \partial_t \sum_i \int_{V_{p_i}} \alpha_{p_i} F \, dV + \int_{S_m} [\beta_m \vec{V}_m F - \gamma_m \vec{\nabla} F] \\
 & \quad \bullet \vec{s}_m dS + \sum_i \int_{S_{p_i}} [\beta_{p_i} \vec{V}_{p_i} F - \gamma_{p_i} \vec{\nabla} F] \\
 & \quad \bullet \vec{s}_{p_i} dS = \int_V S_F - \int_V S_F F \tag{2.6-1}
 \end{aligned}$$

where F is the dependent variable (P, T, or C) and the various other coefficients and source terms are summarized in Table 2-1.

Table 2-1. Coefficients and Source Terms of the General Transport Equation for the Three Dependent Variables of PORMC.

F	α	β	γ	S_F	s_F
P	$R S_s$	0	$R \xi \underline{k}_r$	$W_V + W_T + R_s - \vec{\nabla} z$	0.
T	$\rho_e c_e$	c	$k_e + \rho c \eta T \underline{D}$	S_T	0.
C	θR_d	1	$\theta D_M + \eta \underline{D}$	S_C	$\theta R_d R_C$

An alternative form of Equation 2.6-1 that is more convenient for discussion of numerical solution (Section 2.8) is

$$\begin{aligned} \int_{V_m} \partial_t (\alpha_m F) dV + \sum_i \int_{V_{p_i}} \partial_t (\alpha_{p_i} F) dV \\ + \int_{S_m} [L_{m_x} + L_{m_y} + L_{m_z}] F dS \\ + \sum_i \int_{S_{p_i}} [L_{p_x} + L_{p_y} + L_{p_z}] \end{aligned} \quad (2.6-2)$$

L_x , L_y , and L_z in Equation 2.6-2 are the transport components in the x, y, and z directions, respectively. The form of these components is the same for both the rock matrix and the planar features. Omitting the subscripts m and p, these are as follows:

$$L_x + r^{-1} (r \beta U - r \gamma_x \partial_x) \quad (2.6-3a)$$

$$L_y = (\beta V - \gamma_y \partial_y) \quad (2.6-3b)$$

$$L_z = (\beta W - \gamma_z \partial_z). \quad (2.6-3c)$$

In Equation 2.6-3a, r is the radial distance when the problem is posed in cylindrical coordinates, $r \rightarrow \infty$ in cartesian coordinates.

Numerical solution of the governing equations of PORMC will be discussed with respect to the general transport Equations 2.6-1 and 2.6-2. Auxiliary equations are discussed first.

2.7 AUXILIARY EQUATIONS

In addition to the governing equations described in Sections 2.1 through 2.3, several auxiliary equations are needed for a complete description of the flow and transport processes. These auxiliary equations include a description of the initial and boundary conditions and equations of state that describe the dependence of the fluid and solid properties on pressure, temperature, and saturation. These equations are described in the following sections.

2.7.1 Fluid Properties

2.7.1.1 Fluid Density. The principal fluid for most applications of PORMC is a liquid. In general, fluid density is a function of both temperature and pressure. However, for most liquids, the dependence of density on pressure is much smaller than that on temperature. For example, for water at 100 °C, compressibility is on the order of 10^{-6} , whereas the coefficient of thermal expansion is on the order of 10^{-4} . For this reason, changes in water density caused by pressure variations are ignored in PORMC. However, if the fluid of interest is a gas, the pressure dependence of density may need to be accounted for.

Several equations relating water density to temperature have been published. Three of these are implemented in the PORMC computer program. The first relation is that recommended by Perry and Chilton (1973). With the density of water known to be ρ^* at temperature T^* , the density ρ at temperature T is given by the equation

$$\rho = \rho^* \left[(T_c - T) / (T_c - T^*) \right]^A \quad (2.7-1)$$

where T_c is the critical temperature, and the value of the exponent, A , is obtained from experimental data through regression. With $T_c = 647.3$ K, $T^* = 300$ K, and $\rho^* = 996.59$ kg/m³, the value of exponent A is found to be equal to 0.20. Perry and Chilton (1973) have tabulated the values of water density from experimental data. Comparison of this tabulation with Equation 3.7-1 demonstrates that from 4 to 200 °C the difference between density calculated using Equation 3.7-1 and that determined experimentally is <1%. The maximum error increases to about 2.5% for temperatures up to 350 °C. This error decreases at higher pressures. If fluids other than water are being simulated, suitable values of T_c and A should first be determined.

The second relation for water density is the polynomial expression

$$\rho = A_1 - A_2 T + A_3 T^2 - A_4 T^3 \quad (2.7-2)$$

where A_1 , A_2 , A_3 , and A_4 are empirical constants. The optimal values of these coefficients for water, which are valid for a temperature range of 0 to 50 °C, are given by Burette (1972) (ρ is in kilograms per cubic meter and T is in degrees Celsius) as

$$A_1 = 9.999317011 \times 10^{+2} \quad (2.7-3a)$$

$$A_2 = 4.745080000 \times 10^{-2} \quad (2.7-3b)$$

$$A_3 = 7.393800000 \times 10^{-3} \quad (2.7-3c)$$

$$A_4 = 3.500000000 \times 10^{-5}. \quad (2.7-3d)$$

These are used as default values in the PORMC program. Other values may be specified by the user.

A third relation for density that is incorporated into PORMC is a linear function of temperature and concentration expressed as

$$\rho = \rho^* [1 + A_5(T^* - T) + A_6(C^* - C)] \quad (2.7-4)$$

where A_5 and A_6 are user-specified constants and * denotes a reference value.

2.7.1.2 Fluid Viscosity. In a manner similar to that for fluid density, the viscosity of liquids is, in general, a much stronger function of temperature than it is of pressure. Therefore, in PORMC the pressure dependence of viscosity is neglected. The PORMC program provides three different options for calculating changes in fluid viscosity. The first is that given by Perry and Chilton (1973)

$$\mu = B_1 \exp (B_2/T) \quad (2.7-5)$$

where B_1 and B_2 are empirical constants and T is the temperature in Kelvin. For a temperature range of 0 to 350 °C, the optimal values of the coefficients B_1 and B_2 for water are 6.40×10^{-6} kg/(m•s) and 1436 K, respectively. The water viscosity obtained by using these coefficients is in kilograms per meter per second.

The second option for calculating water viscosity is the polynomial relation

$$\mu = B_3 - B_4 T + B_5 T^2 - B_6 T^3 \quad (2.7-6)$$

where B_3 through B_6 are empirical constants. The optimal values of these coefficients for a temperature range of 0 to 50 °C are given by Buretta (1972) as follows:

$$B_3 = 1.6872274 \times 10^{-3} \quad (2.7-7a)$$

$$B_4 = 4.4676700 \times 10^{-5} \quad (2.7-7b)$$

$$B_5 = 6.0209700 \times 10^{-7} \quad (2.7-7c)$$

$$B_6 = 3.2788000 \times 10^{-9} \quad (2.7-7d)$$

where the viscosity is in kilograms per meter per second and the temperature is in degrees Celsius.

A third option available in PORMC is the second-order exponential relation

$$\mu = \mu^* \exp [B_7 (T^* - T) - B_8 (T^* - T)^2] \quad (2.7-8)$$

where B_7 and B_8 are empirical constants and * denotes a reference value.

2.7.2 Hydraulic Properties of Saturated Media

It is evident from Equation 2.1-17 that the two main parameters in the saturated flow equation are the coefficient of specific storage and the hydraulic conductivity tensor. The dependence of both of these parameters on temperature is through their dependence on liquid properties. This dependency was made explicit in Equation 2.1-17 by using the density and viscosity ratios, R and ξ , respectively. Consequently, only the reference values of S_s and k need to be specified for application of this equation to saturated flow.

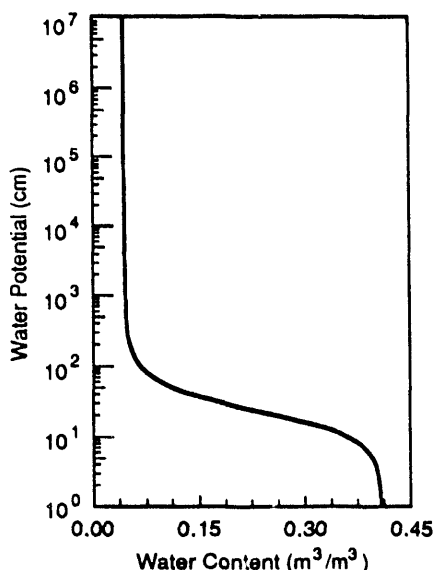
2.7.3 Hydraulic Properties of Partially Saturated Media

Although a single governing equation (Equation 2.1-17) was written for flow in both saturated and unsaturated media, there are two major differences between these two types of flows: (1) in saturated flows, $k_r = 1$ and therefore is eliminated from Equation 2.1-17; but for unsaturated flows, k_r depends on saturation, σ , and is less than 1; and (2) although S_s is directly specified for saturated flows, this is not possible for unsaturated flows because in this case S_s is the (negative) slope of the soil-moisture tension curve and therefore also depends on saturation. As will be discussed, because saturation depends on pressure head, the flow equation for unsaturated flow becomes nonlinear.

Because of the simultaneous presence of both the liquid (e.g., water) and gas (e.g., air) in unsaturated media, liquid-gas interfaces are formed throughout. These concave interfaces extend from grain to grain across each pore channel. The radius of curvature of each interface reflects the surface tension of that interface. Liquid in the unsaturated zone is held by these surface tension forces; the greater this force, the less moisture is retained. The relation between the tension forces and moisture content is dependent on soil (or rock) grain sizes and arrangements. However, this relation often is measured directly in the field and specified as a basic hydraulic property of the medium. In many soils, the θ - Ψ relation is hysteretic; i.e., it has different shapes for wetting and drying episodes. In PORMC, hysteretic effects are neglected.

2.7.3.1 Soil Moisture-Retention Curves. A typical θ - Ψ curve is shown in Figure 2-2. This curve can be specified as either an analytic function or a table. The following three options for analytic functions are provided in PORMC.

Figure 2-2. Typical Soil-Moisture Retention Curve.



- van Genuchten (1978)

$$\theta^* = [1 + (\alpha \Psi)^n]^{-m}, h < 0 \quad (2.7-9a)$$

$$\theta^* = 1, h \geq 0 \quad (2.7-9b)$$

where α , m , and n are empirical constants; $h = -\Psi$ is the pressure head; and θ^* is the normalized water content (or saturation), which is defined as

$$\theta^* = \frac{\theta - \theta_r}{n_b - \theta_r} \quad (2.7-10)$$

in which θ_r is the residual (or immobile) moisture content. In PORMC, because of the way the diffusive and effective porosities have been defined,

$$\theta_r = n_b - n_E \quad (2.7-11a)$$

In addition, the coefficients m and n are related through

$$m = (1 - a/n) \quad (2.7-11b)$$

where a is 1 for Mualem and 2 for Burdine relations for hydraulic conductivity (Section 2.7.3.2).

- Brooks and Corey (1966)

$$A^* = (\Psi/\Psi^*)^{-\beta}, \Psi < -\Psi^* \quad (2.7-12a)$$

$$\theta^* = 1, \Psi \geq -\Psi^* \quad (2.7-12b)$$

where Ψ^* is the air-entry head and β is an empirical constant. From Equation 2.7-12a, it is apparent that when $\Psi = -\Psi^*$, $\theta^* = 1$ (i.e., full saturation is approached as $\Psi = -\Psi^*$). Thus, for $\Psi < -\Psi^*$, the soil is saturated. No analogous cutoff point is stipulated in the van Genuchten relation.

- Gardner (or Exponential) Specification

van Genuchten's Equations 2.7-9a and -9b are used to estimate θ from Ψ .

- Tabular Specification

Any arbitrary soil-moisture curve can be specified in the form of a $\theta - \Psi$ table. The value of θ corresponding to a value of Ψ that is not in the table can be obtained through interpolation. Linear interpolation is used in PORMC.

2.7.3.2 Relative Hydraulic Conductivity Curves. Measurement of in situ unsaturated hydraulic conductivity is difficult. Therefore, unsaturated hydraulic conductivities (or relative conductivity, k_r , of Equation 2.1-17) are usually estimated based on physical attributes of the porous media (e.g., pore radii, porosity, and tortuosity factor). The simplest formula for k_r is based on a generalization of Kozney's approach (Brutsaert 1967)

$$k_r = (\theta^*)^\gamma \quad (2.7-13)$$

where γ is an empirical coefficient. A value for γ of 3.5 has been found to agree well with experimental observations (Averjanov 1950).

Other more complex formulae for k_r have been derived using the basic theory of capillary flow. Burdine (1953) derived the following relation:

$$k_r = (\theta^*)^2 \int_0^{\theta^*} \frac{1}{\Psi^2} d\theta / \int_0^1 \frac{1}{\Psi^2} d\theta. \quad (2.7-14)$$

Substituting the van Genuchten relation, Equation 2.7-9a, into Equation 2.7-14, the

van Genuchten - Burdine Relation,

$$k_r(\theta^*) = (\theta^*)^2 \left[1 - (1 - \theta^{*1/m})^m \right], \quad (2.7-15a)$$

is obtained. If the Brooks and Corey moisture-retention curve, Equation 2.7-12a, is used instead, the

Brooks and Corey - Burdine Relation,

$$k_r(\theta^*) = \theta^{*(3+2/\beta)}, \quad (2.7-15b)$$

results. By setting $\beta = [2/(\gamma-3)]$, Equation 2.7-15b reduces to Equation 2.7-13.

The formulae for k_r also can be written in terms of Ψ . The formula corresponding to the van Genuchten moisture-retention curve is

$$k_r(\Psi) = \frac{1 - (\Psi/\alpha)^{n-2} [1 + (\Psi/\alpha)^n]^m}{[1 + (\Psi/\alpha)^n]^{2m}}, \quad (2.7-16a)$$

while for the Brooks and Corey moisture retention curve, it is

$$k_r(\Psi) = (\Psi/\Psi^*)^{-2-3\beta}. \quad (2.7-16b)$$

Mualem (1976) used a pore-size distribution in the modified form of the Childs and Collis-George (1950) relation to obtain the following for k_r :

$$k_r = (\theta^*)^{1/2} \int_0^{\theta^*} \frac{1}{\Psi^2} d\theta / \int_0^1 \frac{1}{\Psi^2} d\theta. \quad (2.7-17)$$

Using Equation 2.7-17, the relations for k_r in terms of θ are

- van Genuchten - Mualem Relation

$$k_r(\theta^*) = (\theta^*)^{1/2} [1 - (1 - \theta^{*n})^m]^2 \quad (2.7-18a)$$

and

- Brooks and Corey - Mualem Relation

$$k_r = \theta^{*(5/2 + 2/\beta)}. \quad (2.7-18b)$$

The corresponding relations in terms of Ψ become

$$k_r(\Psi) = \frac{\{1 - (\Psi/\alpha)^{n-1} [1 + (\Psi/\alpha)]^{-m}\}^2}{[1 + (\Psi/\alpha)^n]^{m/2}} \quad (2.7-19a)$$

and

$$k_r(\Psi) = (\Psi/\Psi^*)^{-2-3\beta}. \quad (2.7-19b)$$

The Gardner's relation often used for analytic solutions of the unsaturated flow equation is particularly simple:

- Gardner or Exponential Relation

$$k_r(\Psi) = \exp(-\gamma \Psi) \quad (2.7-20)$$

where γ is an empirical constant. Equation 2.7-20 is provided in PORMC to facilitate comparison between analytic and numerical solutions.

In addition, an option is available to specify either the k_r - θ or the k_r - Ψ curve in a table. In this case, linear interpolation is used to obtain the value of k_r for any Ψ .

2.7.4 Mechanical Dispersion

Transport following mechanical dispersion is caused by the nature of flow in the interconnected pores of the media (Bear 1972). This phenomenon occurs only in moving fluid and is the result of the velocity variations at the pore scale.

In general, the coefficient of mechanical dispersion, \underline{D} , is a second-order symmetric tensor and a function of both the media and the fluid (Bear 1972). To simplify this term, a set of parameters of the media, termed the dispersivities, is defined. Based on experimental evidence, longitudinal and transverse dispersivities are defined to represent the process of mechanical dispersion in the direction of the average fluid velocity and orthogonal to it, respectively. As stated in Section 2.1.2, the x, y, and z coordinates in PORMC are assumed to coincide with the principal directions of the hydraulic conductivity. The average fluid velocity does not, in general, coincide with the x, y, or z axes. To obtain the components of the dispersion coefficient in the directions of the axes, the following equations suggested by Scheidegger (1961) are used:

$$D_x = \alpha_L U' + \alpha_T (V' + W') \quad (2.7-21a)$$

$$D_y = \alpha_L V' + \alpha_T (W' + U') \quad (2.7-21b)$$

$$D_z = \alpha_L W' + \alpha_T (U' + V') \quad (2.7-21c)$$

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

$$U' = U^2/\xi \quad (2.7-22a)$$

$$V' = V^2/\xi \quad (2.7-22b)$$

$$W' = W^2/\xi \quad (2.7-22c)$$

where

$$\xi = (U^2 + V^2 + W^2)^{1/2}. \quad (2.7-22d)$$

2.7.5 Boundary and Initial Conditions

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

$$- a\partial F/\partial N = b(F - F_o) + c \quad (2.7-23)$$

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_o are specified constants. By selecting appropriate values of a , b , c , and F_o , three types of boundary conditions can be represented by Equation 2.7-23. These boundary conditions are as follows.

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

$$F = F_o \quad (2.7-24a)$$

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

- Neumann boundary condition: Obtained by specifying that $b = 0$. 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

$$- a\partial F/\partial N = c \quad (2.7-24b)$$

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

- Mixed (or radiation) boundary condition: Obtained by substituting $c = 0$ in Equation 2.7-23, resulting in

$$- a\partial F/\partial N = b(F - F_o). \quad (2.7-24c)$$

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_o is the equilibrium value of F . Using the heat transfer equation as an example, F_o may be specified to be the temperature of the atmosphere to which heat is being lost from the boundary of the domain under consideration.

- Seepage boundary condition: Applicable to the flow equation in the vadose zone. This is a special type of boundary condition defined as

$$\partial F / \partial N = 0; \quad F < F_0 \quad (2.7-25a)$$

$$F = F_0; \quad F \geq F_0. \quad (2.7-25b)$$

Thus it is a Neumann boundary (with zero flux) until the boundary pressure is less than a specified value; after that it becomes a Dirchlet boundary and seepage is allowed.

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; that is,

$$F = a + bx + cy + dz \quad (2.7-26)$$

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.

2.8 DISCRETE ALGEBRAIC FORM OF GOVERNING EQUATIONS

Numerical solution of the governing and auxiliary equations described in Sections 2.1 to 2.3 is by two steps: (1) using the nodal point integration method, the governing equations are discretized into a set of algebraic equations; and (2) the matrix of algebraic equations is solved. Alternative choices of 'integration profiles' in step 1 and different 'matrix solution' methods in step 2 provide the adaptability to solve problems of increasing difficulty. This section discusses these two steps. Equation 2.6-1 (or Equation 2.6-2), the generic mass transport equation, provides a convenient basis for these discussions and will be referenced throughout this chapter.

2.8.1 Discretization Method

The method of nodal point integration is employed to transform the differential equations into their algebraic analogues (Runchal 1969, Gosman et al. 1969, Patankar 1980). The nodal point integration method is also referred to in technical literature as the 'finite-volume' or 'integrated finite-difference' method. The essence of the nodal point integration method is to analytically integrate assumed profiles (polynomials, exponentials, etc.) for the dependent variable (F in Equation 2.6-1) over a time step and finite volume that are defined by the calculational domain. Consequently, the nodal point integration method does not use the Taylor expansion method to represent derivatives, as is typically the case with finite-difference methods. In contrast, the nodal point integration approach resembles the finite-element method. However, it differs from the finite-element method in

that integrations are performed on each finite volume rather than on the total domain. This local nature of integration gives a significant advantage to the nodal point integration method; it intrinsically maintains the mass, momentum, and thermal energy balances at the local scale of an element and thus results in a stable numerical formulation.

The nodal point integration method implemented in PORMC provides a choice of two distinct integration profiles (or schemes) for discretization; the exponential (Spalding 1972) and the hybrid (Runchal 1972). However, the first step of the discretization process is to partition the total spatial domain into a set of finite volumes through the imposition of a grid, as the following explains.

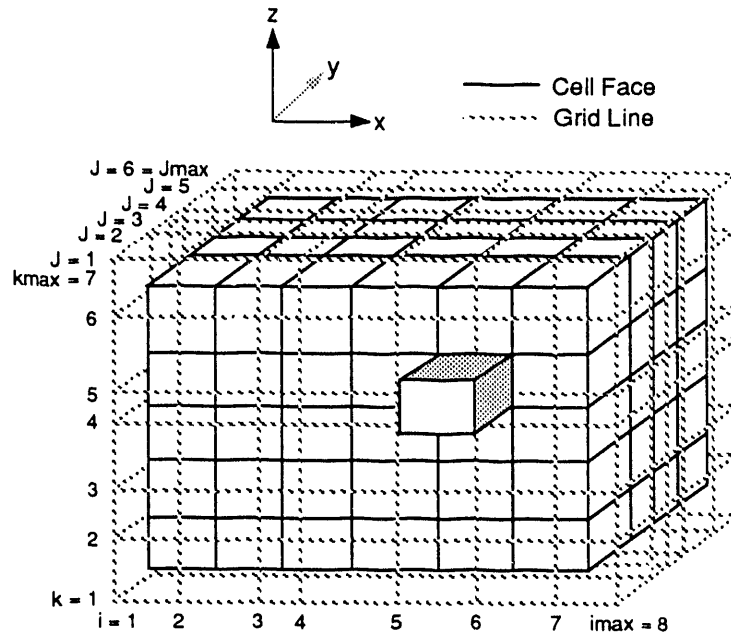
2.8.2 The Spatial Grid

The spatial grid used in PORMC is constructed using three mutually perpendicular surfaces. In the Cartesian coordinate system, these surfaces are identified by right-handed orthogonal (x,y,z) coordinates. In the cylindrical coordinate system, the orthogonal coordinates are (r,θ,z) , and the surface in the θ - z plane is circular. In both coordinate systems, the z -axis is taken to be vertical and is positive in the upward direction. In the following discussion, only the x,y,z notation is used, but the discussion can be applied to the r,θ,z system by substituting r for x and θ for y . The grids are depicted in Figures 2-3 and 2-4 for Cartesian and cylindrical coordinates, respectively. The dashed lines in these figures show the grid surfaces. Horizontal cross sections through these grids are shown in Figures 2-5 and 2-6.

In the following discussion, the grid surfaces (or grid lines in two dimensions) are identified by the indexes I , J , and K in the x , y , and z directions, respectively. Within the domain of interest, these grid surfaces are numbered from 1 to $IMAX$, 1 to $JMAX$, and 1 to $KMAX$ in the three respective directions. Grid nodes are points where the three mutually perpendicular surfaces intersect. The total number of nodes (internal plus boundary) in the domain of interest is thus $IMAX \times JMAX \times KMAX$.

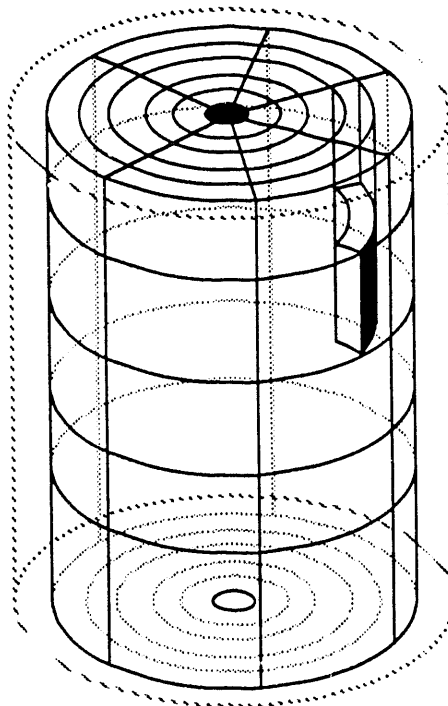
The actual integration and solution of the governing equations of PORMC proceeds not by reference to the grid surfaces or nodes but by reference to the elements. These elements also are variously referred to as the control volumes or cells. An element or control volume is associated with each internal grid node (i.e., all grid nodes except the boundary grid nodes). The control volume for each node is obtained by constructing surfaces that are located exactly midway between the grid surfaces. The cell surfaces are shown as solid lines in Figures 2-3 to 2-6. Because the grid surfaces in PORMC may be unevenly spaced, the control volume sizes associated with nodes may vary from node to node. The actual physical domain of a problem is thus completely encompassed by a discrete number of contiguous elements. The boundary nodes surrounding the physical domain are employed to impose the boundary conditions for the problem.

Figure 2-3. Illustration of Cartesian Grid Arrangement.



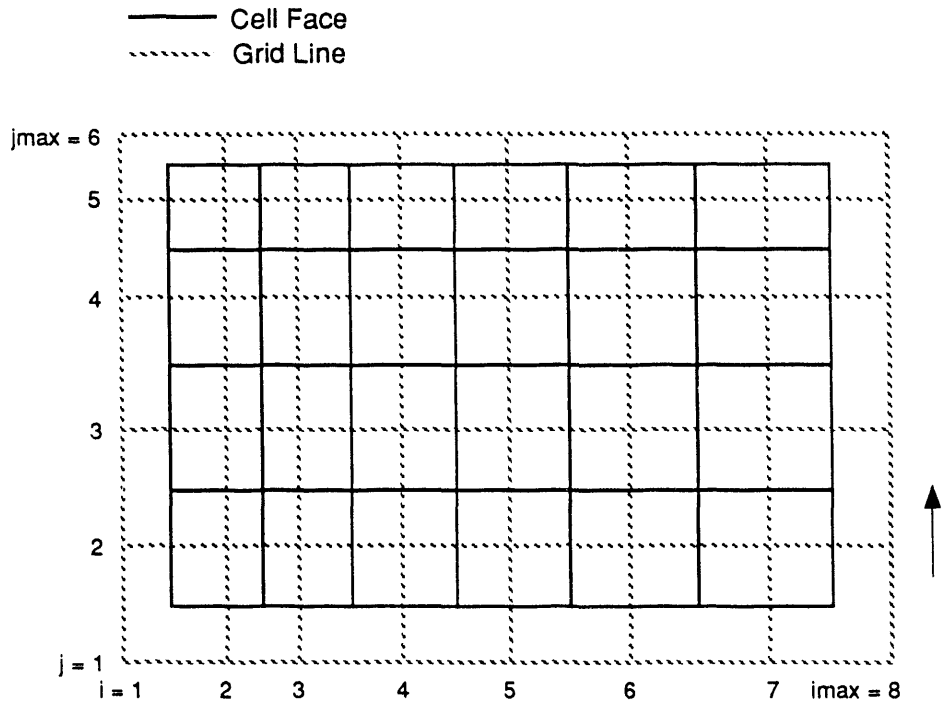
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Figure 2-4. Illustration of Cylindrical Grid Arrangement.



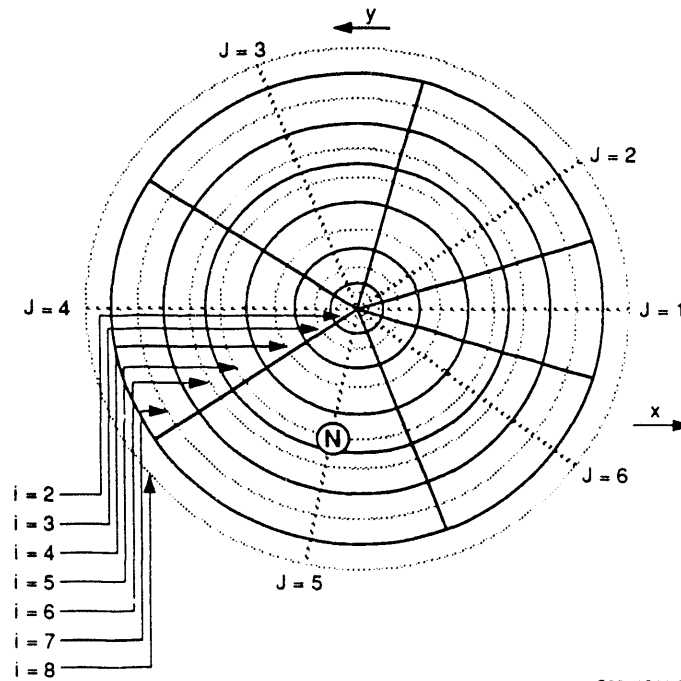
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Figure 2-5. Horizontal Cross Section Through a Cartesian Grid System.



S8911041.7

Figure 2-6. Horizontal Cross Section Through a Cylindrical Grid System.



S8911041.6

A typical cell or element for a Cartesian grid system is shown in Figure 2-7; one for a cylindrical grid system is shown in Figure 2-8. A horizontal cross section through the element of Figure 2-7 is shown in Figure 2-9. The node P, enclosed by the cell, has the grid indexes (I,J,K). The value of the dependent variable, F, at P (and at each internal node) is assumed to be influenced by its six immediate neighbors; these neighbors are denoted by E (east), W (west), N (north), S (south), U (up), and D (down). The respective indexes for these nodes are (I+1,J,K), (I-1,J,K), (I,J+1,K), (I,J-1,K), (I,J,K+1), and (I,J,K-1). The cell faces are denoted, respectively, by e, w, n, s, u, and d. Each cell face lies exactly midway between the elemental node, P, and its nearest neighbor in the direction of the cell face. The number of internal nodes or, equivalently, the number of cells is (IMAX-2)*(JMAX-2)*(KMAX-2).

During numerical manipulations, all the intrinsic property variables, such as pressure head, temperature, concentration, density, and viscosity, are defined at the grid nodes. The flux variables, such as velocity components and heat and mass fluxes, are defined at the cell faces. The U velocity locations are midway between the grid nodes in the x-direction, the V velocity locations are midway between the grid nodes in the y-direction, and the W velocity locations are midway between the grid nodes in the z-direction. The use of this "staggered" grid approach leads to a more natural description of the physical system, whereby the fluxes are defined at the element boundaries, and the intrinsic properties are defined at the element node. The index notation employed is such that the velocity components at the W (west), S (south), and D (down) faces of the control volume are denoted by the same I, J, and K index values as the F values at the associated grid node (Figure 2-9).

2.8.3 General Formula for Discretization

The governing equations are discretized by integrating them over the volume of each cell and time step. Considering Equation 2.6-2 for a node, P, as shown in Figure 2-9, the integral is

$$\begin{aligned}
 \int_t^{t+\delta t} & \left[\int_{V_m} \partial_t(\alpha_m F) dV + \sum_i \int_{V_{p_i}} \partial_t(\alpha_{p_i} F) dV \right. \\
 & + \int_{S_m} [L_{m_x} + L_{m_y} + L_{m_z}] F dS \\
 & + \sum_i \int_{S_{p_i}} [L_{p_x} + L_{p_y} + L_{p_z}] F dS \\
 & \left. - \int_V S_F dV + \int_V s_F F dV \right] dt = 0
 \end{aligned} \tag{2.8-1}$$

Figure 2-7. Typical Grid Cell in Cartesian Coordinates.

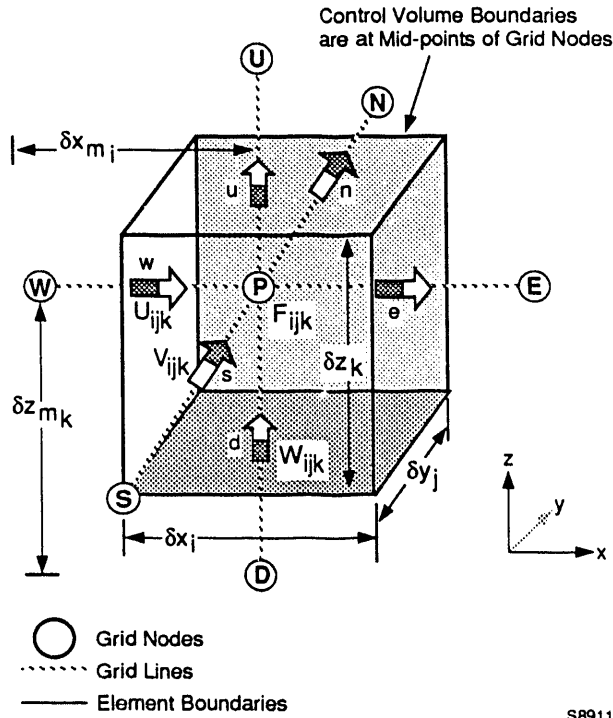


Figure 2-8. Typical Grid Cell in Cylindrical Coordinates.

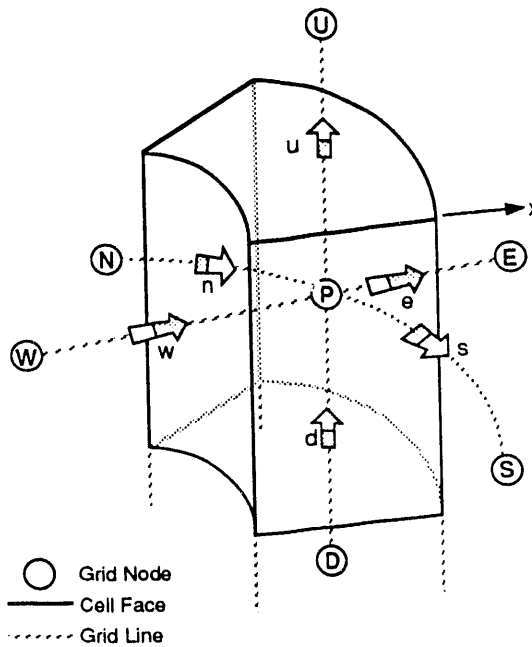
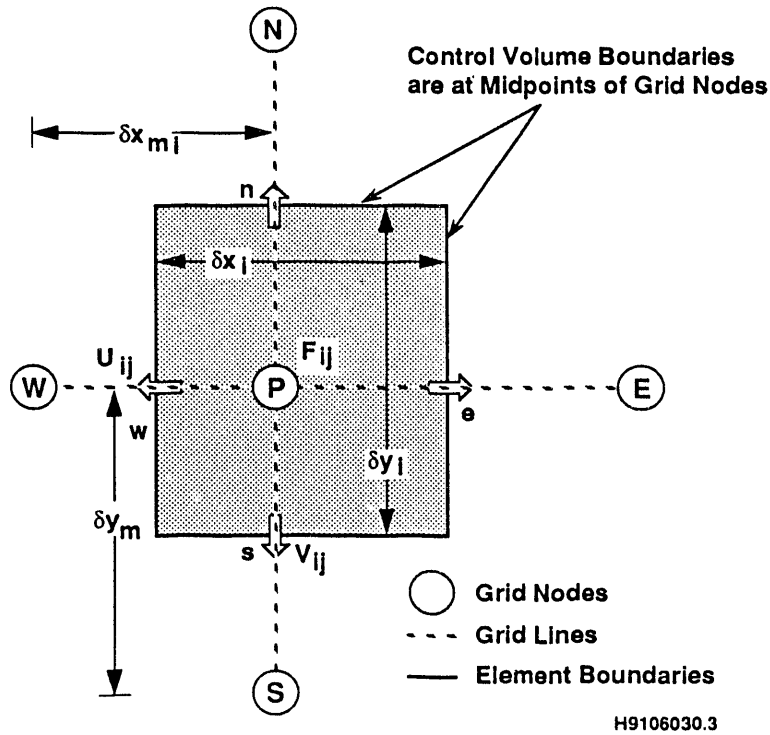


Figure 2-9. Horizontal Cross Section Through a Typical Grid Cell in Cartesian Coordinates.



where, with appropriate subscripts m and p omitted,

$$L_x = r^{-1} \partial_x (r \beta U - r \gamma_x \partial_x) F \quad (2.8-2a)$$

$$L_y = \partial_y (\beta V - \gamma_y \partial_y) F \quad (2.8-2b)$$

$$L_z = (\beta W - \gamma_z \partial_z) F. \quad (2.8-2c)$$

If a profile (polynomial or exponential) for F (and other terms, such as S_F) is assumed within the time interval $[t, t+\delta t]$ and over the volume, V , Equation 2.8-1 can be integrated analytically to obtain an algebraic equation applicable to node P . As will be seen later, different profile shapes for F may be used while integrating the convective (i.e., containing velocity components U , V , and W) and diffusive (containing gradients of F) terms in Equation 2.8-1. A similar procedure is followed to obtain an algebraic

equation for each internal node. In the details provided below, subscripts m and p are omitted, because the integrals proceed in exactly the same manner for the rock matrix (subscript m) and the planar features (subscript p).

2.8.4 Temporal Integration

Assuming a linear time variation of F at node P(I,J,K), the time integral of the term containing the time derivative and the decay term of Equation 2.8-1 is

$$\int_t^{t+\delta t} \int_V [\partial_t (\alpha F) + s_F F] dV dt = \int_V [\alpha (F^{n+1} - F^n) + s_F F^{n+1}] dV. \quad (2.8-3a)$$

In Equation 2.8-3a, F^{n+1} and F^n are the values of F at points in volume dV at time steps (n+1) and n, respectively; i.e., $F^{n+1} = F(t+\delta t)$ and $F^n = F(t)$. For the remaining terms in Equation 2.8-1, the time integral is written as

$$\int_t^{t+\delta t} \int_V (L_x + L_y + L_z - S_f) dV dt = \delta t \left[\int_V (L_x^k + L_y^\ell + L_z^i - S_f^j) dV \right]. \quad (2.8-3b)$$

The superscripts (k, ℓ , i, and j) in Equation 2.8-3b denote the value at a time between t and t+ δt of the specific quantity in which they occur. In terms of time steps, $n \leq k, \ell, i, j \leq n+1$. A choice of values of k, ℓ , i, and j results in different numerical schemes and solution methods. The schemes used in PORMC are as follows.

1. $k = \ell = i = j = n$; that is, all values in Equation 2.8-3b are at the previous time step and, therefore, are known. This is a fully explicit formulation. Only one unknown, F(t+ δt), remains in the equation for a node. The Point Successive Over-Relaxation method used in PORMC uses this type of formulation.
2. $k = \ell = i = j = n+1$; that is, all values in Equation 2.8-3b are at the new time step. In this case, values of F(t+ δt), not only at node P but at all of its neighboring nodes, appear in the equation for node P. This is the fully implicit formulation. The Cholesky Decomposition, Gaussian Elimination, and Reduced-System Conjugate-Gradient methods in PORMC use this formulation.

3. Three substeps are taken to complete the solution for a time step. In the first substep, $k = n+1$; in the second, $l = n+1$; and in the third, $i = n+1$; while all other superscripts are held equal to n . This formulation is used in conjunction with the Alternating Direction Implicit method of solution in PORMC.

The various solution methods mentioned previously have distinctive accuracy and stability characteristics and differ greatly in required computer memory, as discussed in Chapter 3.0.

2.8.5 Spatial Integration

PORMC provides for alternative methods of spatial integration of the terms appearing in Equations 2.8-3a and -3b. From inspection of these equations, it can be seen that the spatial terms fall into four categories: diffusion terms involving derivatives of F , the convection term with fluid velocities, the source and sink terms, and the accumulation terms with first-order time derivatives.

In the nodal point integration method, integration proceeds by assuming a suitable internodal profile for the piecewise variation of the state variables (F of Equation 2.6-1 or 2.6-2) from one grid node to another. There are two approaches to the assumptions of these integration profiles. In the simpler approach, the diffusive and convective terms are considered separately, each with its own characteristic profile. The second approach provides a more comprehensive mathematical treatment by considering both the convective and the diffusive terms in a unified manner. Both approaches are illustrated below for the Cartesian coordinate system. The derivation of the equations proceeds in an identical manner for the cylindrical coordinate system.

The geometry of the two-dimensional fracture and the one-dimensional borehole elements is restricted by the model in two ways. First, these elements must be aligned with the grid lines of the three-dimensional elements; second, they must begin and end at nodes of the three-dimensional grid. The first limitation is restrictive because fractures and boreholes inclined to the grid lines cannot be represented except by ingenious grid designs that allow approximation of inclined fractures as "stair-stepped" features. The second limitation is not severe because grid points can be located anywhere in three-dimensional space.

2.8.5.1 Discretization of the Diffusive Terms. The integral of the x-directional component of the diffusion term in Equation 2.8-3b is written as

$$I_1 = \int_t^{t+\delta t} \int_{S_{ijk}} \partial_x (\gamma_x \partial_x F) \cdot \vec{s} \, dS \, dt \quad (2.8-4)$$

where S_{ijk} is the bounding surface of the element (I,J,K) and \vec{s} is the unit outward, normal to this surface. In the Cartesian coordinate system, the surface is composed of six rectangular surfaces. Because of the orthogonality

of the coordinate system and the rectangular shape of the elements, the contribution to the integral in the y- and z-directions is zero. Therefore, Equation 2.8-4 is written as

$$I_1 = \int_t^{t+\delta t} \left[\int_e \partial_x (\gamma_x \partial_x F) dy dz - \int_w \partial_x (\gamma_x \partial_x F) dy dz \right] dt \quad (2.8-5)$$

where e and w denote the values of the quantity at the e and w faces of the element, as shown in Figure 2-9.

Further integration now proceeds by assuming that in the interval $x_{i-1} \leq x \leq x_{i+1}$, $y_{j-1} \leq y \leq y_{j+1}$, and $z_{k-1} \leq z \leq z_{k+1}$, the state variable, F, is represented by the following piecewise quadratic polynomial

$$F = a_0 + a_1 x + a_2 x^2 + a_3 y + a_4 y^2 + a_5 z + a_6 z^2 \quad (2.8-6)$$

where all of the "a" terms are arbitrary constants. This yields

$$\partial_x F|_w = a_1 + 2 a_2 x_{i-w} \quad (2.8-7a)$$

$$\partial_x F|_e = a_1 + 2 a_2 x_{i+w} \quad (2.8-7b)$$

Equation 2.8-6 also implies that for nodes W, P, and E of Figure 2-9

$$F_w = a_0 + a_1 x_{i-1} + a_2 x_{i-1}^2 + a_3 y_j + a_4 y_j^2 + a_5 z_k + a_6 z_k^2 \quad (2.8-8a)$$

$$F_p = a_0 + a_1 x_i + a_2 x_i^2 + a_3 y_j + a_4 y_j^2 + a_5 z_k + a_6 z_k^2 \quad (2.8-8b)$$

and

$$F_e = a_0 + a_1 x_{i+1} + a_2 x_{i+1}^2 + a_3 y_j + a_4 y_j^2 + a_5 z_k + a_6 z_k^2 \quad (2.8-8c)$$

because

$$x_{i-\frac{1}{2}} = (x_i + x_{i-1}) / 2 \quad (2.8-9a)$$

$$x_{i+\frac{1}{2}} = (x_i + x_{i+1}) / 2. \quad (2.8-9b)$$

Equations 2.8-8a and -8c yield

$$(F_p - F_w) / (x_i - x_{i-1}) = a_1 + 2 a_3 x_{i-\frac{1}{2}} \quad (2.8-10a)$$

$$(F_E - F_p) / (x_{i+1} - x_i) = a_1 + 2 a_3 x_{i+\frac{1}{2}}. \quad (2.8-10b)$$

By comparison of Equations 2.8-7a and -7b and 2.8-10a and -10b

$$\partial_x F|_w = (F_p - F_w) / (x_i - x_{i-1}) \quad (2.8-11a)$$

$$\partial_x F|_e = (F_E - F_p) / (x_{i+1} - x_i). \quad (2.8-11b)$$

In the notation of Figure 2-9, these equations may be written more compactly as

$$\partial_x F|_w = (F_p - F_w) / \delta x_w \quad (2.8-12a)$$

$$\partial_x F|_e = (F_E - F_p) / \delta x_e \quad (2.8-12b)$$

where

$$\delta x_w = x_i - x_{i-1} \quad (2.8-13a)$$

$$\delta x_e = x_{i+1} - x_i. \quad (2.8-13b)$$

Assuming that γ_x remains constant across a cell face, Equation 2.8-5 is now written as

$$I_1 = \int_t^{t+\delta t} \left\{ \left[\gamma_{xe} (F_E - F_P) / \delta x_e \right] A_e - \left[\gamma_{xw} (F_P - F_W) / \delta x_w \right] A_w \right\} dt \quad (2.8-14)$$

where the cell face areas, A_e and A_w , are given by

$$A_w = (y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}) (z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}) = A_e. \quad (2.8-15)$$

Analogous to the discussion of the time integral provided above, to complete the transformation of this integral, assume that a representative value of F^m between $F(t)$ and $F(t+\delta t)$ exists. In general, this may be written as

$$F^m = \alpha F(t) + \beta F(t+\delta t) \quad (2.8-16)$$

where

$$\alpha + \beta = 1. \quad (2.8-17)$$

PORMC provides three choices for α and β ; these are the fully explicit scheme with $\alpha = 1$, the implicit scheme with $\beta = 1$, and the Alternating Direction Implicit scheme with mixed values of α and β . The final form of the integral of Equation 2.8-14 is now written as

$$I_1 = B_w (F_w^l - F_P^l) + B_e (F_E^l - F_P^l) \quad (2.8-18)$$

where

$$B_w = \gamma_{xw} A_w \delta t / \delta x_w \quad (2.8-19a)$$

$$B_e = \gamma_{xe} A_e \delta t / \delta x_e. \quad (2.8-19b)$$

In a similar manner, the integrals for the y and z directional diffusion terms may be written as

$$I_2 = B_s (F_s^l - F_P^l) + B_n (F_N^l - F_P^l) \quad (2.8-20)$$

$$I_3 = B_D(F_D^\ell - F_P^\ell) + B_U(F_U^\ell - F_P^\ell) \quad (2.8-21)$$

where

$$B_S = \gamma_{ys} A_s \delta t / \delta y_s \quad (2.8-22a)$$

$$B_N = \gamma_{yn} A_n \delta t / \delta y_n \quad (2.8-22b)$$

$$B_D = \gamma_{zd} A_d \delta t / \delta y_d \quad (2.8-22c)$$

$$B_U = \gamma_{zu} A_u \delta t / \delta y_u \quad (2.8-22d)$$

with

$$\delta y_s = y_j - y_{j-1} \quad (2.8-23a)$$

$$\delta y_n = y_{j+1} - y_j \quad (2.8-23b)$$

$$\delta z_d = z_k - z_{k-1} \quad (2.8-23c)$$

$$\delta z_u = z_{k+1} - z_k \quad (2.8-23d)$$

$$A_s = (z_{k+1/2} - z_{k-1/2}) (x_{i+1/2} - x_{i-1/2}) = A_n \quad (2.8-23e)$$

$$A_d = (x_{i+1/2} - x_{i-1/2}) (y_{j+1/2} - y_{j-1/2}) = A_u \quad (2.8-23f)$$

The values of the diffusion coefficients at the interfaces (i.e., the " γ " terms of Equations 2.8-19a-b and 2.8-22a-d) are taken to be functions of the values at their nearest neighboring nodes. Four choices for these functions are available in PORMC: (1) harmonic mean, (2) geometric mean, (3) arithmetic mean, and (4) upwind value. For γ_{xw} , these four functional forms are, respectively,

$$\gamma_{xw} = 2 \cdot \gamma_{xw} \gamma_{xp} / (\gamma_{xw} + \gamma_{xp}) \quad (2.8-24a)$$

$$\gamma_{xw} = (\gamma_{xw} \gamma_{xp})^{1/2} \quad (2.8-24b)$$

$$\gamma_{xw} = (\gamma_{xw} + \gamma_{xp}) / 2 \quad (2.8-24c)$$

$$\gamma_{xw} = \gamma_{xw}, \text{ if } U > 0; \gamma_{xw} = \gamma_{xp}, \text{ if } U < 0 \quad (2.8-24d)$$

where γ_{xw} and γ_{xp} are the values of the diffusion coefficient, γ_x , at the nodes W and P (Figure 2-9). For fully saturated flow problems, the harmonic mean option usually produces the best results; for unsaturated flow problems, the geometric mean options generally work best.

2.8.5.2 Discretization of the Convective Term. The integral of the x-directional component of the convection term in Equation 2.8-1 is written as

$$I_4 = - \int_t^{t+\delta t} \int_{V_p} \partial_x(\beta U F) dV dt. \quad (2.8-25)$$

Proceeding in a manner similar to that for the diffusion term, this integral can be written as

$$I_4 = - [\beta_e U_e^\ell F_e^\ell A_e - \beta_w U_w^\ell F_w^\ell A_w] \delta t \quad (2.8-26)$$

where

$$\beta_e = (\beta_E + \beta_P) / 2 \quad (2.8-27a)$$

$$\beta_w = (\beta_W + \beta_P) / 2 \quad (2.8-27b)$$

$$F_e = f_e F_E + (1 - f_e) F_P \quad (2.8-27c)$$

$$F_w = f_w F_W + (1 - f_w) F_P. \quad (2.8-27d)$$

For the second-order polynomial of Equation 2.8-6

$$f_e = f_w = 1/2. \quad (2.8-28)$$

However, the use of the second-order polynomial for the convective terms may lead to numerical instability if the grid Peclet number exceeds a critical value of 2 (Patankar 1980, p. 82). For example, in the present context, the grid Peclet number for the x-direction flux at location e of the control volume is defined by

$$P_e = \beta_e |U_e| \delta x_e / \gamma_{xe} \quad (2.8-29)$$

where x_e is the local grid size and U_e is the velocity component in the x-direction. To combat this instability, PORMC employs a hybrid approach for selecting suitable values for the f 's of Equations 2.8-27c and -27d (Spalding 1972, Runchal 1972). In this approach, the second-order polynomial of Equation 2.8-6 is employed if the local grid Peclet number is less than 2; otherwise, an upwind (or donor) scheme is employed. The values of the f 's of Equations 2.8-27c and -27d are then given by

$$f_e = 0.5 - 0.25 (P_e/|P_e|) \left[1 + (| |P_e| - 2|) / (|P_e| - 2) \right] \quad (2.8-30a)$$

$$f_w = 0.5 + 0.25 (P_w/|P_w|) \left[1 + (| |P_w| - 2|) / (|P_w| - 2) \right] \quad (2.8-30b)$$

The convective integral of Equation 2.8-26 can now be written as

$$I_4 = C_E (F_E^\ell - F_P^\ell) + C_W (F_W^\ell - F_P^\ell) + (C'_W - C'_E) F_P^\ell \quad (2.8-31)$$

where

$$C'_W = \beta_w U_w^\ell A_w \delta t \quad (2.8-32a)$$

$$C'_E = \beta_e U_e^\ell A_e \delta t \quad (2.8-32b)$$

$$C_W = f_w |C'_W| \quad (2.8-32c)$$

$$C_E = f_e |C'_E|. \quad (2.8-32d)$$

The convective integrals in the y- and z-directions are written by analogy as

$$I_5 = C_N (F_N^\ell - F_P^\ell) + C_S (F_S^\ell - F_P^\ell) + (C'_S - C'_N) F_P^\ell \quad (2.8-33)$$

$$I_6 = C_U (F_U^\ell - F_P^\ell) + C_D (F_D^\ell - F_P^\ell) + (C'_D - C'_U) F_P^\ell \quad (2.8-34)$$

where

$$C'_s = \beta_s U_s^\ell A_s \delta t \quad (2.8-35a)$$

$$C'_n = \beta_n U_n^\ell A_n \delta t \quad (2.8-35b)$$

$$C'_d = \beta_d U_d^\ell A_d \delta t \quad (2.8-35c)$$

$$C'_u = \beta_u U_u^\ell A_u \delta t \quad (2.8-35d)$$

$$C_s = f_s |C'_s| \quad (2.8-35e)$$

$$C_n = f_n |C'_n| \quad (2.8-35f)$$

$$C_d = f_d |C'_d| \quad (2.8-35g)$$

$$C_u = f_u |C'_u| \quad (2.8-35h)$$

where the β and f terms are defined in a manner analogous to that of Equations 2.8-27a through -27d and 2.8-30a and -30b.

2.8.5.3 Discretization of the Source Term. The source term S_F of Equation 2.8-1 is discretized as

$$I_7 = \int_t^{t+\delta t} \int_{V_p} S_F dV dt \quad (2.8-36a)$$

$$= S_p^\ell V_p \delta t \quad (2.8-36b)$$

where

$$V_p = (1/8) (x_{i+1} - x_{i-1}) (y_{j+1} - y_{j-1}) (z_{k+1} - z_{k-1}). \quad (2.8-37)$$

2.8.5.4 Discretization of the Decay-Rate Term. As indicated by Equation 2.8-3a, the decay-rate term $s_F F$ of Equation 2.8-1 is always discretized at the time level $t+\delta t$; i.e.,

$$I_8 = \int_t^{t+\delta t} \int_{V_p} s_F F dV dt \quad (2.8-38a)$$

$$= s_p^{n+1} F_p^{n+1} V_p \delta t. \quad (2.8-38b)$$

2.8.5.5 Discretization of Accumulation Term. For this term, the F is assumed to remain constant within the cell so that

$$I_9 = \int_t^{t+\delta t} \int_{V_p} a \partial_t F dV dt \quad (2.8-39a)$$

$$= a_p (F_p^{n+1} - F_p^n) V_p. \quad (2.8-39b)$$

2.8.6 Algebraic Analog of the General Transport Equation

The algebraic analog of the general transport equation (Equation 2.6-1) can be obtained by a combination of Equations 2.8-18 through 2.8-39. For completeness, the subscripts m for rock matrix and p for planar features are reintroduced into Equation 2.8-40.

$$\begin{aligned}
 (F_p^{n+1} - F_p^n) \left[a_{p_m} \psi_{p_m} + \sum_i a_{p_{p_i}} \psi_{p_{p_i}} \right] &= (F_E^\ell - F_p^\ell) \left[A_{E_m} + \sum_i A_{E_{p_i}} \right] \\
 + (F_W^\ell - F_p^\ell) \left[A_{W_m} + \sum_i A_{W_{p_i}} \right] &+ (F_N^\ell - F_p^\ell) \left[A_{N_m} + \sum_i A_{N_{p_i}} \right] \\
 + (F_S^\ell - F_p^\ell) \left[A_{S_m} + \sum_i A_{S_{p_i}} \right] &+ (F_U^\ell - F_p^\ell) \left[A_{U_m} + \sum_i A_{U_{p_i}} \right] \\
 + (F_D^\ell - F_p^\ell) \left[A_{D_m} + \sum_i A_{D_{p_i}} \right] &+ [S_p^\ell \psi_p] \delta t \\
 - S_p^{n+1} F_p^{n+1} \psi_p \delta t - (C_{W_m}^i + \sum_i C_{W_{p_i}}^i) & \\
 - C_{E_m}^i - \sum_i C_{E_{p_i}}^i + C_{S_m}^i + \sum_i C_{S_{p_i}}^i - C_{N_m}^i - \sum_i C_{N_{p_i}}^i & \\
 + C_{D_m}^i + \sum_i C_{D_{p_i}}^i - C_{U_m}^i - \sum_i C_{U_{p_i}}^i) F_p^\ell & \tag{2.8-40}
 \end{aligned}$$

where

$$A_W = B_W + C_W \tag{2.8-41a}$$

$$A_E = B_E + C_E \tag{2.8-41b}$$

$$A_S = B_S + C_S \tag{2.8-41c}$$

$$A_N = B_N + C_N \tag{2.8-41d}$$

$$A_D = B_D + C_D \tag{2.8-41e}$$

$$A_U = B_U + C_U \tag{2.8-41f}$$

and the superscript ℓ indicates the time (equal to n or $n+1$) at which various values are taken.

From the continuity equation, the last term on the right side of Equation 2.8-40 can be shown to be zero for incompressible fluids and negligible for fluids with small compressibility. Equation 2.8-40 can be written in a more compact form as follows:

$$A_p F^{n+1} = a_p v_p F_p^n + \sum_M A_M (F_M^\ell - F_p^\ell) + \sum_M (-1)^k C_M' F_p^\ell + S_p^\ell v_p \delta t \quad (2.8-42)$$

where M takes values of E, W, N, S, U, and D, respectively; $k = +1$ for $M = W, S,$ and D ; and $k = -1$ otherwise; and

$$a_p = a_{p_n} + \sum_i a_{p_i} \quad (2.8-43a)$$

$$A_p = a_p + s_p^{n+1} v_p \delta t \quad (2.8-43b)$$

$$A_M = A_{M_n} + \sum_i A_{M_i} \quad (2.8-43c)$$

$$C_M' = C_{M_n}' + \sum_i C_{M_i}' \quad (2.8-43d)$$

PORMC provides for both the explicit and implicit versions of Equation 2.8-42 to be solved. The methods of solution are described later in Section 2.9.

2.8.7 Exponential Integration Profile

The mathematical description given above employs a second-degree polynomial profile for the state variable F (Equation 2.8-7) for spatial discretization of the convection and diffusion terms. A second alternative available in PORMC relies on piecewise exponential profiles for F .

This choice is inspired by the analytic solution to the steady-state, one-dimensional version of the general transport Equation 2.6-1, which is

$$\partial_x (\beta U F - \gamma_x \partial_x F) = \phi \quad (2.8-44)$$

when

$$F = F_p \text{ at } x = x_p \quad (2.8-45a)$$

$$F = F_E \text{ at } x = x_E \quad (2.8-45b)$$

and ϕ is some constant. The exact solution of Equation 2.8-44, subject to Equations 2.8-45a and -45b, is

$$F = F_p + (F_E - F_p) \left\{ \exp \left[\beta U (x - x_p) / \gamma_{xe} \right] - 1 \right\} / \left[\exp (P_e - 1) \right]. \quad (2.8-46)$$

Now, consider the following composite convection and diffusion integral for the cell face represented by e:

$$I_{10} = \int_t^{t+\delta t} \int_e (\beta U F - \gamma_x \partial_x F) dy dz dt. \quad (2.8-47)$$

Assuming an exponential profile for F, as indicated by Equation 2.8-46, the integral in Equation 2.8-47 can be evaluated as

$$I_{10} = \beta_e U_e \left[(F_E - F_p) / (\exp P_e - 1) - F_p \right] A_e \delta t. \quad (2.8-48)$$

The coefficient A_e of Equation 2.8-42 now can be replaced by

$$A_e = \beta_e U_e / (\exp P_e - 1). \quad (2.8-49)$$

The other integrals are evaluated in a similar manner. The A's of Equation 2.8-42e are thus replaced by expressions similar to those of Equation 2.8-49. All other terms of Equation 2.8-42 are evaluated as before.

2.8.8 Algebraic Analogues of Boundary Conditions

The general form of the boundary condition, as discussed in Section 2.7.5, is

$$- a \partial F / \partial N = b(F - F_o) + c \quad (2.8-50)$$

where N represents a direction normal to a boundary. Suitable choices for a, b, c, and F_o lead to Dirichlet, Neumann, and mixed boundary conditions (Section 2.7.5). The algebraic equations for nodes located next to boundaries are modified to account for Equation 2.8-50. As an example, consider the node W, to the west of node P in Figure 2-9, to be a boundary node. To incorporate Equation 2.8-50 into the algebraic analog for node P, it is written as

$$- a (F_p - F_w) / \delta x_w = b (F_w - F_o) + c \quad (2.8-51)$$

where the value of F_p is taken at the advanced time, $t + \delta t$ (or at time step $n+1$). Equation 2.8-51 is now solved for F_w to obtain

$$F_w = a F_p + [\delta x_w (c - b F_o)] / [a - b \delta x_w]. \quad (2.8-52)$$

Finally, Equation 2.8-52 is substituted into the algebraic Equation 2.8-51 for node P, which eliminates F_w from the latter equation.

Thus, when the coefficient matrix is formed, the boundary conditions are implicitly included in it. Once the equations are solved (i.e., the value of F_p is obtained), Equation 2.8-52 is used again (in case of Neumann and mixed boundary conditions) to obtain the new value of F at the boundary.

2.9 SOLUTION OF ALGEBRAIC EQUATIONS

2.9.1 Explicit Solution Method

For explicit solution of Equation 2.8-42, the superscript l is replaced by n ; i.e., all of the F^l appearing on the right side of Equation 2.8-42 are assumed to be those at time t . Equation 2.8-42 then can be rearranged as

$$F_p = (1/A_p) a_p \psi_p F_p^n + \sum_M A_M (F_M^n - F_p^n) + \sum_M (-1)^k C_M^i F_p^n + S_p^n \psi_p \delta t. \quad (2.9-1)$$

Because all quantities on the right side of Equation 2.9-1 are known from initial conditions at time t , the F_p^{n+1} is easily evaluated by a simple substitution. The substitution is performed in a simple point-by-point manner. Three alternatives are available for the order of this substitution. In the first alternative, the substitution starts along the x-direction ($I=1$ to $IMAX$), then along the y-direction ($J=1$ to $JMAX$), and finally along the z-direction ($K=1$ to $KMAX$). This is called an x-y-z sweep. For the second alternative, the substitution is performed in the order of the y-, z-, and x-directions; whereas, in the third, it is performed in the order of the z-, x-, and y-directions. These last two alternatives are called the z-x and x-y sweeps.

2.9.2 Implicit Solution Method

For implicit solution, the superscript l is replaced by $n+1$. Equation 2.8-42 then can be rearranged as

$$\left(A_p + \sum_M A_M + (-1)^k C_M' \right) F_p^{n+1} = \sum_M A_M F_M^{n+1} + S_p^n \quad (2.9-2a)$$

where

$$S_p^n = a_p \psi_p F_p^n + S_p^n \psi_p \delta t. \quad (2.9-2b)$$

There are no more than seven unknowns (at node P and its six nearest neighbors) in Equation 2.9-2a. The number of unknowns is exactly seven for those nodes that have no boundary node as their neighbor. As explained in Section 2.8.7, values of F are eliminated for equations of those nodes that are located next to domain boundaries. Thus, for these nodes the number of unknowns is less than seven. Writing the set of equations for all of the nodes results in a heptadiagonal matrix. This coefficient matrix is of banded form and is very sparse. The actual band width depends on how the nodes are numbered. In PORMC, nodes are numbered in the order of increasing I, then J, and then K index. In this numbering system, the band width is $2 * (IMAX-2) * (JMAX-2)$.

To visualize the concept of sparsity of the coefficient matrix, consider a grid with dimensions of $10 \times 12 \times 15$. The total number of nodes in this grid is 2400. The number of internal nodes is 1040. Thus the coefficient matrix has $1040 * 1040 = 1,081,600$ elements, of which fewer than $1040 * 7 = 7280$ are nonzero.

Two direct and two iterative methods are available in PORMC. The direct-solution methods are accurate, but have the disadvantage of having elements within the band width that become nonzero during elimination procedures and thus require large amounts of storage. Therefore, these methods can be used only for relatively small grid sizes. The iterative methods, however, can be

implemented using a limited storage space and are preferred for large grids. A brief description of these methods is provided in the following section.

2.9.2.1 Cholesky Decomposition Method. The Cholesky decomposition method is a direct-solution method that is applicable to symmetric matrixes. The governing equation for pressure is always symmetric. The governing equations for temperature and concentration are symmetric only if the convection terms are neglected; otherwise, they are asymmetric. In a matrix form, the set of algebraic equations may be written as

$$[A]\{F\} = \{R\} \quad (2.9-3)$$

where $[A]$ is the symmetric coefficient matrix for elements A_{ij} , $\{F\}$ is the vectors of unknowns, and $\{R\}$ is the right side (or forcing) vector. $[A]$ is of size $N \times N$, where N is the number of internal nodes. Because $[A]$ is symmetric, only half of the band width needs to be stored. In the Cholesky decomposition, $[A]$ is decomposed into the product

$$[A] = [L] [L^T] \quad (2.9-4)$$

where $[L]$ is a lower triangular matrix for elements L_{ij} and $[L^T]$ is the transposition of $[L]$. The general formulas for obtaining L_{ij} are (Jennings 1977)

$$L_{ij} = \left[A_{ij} - \sum_{k=1}^{i-1} L_{ik} \right]^{1/2}, \quad j > i \quad (2.9-5a)$$

and

$$L_{ij} = \left[-\sum_{k=1}^{j-1} L_{ik} L_{jk} \right] / L_{jj}, \quad j > i. \quad (2.9-5b)$$

Having thus decomposed the coefficient matrix $[A]$, solution of the system of equations $[A]\{F\} = \{R\}$ proceeds in two stages. First, $\{G\} = [L^T]\{F\}$ is defined, whereupon the lower triangular system

$$[L]\{G\} = \{R\} \quad (2.9-6a)$$

may be solved for the vector {G} by forward substitution. Then the solution for {F} is obtained from the upper triangular system

$$[L^T] \{F\} = \{G\} \quad (2.9-6b)$$

by back substitution.

2.9.2.2 Gaussian Elimination Method. Gaussian elimination, taking into consideration the special structure of the coefficient matrix but without any pivoting, is used in PORMC. Pivoting is not used because the coefficient matrix is expected to stay diagonally dominant throughout the elimination process.

With respect to Equation 2.9-3, the (k+1)th elimination step is as follows:

$$A_{ik}(k+1) = 0, \quad k < i \leq N \quad (2.9-7a)$$

$$A_{ij}(k+1) = A_{ij}(k) - [A_{ik}(k) A_{kj}(k)] / A_{kk}(k), \quad k < i, j \leq N \quad (2.9-7b)$$

and

$$R_i(k+1) = R_i(k) - [A_{ik}(k) R_k(k)] / A_{kk}(k), \quad k < i \leq N. \quad (2.9-7c)$$

After the reduction phase has been completed, the solution can be written into {R} beginning with the last row. This back substitution is described by the following equation:

$$F_{ij} = \left[R_i - \sum_{k=i+1}^N A_{ik} F_{kj} \right] / A_{ii}. \quad (2.9-8)$$

2.9.2.3 Alternating-Direction-Implicit Method. The alternating-direction-implicit method completes the solution for one time step in three substeps. In the first substep, Equation 2.8-42 is replaced with

$$\left[A_p + \sum_M A_M + (-1)^k C_M' \right] F_p^* = A_E F_E^* + A_W F_W^* + S^n + S_p^n \quad (2.9-9a)$$

where

$$S^* = A_S F_S^n + A_N F_N^n + A_D F_D^n + A_U F_U^n. \quad (2.9-9b)$$

Equation 2.9-9a generates a tridiagonal (no more than three unknowns per node) matrix that is easily solved using the Thomas algorithm to yield values of F^* . For the next substep, another approximation, F^{**} , is obtained from

$$\left(A_P + \sum_M A_M + (-1)^k C_M' \right) F_P^{**} = A_S F_S^{**} + A_N F_N^{**} + S^* + S_P^n \quad (2.9-10a)$$

where

$$S^* = A_W F^* + A_E F^* + A_D F^* + A_U F^*. \quad (2.9-10b)$$

Finally, the solution for δt is completed by a third approximation, F_P^{***} , which is obtained from

$$\begin{aligned} \left(A_P + \sum_M A_M + (-1)^k C_M' \right) F_P^{***} &= A_D F_D^{***} + A_U F_U^{***} \\ &+ S^{**} + S_P^n \end{aligned} \quad (2.9-11a)$$

where

$$S^{**} = A_W F_W^{**} + A_E F_E^{**} + A_S F_S^{**} + A_N F_N^{**}. \quad (2.9-11b)$$

In many instances, F_P^{***} provides an acceptable approximation to F_P^{n+1} ; however, PORMC provides for iterative solution of Equations 2.9-9a and -9b through 2.9-11a and -11b, for a prespecified number of cycles at each time step.

The procedure above describes the solution process that first proceeds in the x-direction (Equation 2.9-9a), then in the y-direction (Equation 2.9-10a), and finally in the z-direction (Equation 2.9-11a). In a manner similar to that for the explicit-solution method, PORMC also provides for the sweeps to be conducted in the y-z-x and z-x-y directions.

2.9.2.4 Reduced-System Conjugate-Gradient Method. The reduced-system conjugate-gradient method provides an accelerated iterative solution that is

well suited to sparse matrixes. In PORMC, the reduced-system conjugate-gradient algorithm developed by Kincaid et al. (1982) is used. Application of this method requires that the algebraic equations be reordered into a "red-black" system (Hageman and Young 1981). In this ordering, components of {F} are considered to be either red or black. A red-black ordering rearranges the vector {F} such that every black unknown follows all of the red unknowns. This ordering leads to a 2 x 2 red-black partitioning of [A]; i.e.,

$$[A] = \begin{vmatrix} [A_{D1}] & [A_B] \\ [A_R] & [A_{D2}] \end{vmatrix} \quad (2.9-12)$$

where $[A_{D1}]$ and $[A_{D2}]$ are diagonal submatrixes, and $[A_B]$ and $[A_R]$ are, respectively, the black and red submatrixes.

The conjugate-gradient algorithm follows the following steps (Reid 1972). The residual at iteration k, $r(k)$, is

$$\{r(k)\} = \{R\} - [A]\{F(k-1)\} \quad (2.9-13)$$

where $F(0)$ is the initial approximation of the solution. The following steps are then followed:

$$q(k) = \frac{\langle \{r(k)\}, [A]\{r(k)\} \rangle}{\langle \{r(k)\}, \{r(k)\} \rangle} - e(k-1) \quad (2.9-14a)$$

$$\{r(k+1)\} = \{r(k)\} + [1/q(k)] [-[A]\{r(k)\} + e(k+1)(\{r(k)\} - \{r(k-1)\})] \quad (2.9-14b)$$

$$\{F(k+1)\} = \{F(k)\} + (1/q(k)) [\{r(k)\} + e(k-1) (\{F(k)\} - \{F(k-1)\})] \quad (2.9-14c)$$

$$e(k) = q(k) [\langle \{r(k+1)\}, \{r(k+1)\} \rangle / \langle \{r(k)\}, \{r(k)\} \rangle]. \quad (2.9-14d)$$

In Equations 2.9-14a through -14d, $\langle \{r\}, \{s\} \rangle$ denotes the inner product of the two vectors, $\{r\}$ and $\{s\}$. The iterations are performed until the solution satisfies a tolerance limit on the residual, $\{r\}$.

2.10 TREATMENT OF NONLINEARITIES

The governing equations for temperature and concentration (Equations 2.2-11 and 2.3-13) have slight nonlinearities. These nonlinearities stem from the fact that the convective velocities, U, V, and W, can be functions of temperature and concentration. With suitably selected time steps, these minor nonlinearities are of no consequence in solution of the equations. In general, it is assumed that the values of the quantities that rely on the dependent variable are available from the calculation at the previous time step, i.e., these quantities lag behind the solution by one time step.

The governing equation for pressure (Equation 2.1-17), however, can be highly nonlinear for conditions of partial saturation. This is apparent from the soil-moisture relations discussed in Section 2.7.3. For most soils and rocks, the degree of nonlinearity increases as the saturation decreases. To deal with these nonlinearities, an iterative method is followed in PORMC.

Three iterative methods for nonlinear equations are discussed in Huyakorn and Pinder (1983): (1) Picard, (2) Newton-Raphson, and (3) chord slope. Of these, the Picard method is the simplest and requires no additional storage; it is currently implemented in PORMC.

Using the Picard method, solution is begun with an initial "guess," which usually consists of the initial conditions specified by the user. Values of parameters that are functions of the dependent variable are calculated using this guess and substituted into Equation 2.8-42. Solution of Equation 2.8-42 provides a new estimate of the solution, and the process is repeated until specified convergence criteria are satisfied.

The following two options for determining convergence are provided by PORMC:

$$\max_{i=1,N} | [1 - F_i(k+1)/F_i(k)] | \leq \epsilon \quad (2.10-1)$$

and

$$(1/N) \left[\sum_{i=1}^N \left\{ 1 - [F_i(k+1)/F_i(k)] \right\}^2 \right]^{1/2} \leq \epsilon \quad (2.10-2)$$

where

N = the total number of internal nodes

k = the iteration number

ϵ = the specified convergence limit.

2.11 TREATMENT OF PARAMETER UNCERTAINTIES

There are three major steps in the uncertainty analysis of groundwater flow and contaminant transport in the vadose zone: (1) characterization of uncertain inputs, (2) propagation of uncertain inputs through the numerical model, and (3) characterization of output. The first step requires that the uncertainties in various inputs be quantified possibly in the form of multidimensional probability distributions. In most instances, this step would involve analysis of field and laboratory data as well as some conceptualization of the underlying model that represents the variation of a property in space. It may require application of geostatistical techniques such as Kriging. Some discussion of this aspect is provided in the following passages. Although geostatistical analysis is not a part of PORMC, options are available to use geostatistical models to generate spatially correlated samples. If geostatistical analysis is needed to determine geostatistical models, this step should be accomplished in a preprocessor to prepare the input for PORMC.

Currently, there are two broad approaches for propagation of uncertain inputs through a numerical model: perturbation techniques and Monte Carlo simulations. Perturbation techniques are usually applicable in cases in which the magnitude of parameter variability is small. Taking expectation of the first-order perturbation of the isothermal form of Equation 2.1-17, Mantoglou and Gelhar (1987a, 1987b, 1987c) obtained an equation for the mean value of the soil moisture tension (Ψ). The form of the equation for the expected value of Ψ remained the same as Equation 2.1-17, but the hydraulic parameters in the new equation became complicated nonlinear functions of gradients of Ψ . In applying the perturbation approach to field data, several additional assumptions may be required before a solution is obtained.

The approach for uncertainty propagation implemented in PORMC is to use a Monte Carlo method to calculate sample estimates for the statistics of the dependent variables (P, T, and C). This is accomplished by generating vectors of samples from the distributions of the uncertain input quantities. These samples are then used in Equations 2.1-17, 2.2-11, and 2.3-13; and the solutions are used to form an ensemble for the dependent variables, which can be analyzed to obtain uncertainties in the output. This approach is straightforward and has been demonstrated previously (Dagan and Bresler 1983, Andersson and Shapiro 1983, Sharma et al. 1987).

The third step involves application of standard statistical techniques to estimate mean, covariance, and probability distributions of the model output, and will be performed in a postprocessor.

Both a pre- and postprocessor for use with PORMC have been developed at Pacific Northwest Laboratory. The preprocessor is intended to provide an automated tool for generating a statistical cumulative distribution function (CDF) that describes a set of field data. Generating a CDF with the preprocessor allows field data to be used in PORMC without assigning an appropriate analytic form (e.g., lognormal) for the statistical distribution. The postprocessor is designed to perform statistical analysis on output files written by PORMC. This allows PORMC data of the dependent variables (P, T, and C) to be summarized in terms of means, variances, standard deviations, or statistical distributions.

2.11.1 Representation of Uncertain Parameters

To deal with parameter uncertainties quantitatively, several parameters will be treated as random variables. In Section 2.8, the spatial domain of interest was divided into a finite number (N) of elements (or cells) over which the governing equations were discretized to obtain a set of N algebraic equations. An uncertain parameter (e.g., porosity) is treated as a random variable within each cell. Thus, any one of the uncertain properties will be represented by a set of N random variables. If M parameters are simultaneously uncertain, then M x N random variables will represent the random field. Problems become increasingly complex as statistical dependence between these random variables is considered. The following cases may arise.

1. Parameters are Statistically Independent. The property in a region is represented by a single random variable (i.e., the same realization of the random variable represents the property in many elements of the computational grid). A one-dimensional probability distribution function (PDF) provides all the required statistical information about the parameter. When a soil (or rock) layer is homogeneous with respect to a property, one may assume that within the layer that property has a single value that will be obtained by sampling from its PDF.
2. Parameters are Cross Correlated. If a parameter is correlated with another (e.g., porosity with hydraulic conductivity), it cannot be sampled independently of the other. Two variations of this case may arise. In the first case, the two parameters may be perfectly correlated. This implies that once the value of one of them is known, the value of the other can be determined from a linear relation

$$A = \alpha + B \beta \quad (2.11-2)$$

where A and B are the perfectly correlated variables and α and β are known constants. In this case, only one of the two variables needs to be sampled; the other variable is then computed using the linear relationship.

In the second case, a correlation between A and B may exist:

$$\rho_{AB} = c(A,B)/[(\sigma_A \cdot \sigma_B)] \quad (2.11-3)$$

where $c(A,B)$ represents the covariance between A and B

$$c(A,B) = E\{[A - \mu_A] \cdot [B - \mu_B]\} \quad (2.11-4)$$

where E is the expectation operator and μ is the expected value.

With $f(u)$ representing the PDF of A,

$$E(A) = \mu_A \int_{-\infty}^{\infty} uf(u)du \quad (2.11-5a)$$

and

$$\sigma_A^2 = E\{[A - \mu_A]^2\} = \int_{-\infty}^{+\infty} (u - \mu_A)^2 f(u) du \quad (2.11-5b)$$

is the variance of A. In this case, A and B have to be sampled simultaneously, maintaining the relation of Equation 2.11-3. For a full description of the dependence between A and B, a bivariate PDF is needed. However, in PORMC, sampling is done using the univariate marginal PDFs of A and B and the coefficient of correlation ρ_{AB} . The marginal PDF of A (and analogously, the marginal PDF of B) is obtained from the bivariate PDF, $f(u,v)$, of A and B using the operation

$$f(u) = \int_{-\infty}^{\infty} f(u,v)dv. \quad (2.11-5b)$$

3. Parameters are Autocorrelated. The N (or a subset) of the random variables representing a property (e.g., porosity) in a spatial region of interest are correlated. Again, a multidimensional PDF is required to fully describe the relationship between these random variables. In most practical applications, it is not feasible to specify the multidimensional PDF. A spatially variable parameter in PORMC is assumed to be statistically homogenous (i.e., the mean is constant over the domain); and the covariance is dependent only on the separation, h , between two points, not the absolute location. In a one-dimensional setting, this can be represented by

$$c[A(x),A(x+h)] = c(h). \quad (2.11-6)$$

The internodal distances of the spatial grid determine the distance h . $c(h)$ can be anisotropic; however, in PORMC only geometric anisotropies are considered. Geometric anisotropies have the principal directions of anisotropy coinciding with the major coordinate axes.

When the above two assumptions are made (i.e., statistical homogeneity and covariance is independent of absolute location), the relationship between the covariance and the semivariogram is

$$\gamma(h) = c(0) - c(h) \quad (2.11-7)$$

where $\gamma(h)$ and $c(h)$ are the values of the semivariogram and covariance, respectively, at distance h , and $c(0)$ is the value of the covariance at $h=0$ (Journel and Huijbregts 1978). PORMC uses semivariogram models to describe autocorrelation. PORMC does not perform any geostatistical analysis; therefore, only the parameters that define semivariogram models are input into the code. The semivariogram models are then used to define the correlation matrix for autocorrelated parameters.

The four most commonly used semivariogram models are referred to as the linear, exponential, spherical, and Gaussian models. The typical definitions for these models are as follows:

- Linear Variogram Model

$$\gamma(h) = c(0) + w \left[\frac{h}{2} \right] \quad (2.11-8a)$$

- Exponential Variogram Model

$$\gamma(h) = c(0) + w \left[1 - \exp \left[-\frac{h}{a} \right] \right] \quad (2.11-8b)$$

- Spherical Variogram Model

$$\begin{aligned} \gamma(h) &= c(0) + w \left[\frac{3}{2} \left(\frac{h}{a} \right) - \frac{1}{2} \left(\frac{h}{a} \right)^3 \right] \text{ for } h \leq a \\ &= c(0) + w \quad \text{for } h > a \end{aligned} \quad (2.11-8c)$$

- Gaussian Variogram Model

$$\gamma(h) = c(0) + w \left[1 - \exp \left[-\left(\frac{h}{a}\right)^2 \right] \right] \quad (2.11-8d)$$

where

$c(0)$ = the "nugget"

w = the sill value

a = the correlation range.

The combined value of $c(0)$ and w is equivalent to the sample variance. Theoretically, the value of the semivariogram at $h=0$ is 0; however, in practice, there usually is a discontinuity at $h=0$. The discontinuity, or nugget, traditionally has been attributed to the combined effect of measurement error in obtaining data and spatial variability of a parameter on a scale below the sampling scale (Journel and Huijbregts 1978).

Equations 2.11-8a through -8d are written for isotropic semivariograms. PORMC, as noted previously, considers geometric anisotropic forms of semivariogram models. In addition, the semivariogram models are merely an intermediate step to defining correlation matrices for autocorrelated parameters. In three-dimensional space, where

$$h = (\Delta x^2 + \Delta y^2 + \Delta z^2)^{1/2} \quad (2.11-9a)$$

and letting

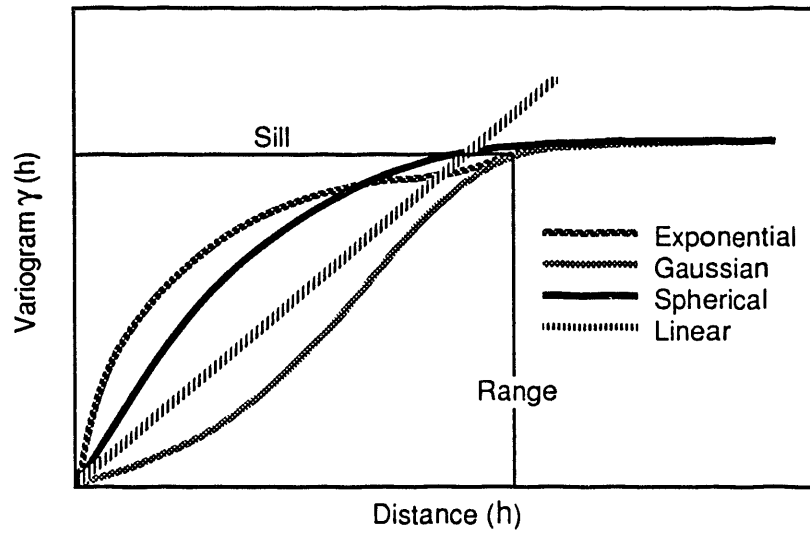
$$h_1 = \left[\left(\frac{\Delta x}{a_x}\right)^2 + \left(\frac{\Delta y}{a_y}\right)^2 + \left(\frac{\Delta z}{a_z}\right)^2 \right]^{1/2}, \quad (2.11-9b)$$

Equations 2.11-8a through -8d are then modified to take the form

- Linear Variogram Model

$$\begin{aligned} \gamma(\Delta x, \Delta y, \Delta z) &= c(0) + w (h_1) \text{ for } h_1 \leq 1 \\ &= c(0) + w \quad \text{for } h_1 > 1 \end{aligned} \quad (2.11-10a)$$

Figure 2-10. Typical Variograms with No Nugget Effect for Autocorrelated Variables.



S9101070.4

- Exponential Variogram Model

$$\gamma(\Delta x, \Delta y, \Delta z) = c(0) + w \left[1 - \exp(-h_1) \right] \quad (2.11-10b)$$

- Spherical Variogram Model

$$\begin{aligned} \gamma(\Delta x, \Delta y, \Delta z) &= c(0) + w \left[\frac{3}{2}(h_1) - \frac{1}{2}(h_1)^2 \right] \text{ for } h_1 \leq 1 \\ &= c(0) + w \quad \text{for } h_1 > 1 \end{aligned} \quad (2.11-10c)$$

- Gaussian Variogram Model

$$\gamma(\Delta x, \Delta y, \Delta z) = c(0) + w \left[1 - \exp(-h_1^2) \right]. \quad (2.11-10d)$$

Correlations, as a function of distance, are computed as

$$\rho(h_1) = 1 \text{ for } h_1 = 0 \quad (2.11-10e)$$

$$\rho(h_1) = 1 - \left[\frac{\gamma(\Delta x, \Delta y, \Delta z)}{c(0) + w} \right] \text{ for } h_1 > 0 \quad (2.11-10f)$$

for each of the semivariogram models. The linear semivariogram model was modified to have a sill; correlations cannot be computed from unbounded variances.

For the linear and spherical models, the inputs a_x , a_y and a_z , typically called "correlation lengths," denote the distance to the sill along each of the principal axes. For the exponential and Gaussian models, a_x , a_y , and a_z are typically chosen to satisfy

$$\gamma(\Delta x, 0, 0) = .95w \quad (2.11-10g)$$

$$\gamma(0, \Delta y, 0) = .95w \quad (2.11-10h)$$

$$\gamma(0, 0, \Delta z) = .95w \quad (2.11-10i)$$

at a specified distance Δx (or Δy or Δz). Thus, a_x is the input required to obtain a correlation of .05 at distance Δx .

The nugget, $c(0)$, is set to zero in $\gamma(\Delta x, \Delta y, \Delta z)$ when choosing values for a_x , a_y and a_z ; i.e., for the Gaussian model, a_x is found from

$$1 - \exp \left[- \left(\frac{\Delta x}{a_x} \right)^2 \right] = .95 \quad (2.11-10j)$$

thus,

$$1.7308 a_x = \Delta x. \quad (2.11-10k)$$

For uncertain parameters, the input to PORMC consists of the marginal PDFs and either the cross-correlation coefficients or the semivariograms.

2.11.2 Representation of Stochastic Hydraulic Properties

Stochastic hydraulic properties of the vadose zone may present a special problem because these are functions of Ψ , the soil-moisture suction, which itself varies stochastically. In PORMC, the $\theta - \Psi$ and $k_r - \Psi$ functions are assumed to take on the functional forms discussed in Section 2.7.3. The parameters of these functional forms (e.g., α and n of the van Genuchten relation) are considered to be stochastic and are described in Section 2.11.1.

An alternate representation of hydraulic properties in PORMC is the use of similarity theory. When the porous medium has similar hydraulic properties at different locations, in the sense of Miller and Miller (Sharma et al. 1987, Sposito and Jury 1985), the hydraulic property functions at each location can be scaled with a factor called α . This scaling factor reduces the curves at various locations to a single mean curve. The scaling equations for the hydraulic head and the hydraulic conductivity are

$$\Psi_i = \Psi^*/\alpha_i \quad (2.11-11a)$$

$$K_i = K^*\alpha_i^2 \quad (2.11-11b)$$

for location index $i = 1, \dots, N$; where $\Psi^*(\theta)$ and $K^*(\theta)$ are the reference (or mean) hydraulic properties. Once reference properties are determined, corresponding properties at various locations are obtained by applying the scale factor α_i as indicated by Equations 2.11-10a and -10b. By using scaling when applicable, the spatial variability can be entirely characterized in terms of the statistical attributes of the single parameter α . Many efforts to assess the impact of spatial variability on unsaturated flow predictions have used the scaling concept. Jury et al. (1987) discuss the technical issues and limitations in applying the scaling method. A significant issue is that the scale relations of Equations 2.11-11a and -11b usually apply only approximately at the field scale. Furthermore, the scale factors defined by using different hydraulic properties are not necessarily equal in value or equivalent in their definition. In some situations, it may become necessary to introduce two scale factors to explain departures from Equations 2.11-11a and -11b. In spite of its shortcomings, the scaling method has been found to be a simple expedient for quantitatively evaluating variability at the first stage of analysis. Sharma et al. (1987) have reviewed past applications of the scaling concept and employed it to evaluate the response of an entire hill slope watershed while accounting for areal correlation in scale factors. Although limited to media for which similarity holds, this method could be a potentially inexpensive way of performing the Monte Carlo simulations.

2.11.3 Probability Distribution Functions of Random Properties

Several standard forms for PDFs are available in PORMC and are described below. In addition to the standard forms, PDFs can also be specified in a table.

- Constant

$$p\{A = a\} = 1. \quad (2.11-12)$$

In this case, variable A is constant with a value equal to a. No sampling is done for this specification.

- Uniform Distribution

This is also known as the equally likely or the rectangular distribution. The PDF for the uniform distribution is

$$f_A(a) = \begin{cases} 1/(a_{\max} + a_{\min}) & a_{\min} \leq a \leq a_{\max} \\ 0 & \text{elsewhere.} \end{cases} \quad (2.11-13)$$

The mean and variance of this distribution are given by

$$\mu_A = a_{\min} + [(a_{\max} - a_{\min})/2] \quad (2.11-14a)$$

$$\sigma_A^2 = (a_{\max} - a_{\min})^2/12. \quad (2.11-14b)$$

- Log Uniform Distribution (base 10)

This distribution assigns equal likelihood to $\log_{10}A$. Equation 2.11-13 applies, except that instead of A, $\log_{10}A$ is used.

- Log Uniform Distribution (base e)

Again, Equation 2.11-13 applies, except that $\log_e A$ is used instead of A.

- Normal Distribution

The distribution function is given by

$$f_A(a) = (1/\sigma_A \sqrt{2\pi}) \exp[-1/2\{(a - \mu_A)/\sigma_A\}^2]; \quad -\infty \leq a \leq +\infty. \quad (2.11-15)$$

The normal distribution is symmetric about its mean μ . The Central Limit Theorem states that under very general conditions, the distribution of the sum of random variables will approach the normal distribution as the number of random variables in the sum increases. In fact, the distribution of a sum of 12 uniformly distributed variables approximates the normal distribution very well.

- Lognormal Distribution (base 10)

In this case, the distribution of $B = \log_{10} A$ is given by Equation 2.11-15. The distribution of A is given by

$$f_A(a) = (1/a\sqrt{2\pi} \sigma_{\log A}) \exp \{-1/2[(1/\sigma_{\log A}) \log(a/m_A)]^2\}, \quad (2.11-16a)$$

or alternatively,

$$f_A(a) = (1/a \sigma_B \sqrt{2\pi}) \exp \{-1/2[(\log a - \mu_B)/\sigma_B]^2\}; a \geq 0. \quad (2.11-16b)$$

In Equation 2.11-16a, m_A is the median of the distribution; i.e.,

$$p(A \leq m_A) = 0.5 \quad (2.11-16c)$$

$$\text{and } \log m_A = \mu_B. \quad (2.11-16d)$$

The lognormal distribution is restricted to positive values of the random variable. Depending on σ_B , it can take a variety of shapes as shown in Figure 2-11.

- Lognormal Distribution (base e)

The previous description for base 10 lognormal variables applies to this distribution also.

- Exponential Distribution

This distribution is

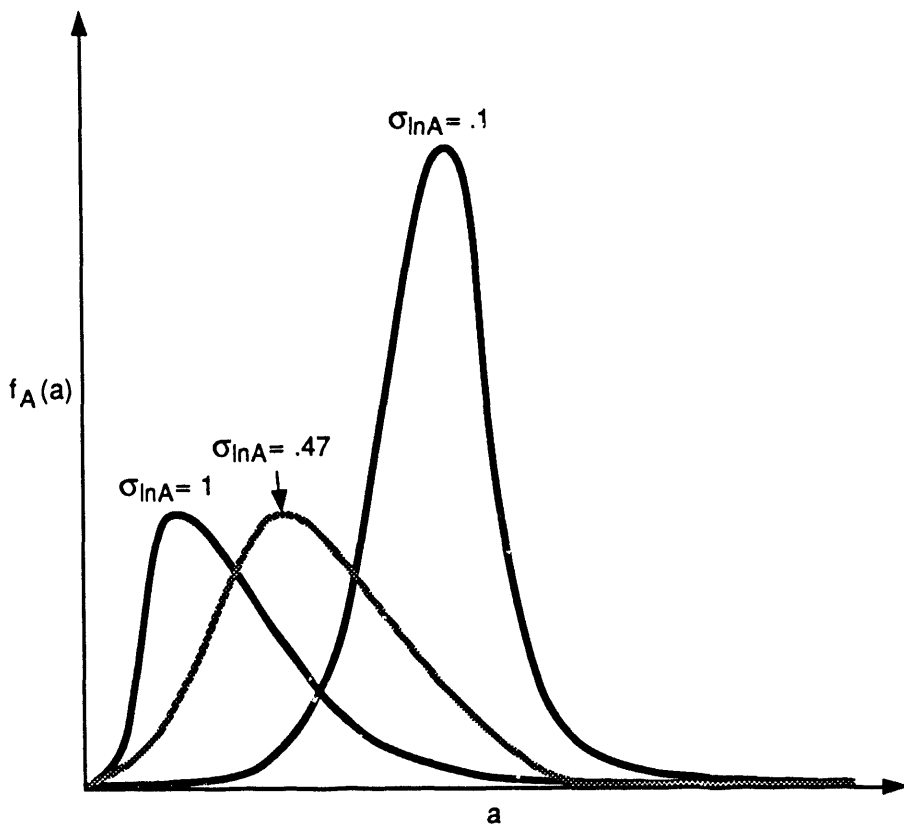
$$f_A(a) = \lambda \exp(-\lambda a); a \geq 0 \quad (2.11-17)$$

with mean = $1/\lambda$ and variance = $1/(\lambda^2)$.

- Tabular Distribution

If one of the above standard distributions cannot be fitted or is not appropriate for a variable, the CDF can be provided in a table. The CDF is arranged in an ascending order.

Figure 2-11. Illustration of Lognormal Distribution.



S91101070.1a

In certain situations, truncated distributions may be more appropriate. For example, the PDF for porosity may be normal, but because porosity values can lie between 0 and 1 only, the specified normal distribution must be specified with lower and upper limits. The truncated PDF of a random variable A ($a_{\min} \leq A \leq a_{\max}$) is obtained by renormalizing; i.e.,

$$f_A(a) = \begin{cases} 0; & a < a_{\min} \\ k f_B(a); & a_{\min} \leq a \leq a_{\max} \\ 0; & a > a_{\max} \end{cases} \quad (2.11-18a)$$

where k is the renormalizing factor

$$k = 1 / [1 - F_B(a_{\min}) - F_B(a_{\max})]. \quad (2.11-18b)$$

In Equations 2.11-18a and -18b, B is the random variable with its PDF defined over the entire range (in the case of normal, from $-\infty$ to $+\infty$) and A is the transformed variable with lower and upper limits. $F_B(a)$ is the CDF of B. In PORMC, one or both of the truncation limits may be specified.

2.11.4 Method of Sampling

2.11.4.1 Random Number Generator. The first step in obtaining samples of random variables is to generate a sequence of random numbers, $U_i(0,1)$, between 0 and 1 that are uniformly distributed. Because these numbers are generated through a recursive deterministic relation on a computer, it is impossible to generate sequences that are truly random. Only pseudo- or quasi-random sequences can be generated. A pseudo-random sequence is defined as a deterministic sequence of numbers in $[0,1]$ having the same relevant statistical properties as a sequence of random numbers. All such pseudo-random sequences are periodic (i.e., they repeat themselves). An effort is made to make this period as large as possible.

Congruential generators are the most common for obtaining the random sequence (Ripley 1987). The general form of these generators is

$$d_i = (a d_{i-1} + c) \text{mod } M \quad (2.11-19a)$$

$$u_i = d_i/M \quad (2.11-19b)$$

where

a = the multiplier

c = the shift

M = a large integer.

Given an initial value of the seed d_0 , a sequence of d_i and U_i can be generated. In PORMC

$$a = 16807 \quad (2.11-20a)$$

$$c = 0 \quad (2.11-20b)$$

$$M = 2147483647. \quad (2.11-20c)$$

The value of the seed d_0 can be any integer between 1 and 2147483647.

2.11.4.3 Samples from Marginal Distributions. Once $U_i(0,1)$ is obtained, a well-known theorem of statistics can be used to obtain samples from various distributions. This theorem states that if $F_A(a)$ is the CDF of A, and u in a number from $U(0,1)$, then $a = \min\{x | F(x) \geq u\}$ is a sample from F (Ripley 1987). Thus, for normal distributions

$$a_i = \mu + \sigma F^{-1}(u_i) \quad (2.11-21a)$$

and for exponential distribution

$$a_i = -(1/\lambda) \ln u_i. \quad (2.11-21b)$$

Two possible schemes can be used to generate a sequence of samples. The simple random sampling scheme consists of obtaining repeatedly a sample from the entire range of the variable; a fairly large number of samples is needed to obtain samples from the low-probability tails of the distribution. An alternate scheme is to use some form of a stratified sampling scheme. In PORMC, a slightly modified form of the Latin Hypercube Sampling scheme is used (Iman and Conover 1982).

To obtain a stratified sample of size N for variable A, a sequence of uniformly distributed random numbers, a_i , $0 \leq a_i \leq 1$; $i = 1, 2, \dots, N$ are first generated. The a_i are random and are not ordered according to their magnitude. Let r_i be the ranks of a_i . Now the range of the variable A is divided into N equiprobable intervals, and one sample is then generated in each one of these intervals. The nth such sample will be

$$s_n = [(n-1) + u_n]/N \quad (2.11-22)$$

where u_n is a freshly generated (i.e., it is not the same as a_i), uniformly distributed number between 0 and 1. The s_n generated by Equation 2.11-22 are ordered according to their magnitude (i.e., $s_1 < s_2 \dots < s_N$). In the final step, the s_i are reshuffled according to the rank vector r_i . The final sample set thus obtained is random and stratified, lies between 0 and 1, and is uniformly distributed.

2.11.4.4 Samples of Correlated Variables. For correlated variables, the Latin Hypercube Scheme method described by Iman and Conover (1982) is used in PORMC. To briefly explain this method, assume that A_i , $i = 1, 2, \dots, K$ are random variables (e.g., porosities at K nodes) that are correlated. Their (K x K) correlation matrix is [C]. As explained before, [C] is obtained from their specified semivariogram. Assume that N samples are to be obtained. First, samples of A_i are obtained as if they are independent, as explained in Section 2.11.4.3. Let these samples be $[A] = a_{ij}$; $i = 1, 2, \dots, K$, and $J = 1, 2, \dots, N$. In other words, there are N sample vectors, each vector having K elements, or

$$[A] = \begin{vmatrix} a_{11} & a_{12} & \cdot & \cdot & \cdot & a_{1K} \\ a_{21} & a_{22} & \cdot & \cdot & \cdot & a_{2K} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{N1} & a_{N2} & \cdot & \cdot & \cdot & a_{NK} \end{vmatrix} \quad (2.11-23)$$

Note that elements in the jth column of [A] are the samples of A_j , and each row of [A] is a sample vector of all the K random variables. The objective is

to rearrange the elements of columns of [A] so that the correlation will be as close to [C] as possible.

The first step in the method of Iman and Conover (1982) is to create a rank matrix [R] = r_{ij} by replacing samples a_{ij} in each column j by their ranks. Because there are N samples of each random variable, r_{ij} will be integers between {1, 2, ..., N}. The next step is to obtain a Cholesky decomposition of [C] as follows (because [C] is symmetric and nonnegative definite, such a decomposition always exists):

$$[C] = [P] [P^T] \quad (2.11-24)$$

where [P] is the lower triangular matrix and [P^T] is its transpose. Next a score matrix [S] is generated by using van der Waarden scores, which are

$$s_{ij} = \phi^{-1} [r_{ij} / (N+1)] \quad (2.11-25)$$

where ϕ^{-1} is the inverse of the standard normal CDF. [S] has the same rank correlation matrix as [A] (i.e., [R]). Let [U] be the correlation matrix of [S], whose Choleski decomposition can be written as

$$[U] = [Q] [Q^T]. \quad (2.1-26)$$

We want to determine a matrix [T] such that

$$[C] = [T] [U] [T^T]. \quad (2.1-27)$$

Substituting for [C] from Equation 2.11-24 and for [U] from Equation 2.1-26, Equation 2.1-27 becomes

$$[P] [P^T] = [T] [Q] [Q^T] [T^T] \quad (2.1-28a)$$

which gives

$$[T] = [P] [Q^{-1}]. \quad (2.1-28b)$$

A new score matrix [S*] is now determined

$$[S^*] = [S] [T^T] \quad (2.1-29)$$

which has a correlation matrix $[C]$. A new rank matrix $[R^*]$ is now obtained by replacing elements of $[S^*]$ by their column ranks. Finally, the columns of the sample matrix $[A]$ are rearranged to obtain the required sample matrix $[A^*]$ that has rank matrix $[R^*]$.

The method described previously has a number of desirable properties, such as the following.

- The method does not require specification of the joint distribution function of the correlated variables.
- The method can be used in conjunction with stratified schemes such as the Latin Hypercube Scheme.
- Marginal distributions of the random variables are preserved.

2.12 SUMMARY

Continuum mechanics provide the mathematical basis for the PORMC 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.

All the parameters in the governing equations of PORMC can be specified as stochastic processes. These parameters include porosities, saturated hydraulic conductivities, thermal conductivities, dispersivities, and the properties of the unsaturated medium. In addition, the source terms can also be treated as stochastic quantities.

3.0 DESCRIPTION OF COMPUTER CODE AND ITS USE

3.1 SUBROUTINES AND THEIR FUNCTIONS

The PORMC computer code currently is made up of 118 subroutines and functions that hereafter are referred to as modules. To the extent possible, each module has been assigned a single, distinct function. The names of these modules and their assigned functions are listed alphabetically in Table 3-1. A brief description of the information flow between modules is given in the next section.

3.2 INFORMATION FLOW BETWEEN SUBROUTINES

The main program is named PORMC. The sizes of various arrays are declared in this program. The problem title, user identification, grid size, and number of realizations to be obtained are read. Default names to output data files are assigned. Finally, 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. The INIT subroutine is executed only during the first realization. Variables that require repeated initialization (i.e., in each realization) are initialized in AFLOW itself. Some or all of these default values subsequently change because of the user-supplied data. The default values are discussed in Chapter 4.0. 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. INPUT is the main routine that interprets the data from each input command.

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 4.0, 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 when these are deterministic; PROPS for matrix properties when these are stochastic; 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.

For problems with stochastic parameters, a call to SAMPLE is made to obtain an ensemble of values from the prescribed probability distribution. Statistics of the samples are calculated in SSTAT and printed in the output file. Values of perfectly correlated variables are obtained in SAMP2 and

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 1 of 8)

Number	Module	Function of module
1	ADATA	Format-free input data is read and interpreted. All characters comprising an input command are read and separated into numeric and nonnumeric data.
2	AFLOW	Solution of governing equations is coordinated; new properties assigned for each realization; iterations controlled and convergence checked. Most subroutines are called from AFLOW.
3	ALNORM	Area under a standard normal probability density curve is computed. ALNORM is written as a real function.
4	ARCHIV	Header and grid information is read from or written to the data archive files.
5	ARCHV2	Field arrays (i.e., data defined at each grid node in a three-dimensional field) are read from or written to archive files.
6	ARRAYS	A utility subroutine is used to initialize three-dimensional field arrays. Either a part or the full array may be initialized.
7	ATITL	Problem title is read for printing on the first page of the output.
8	BCDCAY	Radioactive decay is implemented for concentration boundary conditions.
9	BCDFLT	Default boundary conditions are assigned. Default boundary conditions are equal to the initial values of variables at the boundary nodes.
10	BCEDGE	Values of variables at the eight corners of the solution domain are calculated. Values at these eight nodes actually do not appear in the discrete equations.
11	BCFO	Boundary conditions are processed so that these can be incorporated in the discrete equations. The flux type boundary conditions are multiplied by cell-face areas.
12	BCPOST	Variable values at the boundaries are computed after the solution is obtained in the interior of the domain.
13	BCPRE	Boundary values are incorporated into the coefficient matrix. The size of the coefficient matrix is equal to the number of internal nodes and no equations are written for the boundary nodes.
14	BCUSER	User-specified boundary conditions are read, interpreted, and stored for later use.

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 2 of 8)

Number	Module	Function of module
15	BCUVW	Velocity arrays for surfaces represented by $I = 1$, $J = 1$, and $K = 1$ are filled in. This is for convenience only because these values are not truly calculated. In PORMC, velocities are calculated midway between nodes.
16	BLKPRT	Problem title read in ATITL is printed on the first page of output file. The title is written in letters of height equivalent to five lines.
17	BUGSET	User-specified debugging command is interpreted and stored for later use.
18	CHOLP	A Cholesky decomposition is performed on a symmetric positive definite matrix that is stored as a vector. The input matrix is overwritten by the decomposed matrix.
19	COND	Sample of a nodal autocorrelated conductivity is picked before calculating conductivity cell-face values.
20	DATTIM	The system time and date routine is called. The time and date is printed on the output and archive files.
21	DCLAIM	The status of verification/benchmarking of the code is printed; normally it is used to print any disclaimer or other desired notice.
22	DELXYZ	Fracture length between grid nodes is calculated. In PORMC, fractures must begin and end at grid nodes.
23	DENSTY	The thermal buoyancy term and the pressure source term are computed for nonisothermal flow problems.
24	DIFH	Temperature effects on hydraulic conductivities are incorporated.
25	DISPER	From dispersivities and velocities, dispersion coefficients for material zones are calculated using Scheidegger's relations.
26	DOMAIN	The subdomain of interest for the heat and concentration equations is determined.
27	DZONE	Material zone number in which a particular node lies is determined.
28	ERROR1	Error conditions during input for FORTRAN INTEGER variables are printed.
29	ERROR1	Error conditions during input for FORTRAN INTEGER variables are printed.

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 3 of 8)

Number	Module	Function of module
30	ERROR3	Error conditions during input for specification of planar elements and sources are printed.
31	EXIST	Existence of a command modifier on an input command is detected.
32	EXMP	A second-order expansion is used to estimate the value of an exponential function.
33	FCOV	Correlation matrix is calculated for one of several specified covariance functions.
34	FDS	Coefficient matrix for the heat and concentration equations is assembled and filled into a one-dimensional array for later processing.
35	FDSEXP	Performs calculations for matrix coefficients for the heat and concentration equations when exponential discretization scheme is used.
36	FDSP	Coefficient matrix for the pressure equation is stored in a one-dimensional array.
37	FIX	Coefficient matrix is modified for incorporating nodes where the user wants certain variables to be fixed. The nodes where values are fixed remain in the set of equations to be solved.
38	FLOW	Amount of fluid flow through cell faces is computed.
39	FLUX	Convective and diffusive fluxes of fluid, heat, and mass through user-specified surfaces are computed. Mass and energy balance (if asked for) is also computed in FLUX.
40	FLUX1	Certain repetitive calculations required by FLUX are performed.
41	FLUXP	Following user instructions, fluxes calculated in FLUX are printed to user-specified file.
42	GEODEF	The FIX command for fixing variable values at certain internal nodes is interpreted.
43	GEOM	Geometric quantities such as lengths, areas, and volumes associated with computational elements are computed.
44	GETROW	Elements of a selected row from the coefficient matrix are read for processing. Used by direct solvers only.
45	GRID	The GRID command is interpreted. x-, y-, and z-coordinates of grid nodes are read or calculated and stored.

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 4 of 8)

Number	Module	Function of module
46	HARMON	Hydraulic and thermal conductivities and mass diffusivities are calculated at the cell faces. Conductivities and diffusivities are specified at nodes. Values at cell faces are calculated using user-specified options (e.g., arithmetic, geometric or harmonic means).
47	HISTORY	Command for recording time-history of output variables is interpreted.
48	HISTR2	Time-history data is prepared for time plots and tabular output.
49	INIT	Initialization of various variables is performed. Default values are assigned in INIT. Some initialization is also performed in AFLOW.
50	INPUT	This is the main input routine. Some inputs are also read in program PORMC and in AFLOW. The input commands read by ADATA are interpreted in INPUT.
51	INPUT2	A real or an integer one-dimensional array is updated depending on instructions contained in the input command.
52	INPUT3	Tabular input, containing data in two columns, is read.
53	INTABL	The value of a variable read in a tabular form by using INPUT3 is computed through linear interpolation.
54	INVERT	Tridiagonal coefficient matrixes formed in the application of the ADI method are solved.
55	IOFILE	File name and format type is interpreted on an input command. If archived data is large, more than one file may be assigned by using multiple SOLVE commands.
56	IOUNIT	I/O files are opened.
57	LOCNP	Grid indexes transformed from three-dimensional to one-dimensional space and vice versa.
58	MCORR	Correlations between the columns of the score matrix are calculated.
59	MULTAB	A full matrix is multiplied with a lower triangular matrix. The input full matrix is overwritten on output.
60	NEWPRO	Stochastic variables, except for the source terms, are assigned sample values for the realization before computations for that realization are started.
61	OUTALL	Printing of tables for field arrays is coordinated.

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 5 of 8)

Number	Module	Function of module
62	OUTF1	Output options for field variables are set based on user instructions in the input deck.
63	OUTF2	Default options for the output of field variables are selected.
64	OUTR	Particle travel times are written to output file.
65	OUTSAV	Coordinates the reading and writing of data archives.
66	OUTVAR	Input commands are interpreted to find the variables to which these commands apply.
67	PLALFA	The storage term for planar and linear elements is computed.
68	PLAREA	The area of planar elements is calculated.
69	PLPRF	Effects of planar and linear elements are incorporated into the coefficient matrixes for the temperature and concentration equations.
70	PLPRF2	Repetitive calculations required in PLPRF are performed.
71	PLPRP	Effects of one- and two-dimensional elements are incorporated into the pressure equation.
72	PORMC	It coordinates memory allocation, reads title and grid data, and calls AFLOW.
73	PPND	The standard normal deviate corresponding to a specified lower tail area is evaluated.
74	PRINT	A record of key variables and parameters at the reference node is printed out.
77	PRNTZN	The component and matrix properties for each zone are printed.
78	PROPER	Volumetric and effective properties of soil/water matrix are calculated.
79	PROPS	All input commands associated with stochastic properties (but not stochastic sources) are interpreted in PROPS.
80	PROPZ	Zonal properties from user input are interpreted.
81	PROPO	Default values for density and viscosity are incorporated.

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 6 of 8)

Number	Module	Function of module
82	PUTF	This is a utility subroutine to perform internal three-dimensional array manipulations. Variables of an array can be assigned a constant value, replaced by values in another array, or transformed through a linear transformation.
83	RANGEN	Uniform (0,1) variables are transformed to other specified distribution types.
84	RESDU2	For iterative solution of the pressure equation, the residual is calculated.
85	ROUND	Written as a real function, it rounds off numeric labels on plots.
86	SAMCOR	Latin Hypercube algorithm is applied to obtain samples of autocorrelated variables.
87	SAMPLE	Stochastic inputs interpreted and sample generating routines are called.
88	SAMP2	Values of a variable that is perfectly correlated with another variable are obtained.
89	SLVADI	It solves the matrix of equations by the ADI method.
90	SLVCHL	The matrix of equations is solved by the method of Cholesky decomposition.
91	SLVGSE	The matrix of equations is solved by method of Gaussian elimination.
92	SLVSOR	The matrix of equations is solved by the PSOR method.
93	SLVITP	The matrix of equations is solved by the RSCG method. Subroutines needed for this method are external to PORMC. These are compiled separately and then linked.
94	SOLVE	It coordinates the solution of the set of algebraic equations. Calls to SLVADI, SLVCHL, SLVGSE, SLVSOR, and SLVITP are made from this subroutine.
95	SORCIN	Source data (including stochastic source) is read and stored into appropriate arrays.
96	SOURCE	The current value of source and sink terms is computed.
97	SOURC9	The current value of the inventory-limited source term is computed.
98	SSORT	An array is sorted into increasing or decreasing format.

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 7 of 8)

Number	Module	Function of module
99	SSTAT	This computes statistics of samples and writes them to output file.
100	TABLES	Headings for the printing of three-dimensional field variables are set up.
101	TABLE2	Tables of the three-dimensional field variables are printed.
102	TIMSTP	Written as a real function, the time step for fluid particle travel time is calculated if the current time step is larger than that required to traverse an element.
103	TRAVEL	Travel times for fluid particles are computed.
104	TRMINO	It computes the inverse of a lower triangular matrix and is needed for sampling purposes.
105	TRMULO	Two lower triangular matrixes are multiplied.
106	TSTAT	Central processing unit time taken by the problem is obtained.
107	U01	A uniform (0,1) random number is generated from a given seed; it is written as a real function.
108	U01S1	A vector of uniform (0,1) random numbers with stratification is generated.
109	USPIN	The hydraulic conductivity and moisture content of unsaturated media are computed.
110	USPRP	Soil properties for unsaturated media are processed.
111	VEL	Darcy velocity components and stream function are calculated.
112	WINDOW	The input specification of a window or subdomain is incorporated.
113	XALFA	The volumetric storage term (including retardation coefficient for the concentration equation) for the general equation is calculated.
114	XNEXT	The coordinate of the particle at the end of current time step, a real function, is calculated.
115	XSIDE	The side of an element that a fluid particle will exit on during its travel path is found.
116	XYPLOT	Time-history printer plots are produced.

Table 3-1. PORMC Modules and Their Primary Functions. (sheet 8 of 8)

Number	Module	Function of module
117	ZNAME	The names of the output variables to be printed are provided. These names are printed as the title of the tables.
118	ZONE	The ZONE command interprets input data and assigns a zone-designation index to various regions of flow.

those of autocorrelated variables in subroutine SAMCOR. The ensemble of values is stored for later use. New values are assigned to stochastic variables in NEWPRO, which is called from AFLOW. Once a set of values for the stochastic variables is picked, calculations proceed in the same manner as in the deterministic case.

In the GEOM subroutine, 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 is 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 2.8). 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, and the fluid source term is assigned in the SOURCE subroutine. At this stage, the SOLVE subroutine is called upon 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 (Gaussian elimination), SLVSOR (PSOR), or SLVITP (Conjugate Gradient) subroutine for the actual solution. The values of the hydraulic head at domain boundaries are calculated in the BCPOST subroutine. The solution of the nonlinear pressure equation is obtained iteratively by calculating the residues in each iteration in the RESDUE subroutine.

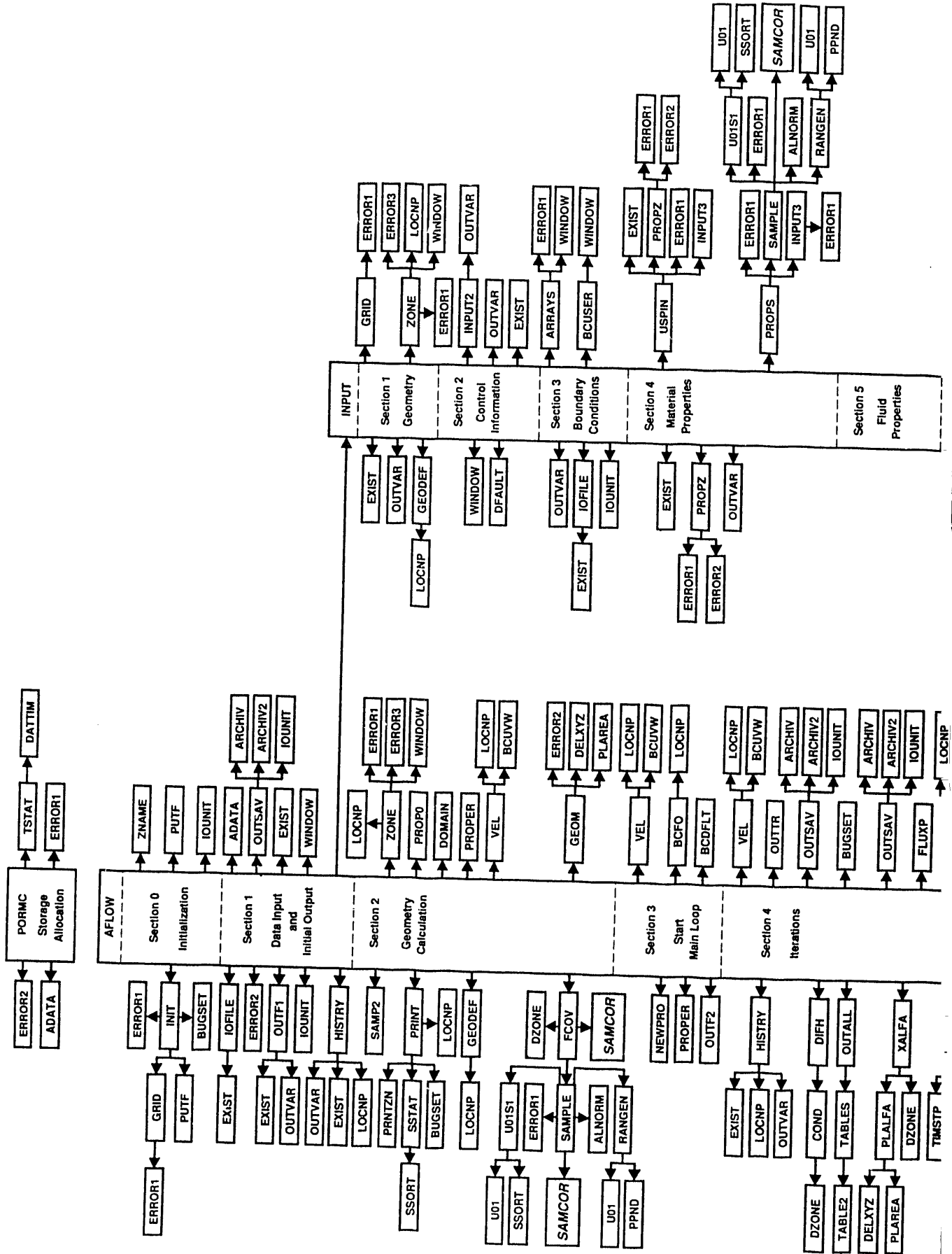
The solution of the heat transfer and mass transport equations proceeds in a similar manner through the same subroutine, except that the hydrodynamic dispersion coefficients are calculated in the DISPER subroutine, and the final values of the coefficients of the algebraic equations are obtained in the 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.

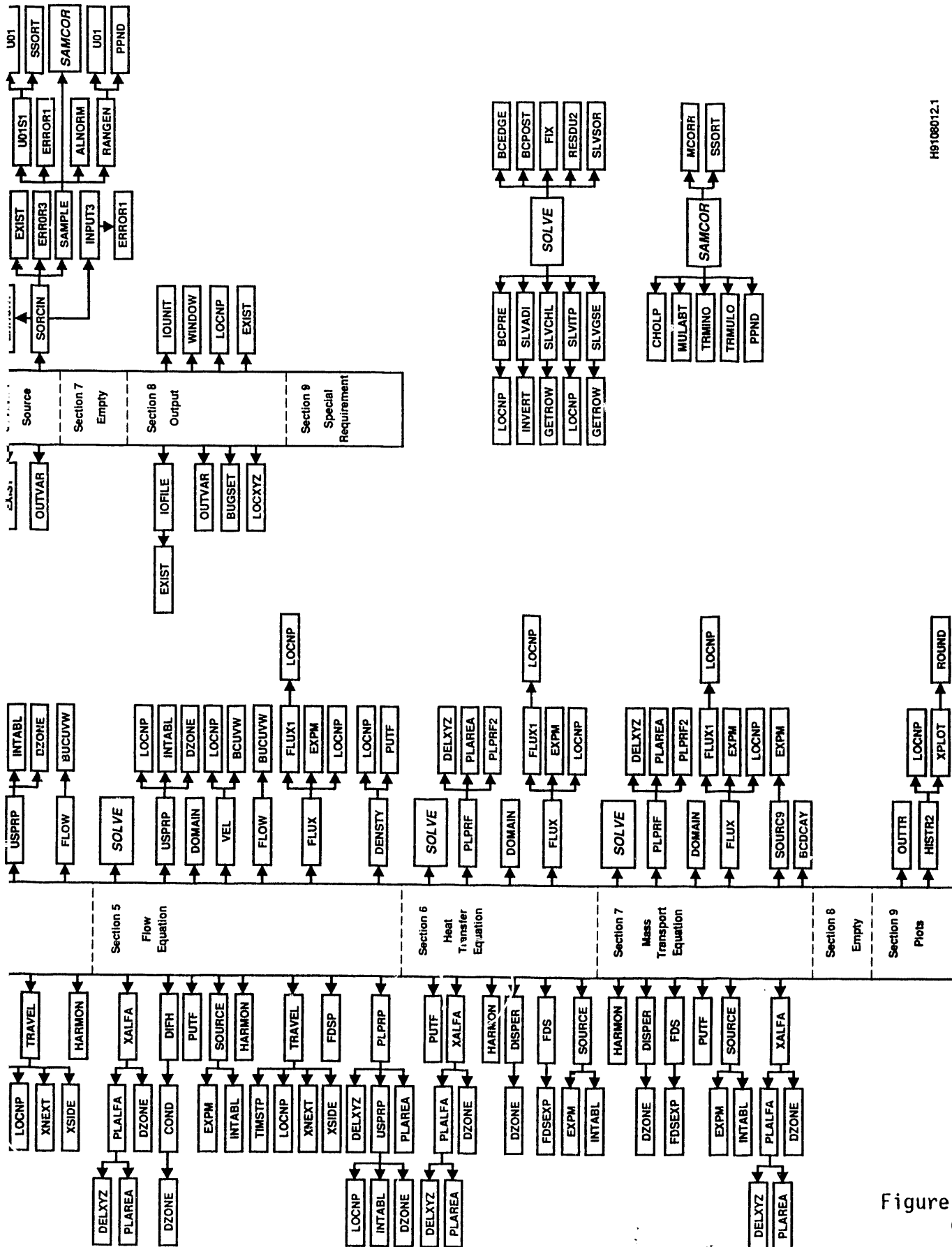
Fluxes of fluid, heat, and chemical species are calculated in FLUX and printed in FLUXP. Tabular outputs are obtained in TABLES, and plot files are written in ARCHIV and ARCHIV2.

The subroutine structure of PORMC is shown in Figure 3-1. The two larger subroutines, AFLOW and INPUT, are shown in segments, each having a distinct function.

3.3 INPUT AND OUTPUT FILE UNITS

To accommodate the large output expected in Monte Carlo runs, PORMC employs many I/O units. The functions of all the I/O units are assigned by default. Table 3-2 lists their names and functions. The user can





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Figure 3-1. Structure of PORMC.

Table 3-2. I/O File Units of PORMC. (sheet 1 of 2)

Unit number	Symbolic name	Default assignment		Function
		File name	Data type	
1	NUNIT1	RESTART	Unformatted	Read data for restart option.
2	NUNIT2	ARCHIVE	Unformatted	Write data file for restart, archive, and postprocessing.
3	NUNIT3	TIMEHIS	Unformatted	Write time-history data.
4	NUNIT4	FLUXBAL	Formatted	Write data on fluxes crossing specified planes and mass and energy balance.
5	IRD	Console	Formatted	Read user input commands. This is unit number 20 on a VAX* computer.
6	IWR	Printer	Formatted	Write output from PORMC. This is unit number 21 on a VAX* computer.
8	NUNIT5	MONTEIN	Unformatted	Write input file for reading in multiple realizations. This file is automatically deleted at the end of run.
31	NUNIT31	STOCH.1	Unformatted	Write data on x-direction velocity, U. This file is automatically opened if output of U is asked for on the WRITE command.
32	NUNIT32	STOCH.2	Unformatted	Write data on y-direction velocity, V. This file is automatically opened if output of V is asked for on the WRITE command.
33	NUNIT33	STOCH.3	Unformatted	Write data on z-direction velocity, W. This file is automatically opened if output of W is asked for on the WRITE command.

Table 3-2. I/O File Units of PORMC. (sheet 2 of 2)

Unit number	Symbolic name	Default assignment		Function
		File name	Data type	
34	NUNIT34	STOCH.4	Unformatted	Write data on pressure, P. This file is automatically opened if output of P is asked for on the WRITE command.
35	NUNIT35	STOCH.5	Unformatted	Write data on temperature, T. This file is automatically opened if output of T is asked for on the WRITE command.
36	NUNIT36	STOCH.6	Unformatted	Write data on concentration, C. This file is automatically opened if output of C is asked for on the WRITE command.
37	NUNIT37	STOCH.7	Unformatted	Write data on relative saturation, TH. This file is automatically opened if output of TH is asked for on the WRITE command.

*VAX is a trademark of the Digital Equipment Corporation.

provide his or her own names to the first six of these units. The opening of the STOCH.x files is triggered by the WRITE command. As many STOCH.x files are opened as there are variables to be output. The names of these files are fixed and the code user cannot change them. In each STOCH.x file, output of a particular variable is written for various realizations. For example, output on pressure is written in STOCH.4. A postprocessor to calculate statistical features (means, variances, correlations, probability distributions, etc.) has been developed (Eslinger and Didier 1991).

No check is made in PORMC to see if an output file already exists in the user's directory. Any time a user executes PORMC, the existing files will be overwritten. This is especially true of the STOCH.x files, because the user cannot provide the file names of his or her choosing. It is recommended that the names of the files be changed if they are to be saved.

Except for units 5 and 6 (VAX¹ units 20 and 21), the code user does not need to open the remaining I/O files. Regarding units 5 and 6, different conventions are followed by various computer systems. For example, on a VAX system, by default, the input and output file names are taken to be FOR020 and FOR021, respectively. These names can, however, be changed. For example, if the VAX user's input and output files are to be named PROB.INP and PROB.OUT, respectively, the following instructions will accomplish this.

```
ASSIGN PROB.INP FOR020
```

```
ASSIGN PROB.OUT FOR021
```

3.4 DIMENSION PARAMETERS

The PORMC code employs FORTRAN PARAMETER statements to change the dimensions of various arrays. These dimension parameters are described in 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 CHOICE OF 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 computer resource limitations (memory and execution time) restrict their use. In practice, considerations of computational cost, accuracy, and stability of numerical solutions; 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.

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Table 3-3. Description of Modifiable Dimension Parameters.
(sheet 1 of 2)

Parameter	Description
LADDF	Storage required for using Cholesky and Gaussian elimination solution methods. For Cholesky method, $LADDF = 1/2 * \text{band width} * LFLD$; for Gaussian method, $LADDF = 1/2 * (LFLD+1) * LFLD$ for pressure equation and twice that for temperature and concentration equations.
LANOD	Maximum number of nodes (in a zone) over which a stochastic property may have spatial autocorrelation.
LAVAR	Maximum number of stochastic variables that can have spatial autocorrelation.
LAZN	Maximum number of zones in which any one of the LAVAR variables can be autocorrelated.
LBC	Maximum number of locations where boundaries are specified. This is equal to $2 * (IMAX * JMAX + JMAX * KMAX + KMAX * IMAX)$ and is calculated by PORMC.
LFLD	Maximum number of internal nodes. This is equal to $(IMAX-2) * (JMAX-2) * (KMAX-2)$, and is calculated by PORMC.
LMAX	Maximum number of nodes in the problem domain. This is equal to $LX * LY * LZ$, and is calculated by PORMC.
LMX	Largest of LX, LY, and LZ.
LREL	Maximum number of Monte Carlo realizations. Must be less than $(2*LANOD)$.
LSO	Maximum number of sets (two values per set) in a time-source table.
LSS	Maximum number of sources for a variable.
LTRA	Maximum number of fluid particles for which travel time can be calculated.
LUD	Maximum number of pairs in an empirical probability table.
LUS	Maximum number of sets (two values per set) in a table of properties of the unsaturated zone.
LVALUE	Maximum number of numerical values that can be interpreted by an input command.
LX	Maximum number of grid coordinates in the x-direction.

Table 3-3. Description of Modifiable Dimension Parameters.
(sheet 2 of 2)

Parameter	Description
LY	Maximum number of grid coordinates in the y-direction.
LZ	Maximum number of grid coordinates in the z-direction.
LZN	Maximum number of zones.

In solving stochastic problems with the Monte Carlo method as is done in PORMC, one makes multiple simulations with values of stochastic variables assigned for each simulation from the ensemble of parameters. The characteristic times discussed in the following sections, therefore, will vary from simulation to simulation. In fact, it is practically impossible to design a perfect grid and choose correct time steps for all realizations of PORMC. As a result, some of the realizations may fail to provide a correct answer, either because the grid and time steps are not appropriate to the particular set of parameters or because the parameter combination itself is not physically realizable. In the current version of PORMC, no check is made of whether the parameter vectors selected through Latin Hypercube sampling are physically realizable. Because of this, the following discussion is provided only as a guide.

3.5.1 Design Of Spatial Grid

The spatial grid in PORMC 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, it is written as $(\Delta r_i, \Delta \theta_j, \Delta z_k)$. The value of the element size depends on the factors described in the following sections.

3.5.1.1 Scale of Heterogeneity. The spatial variation in hydraulic, thermal, and mass-transport properties should be represented adequately by the grid. The material properties are specified at grid nodes (see Section 2.8.2) 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. Position the cell face midway (equidistant) between two nodes.

3.5.1.2 Scale of Resolution. For a variety of reasons, in specific parts of the domain, solutions may be needed at a finer scale than that needed 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.

3.5.1.3 Scale of Geologic Features. Geologic or manmade features such as fractures and clastic dikes, and boreholes, 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.

3.5.1.4 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.

3.5.1.5 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 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.

3.5.1.6 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 3.5.1.1 to 3.5.1.5, may require subsequent adjustment to remain within this limit.

3.5.1.7 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.

3.5.2 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 3.5.1 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 2.9) may be more economical.

3.5.2.1 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

$$\delta t_{pL} = S_s \Delta L^2 / K_L. \quad (3.5-1)$$

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 2.9) 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 10 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.

3.5.2.2 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 3.5.2.1

$$\delta t_D = \Delta L^2 / (2D_L) \quad (3.5-2)$$

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 2.7.4). For reasons analogous to those discussed in Section 3.5.1, 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 10 times δt_D .

3.5.2.3 Time Scale of Convection. The time scale of convection is based on the flow velocity of fluid and is defined as

$$\delta t_c = \Delta L / U_L \quad (3.5-3)$$

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 3.5-3, is often stated in terms of the Courant number, Co , which is defined as,

$$Co = \Delta t / \delta t_c = (U_L \Delta t) / \Delta L. \quad (3.5-4)$$

For the PSOR method to remain stable, Co must not exceed unity. For other methods, Δt must not exceed 10 times δt_c .

3.5.2.4 Other Time Scales. The time scales defined in Sections 3.5.2.1 through 3.5.2.3 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.

3.6 COMMAND STRUCTURE FOR DATA INPUT

The method of providing input data to PORMC is based on the FREEFORM command language developed by Analytic and Computational Research, Inc. (Runchal 1987a). Details of FREEFORM 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 PORMC.

- BOLD** The keywords of PORMC are shown in uppercase characters in bold typeface. The string of keyword characters may be specified by the user in upper- or lowercase. Boldface is used here only for notational purposes; it must not be used as operator input.
- CAPS** Uppercase characters in standard typeface are modifiers of the PORMC 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 lowercase.
- char** Lowercase 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 uppercase.

- | 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 nth numeric value is associated with an input command.

3.6.1 Keyword-Based Input Commands

All input data for PORMC 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 lowercase. A keyword always begins in the first column of an 80-column record. The keywords of PORMC and their functions are summarized in Table 3-4. The keywords are abbreviations of commonly used words. Details are provided in Chapter 4.0.

A simplified logic for interpreting a given keyword-based data input is given in Figure 3-2. 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 3-4. 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 4.0. Separators (identified in Figure 3-2 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 3-1. However, keywords consisting of fewer than four characters cannot be extended in this manner.

Table 3-4. Keywords of PORMC and Their Functions.
(sheet 1 of 3)

Number	Keyword ^a	Input function	Type ^b
1	AUTO correlation	Specify spatial autocorrelation based on a specified covariance function	C
2	BAL Ance	Obtain mass and energy balance	C
3	BOUND ary	Implement user-specified boundary conditions	C
4	CHAR acteristic	Characteristic curves for unsaturated soil	C
5	CONV ergence	Specify convergence criterion for P equation	C
6	CYL indrical	Select cylindrical (axi-symmetric) geometry	F
7	DAT um	Datum for vertical (z) distance	F
8	DEBU g	Specify debug options	C
9	DENS ity	Select options for mass density of fluid	C
10	DIS able	Disable solution of certain equations	C
11	END	End of a problem	F
12	FIX Ed	Fix values of state variables at some nodes	C
13	FLUI d	Physical properties of the principal fluid	C
14	FLUX	Calculate mass and energy fluxes across planes	C
15	FOR	Specify zone designation for property input	C
16	GRID	Number of grid nodes in the x and y directions	F
17	HALF life	Half-life of radioactive decay	F
18	HIST ory	Provide time-history output at selected nodes	F
19	HYDR aulic	Saturated hydraulic properties	C
20	INIT ial	Initial conditions for state variables	F
21	INTE gration	Index for selection of integration profile	C
22	MATR ix	Specify option for matrix inversion	C
23	OUTP ut	Frequency and extent of tabular output	C
24	PAUSE	Cause a temporary pause in processing	C
25	PERI odic	Specify periodic boundary conditions	F
26	PROP erty	Option for mode of property specification	F

Table 3-4. Keywords of PORMC and Their Functions.
(sheet 2 of 3)

Number	Keyword ^a	Input function	Type ^b
27	QUIT	Exit the program	F
28	R	Radial coordinates for cylindrical geometry	F
29	READ	Read initial conditions from archive file	F
30	REFERence	Reference node for diagnostic output	C
31	RELAX	Relaxation factors for governing variables	C
32	ROCK	Material properties of soil or rock	C
33	SAVE	Output to archive file	C
34	SCALE	Internal scaling of specified input	F
35	SCREen	Echo some of the diagnostic output to screen	F
36	SOIL	Material properties of soil or rock	C
37	SOLVE	Start of solution of equations	C
38	SOURce	Specify source, injection, or withdrawal terms	F
39	SUBDomain	Select subdomain option for solution	F
40	THERmal	Thermal properties of soil or rock	C
41	THETA	Tangential coordinate in angular units	C
42	TIME	Set initial time for simulations	C
43	TITLE	Problem title specification	C
44	TRANsport	Transport properties of porous matrix	C
45	TRAVel	Travel time for fluid particles	F
46	UNSAturated	Selection of unsaturated soil functions	C
47	USER	User identification for input and output files	C
48	VISCosity	Select fluid viscosity option	C
49	WINDow	Set subdomain for output purposes	C
50	WRITe	Write plot files from Monte Carlo run	F
51	X	X-direction grid coordinates	F
52	Y	Y-direction grid coordinates	F

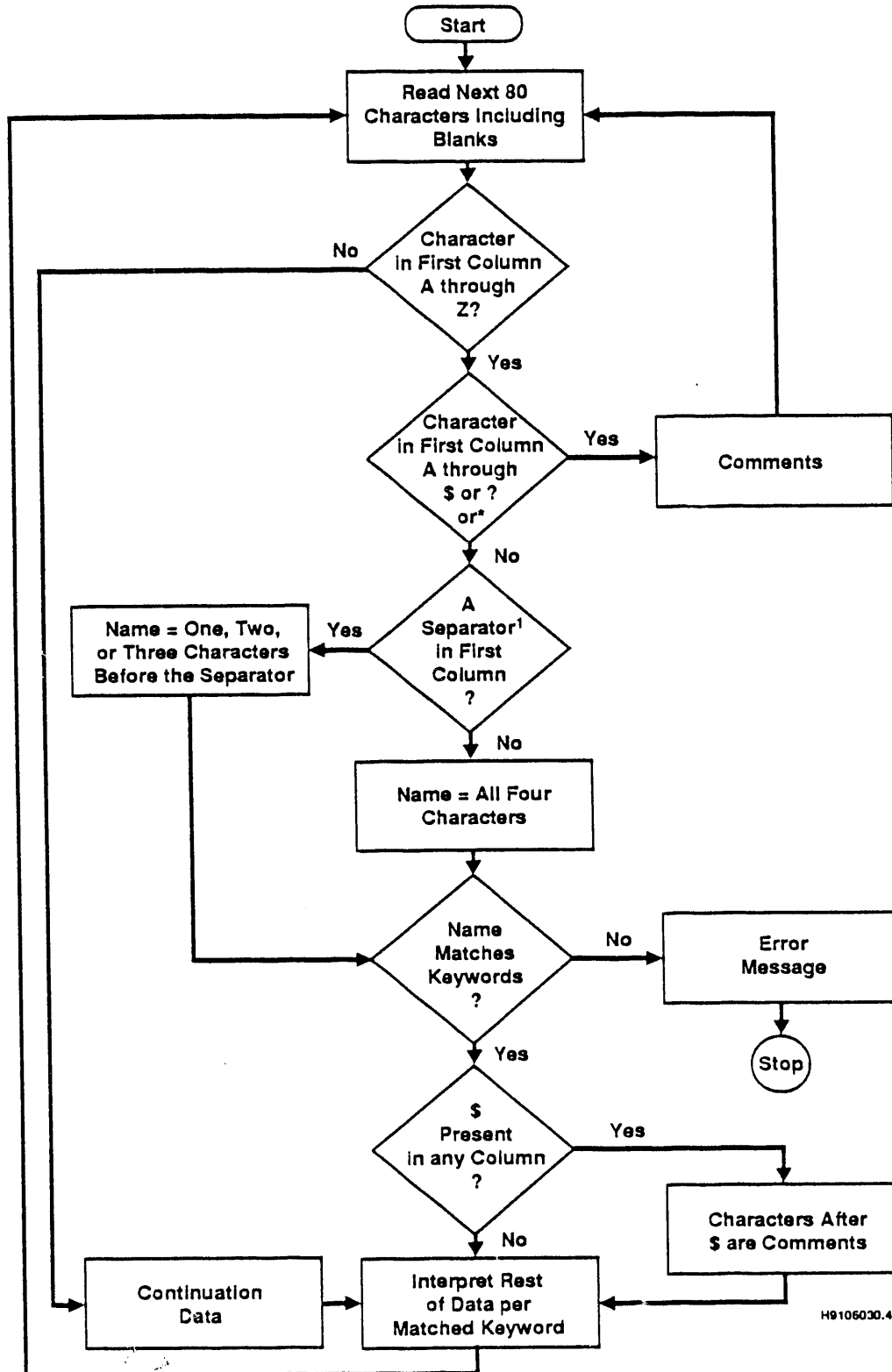
Table 3-4. Keywords of PORMC and Their Functions.
(sheet 3 of 3)

Number	Keyword ^a	Input function	Type ^b
53	Z	Z-direction grid coordinates	F
54	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 are 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 a simulation. This is done by structuring the input data set with multiple SOLVE commands.

Figure 3-2. Interpretation of Keyword-Based Input.



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

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). However, a hyphen (-) must not be used, because this will be interpreted as a negative sign and will be associated with the first numeric value on the command. Thus, X-coordinate will still be an error. Note that the hyphen (-) is not a separator.

The numeric data following a keyword must be entered in a fixed order, but they can be typed in any format; no fixed-column numbers are 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 PORMC.

The PORMC user is warned that the easier the data entry, the easier it is to make mistakes. In Version 1.0 of PORMC, error checks of input data are perfunctory in nature, and therefore the user should carefully debug his/her input data.

3.6.2 Order Of Input Commands

With few exceptions, the input records may be specified in any convenient order (but the numerical values within a record must follow a strict order, which is described in Chapter 4.0). The exceptions are as follows.

- **TITLE**, **USER**, and **GRID** must be the first three commands and in that order. A user may elect to omit the **TITLE** and **USER** command, but the **GRID** command must be provided.
- The **SOLVE** command initiates problem solution and must follow all commands that provide data for that problem.
- 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 **HYDR**aulic 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 before using the **HYDR**aulic property command.

Although the order of input commands is largely arbitrary, a natural order is recommended to facilitate debugging of input data. The recommended order is indicated in Table 3-5.

3.6.3 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 International System of Units 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.

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

Order	Function	Related keyword command
1	Identification	TITLE, USER
2	Grid specification and number of realizations	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	AUTOCORRELATION, 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, TRAVEL, WINDOW, WRITE
10	Operational control	CONVERGENCE, SOLVE, PAUSE, END

3.6.4 Commands For Output

3.6.4.1 General Description of Output Commands. Nine commands generate various types of output in PORMC. These are the BALANCE, DEBUG, FLUX, OUTPUT, REFERENCE, SAVE, TRAVEL, WINDOW, and WRITE commands. The BALANCE command provides output of convective and diffusive fluxes crossing the six boundaries of a specified rectangular tetrahedron within the solution domain. In addition, residual errors of mass and energy balance in the solution of the governing equations are also printed. The FLUX command also leads to the calculation of fluid, heat, or chemical species across user-specified planes. Output from the BALANCE and FLUX commands is printed in a file whose default name is FLUXBAL. The DEBUG command can be used for troubleshooting. It provides a traceback function and initiates diagnostic output from different parts of the code. The DEBUG command can, however, produce enormous amounts of output and should be used with care.

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 **WINDow** command, in conjunction with the **OUTPut** commands, provides output of only a subregion of the master arrays. The **SAVE** and **WRITE** commands provide archive data that can be used to either restart a run or for postprocessing. For deterministic runs, the **SAVE** command should be used, whereas for a stochastic problem, the **WRIT** command should be employed. The **SAVE** command will write in a file whose default name is ARCHIV. The **WRIT** command, on the other hand, writes on multiple files named STOCH.x where x = 1,2,..., 7. The **TRAVel** command will cause particle tracking; the calculated travel times will be written to the main output file (IWR).

3.6.4.2 Commands for Tabular Output of Field Variables. The user may obtain tabular output of up to seven field variables at various stages of the calculations. Table 3-6 lists all the field variables of PORMC, the first seven of which can be obtained in the tabular form. The order in which these variables are written to the output file is the listing order of Table 3-6. 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.

3.6.4.3 Commands for Creating Archive File. Using the **SAVE** and **WRITE** commands, the user may generate archive files consisting of basic problem specifications and the values of up to 22 variables listed in Table 3-6. Note that some of the variables listed in Table 3-6 change during program execution as the solution proceeds from equation to equation. That is, these variables are overwritten during the solution process. These archive files 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 files are self-documenting. They contain 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 these files. The archive information is written to file units NUNIT2 (see Section 3.3) with the **SAVE** command, and to NUNIT31 to NUNIT37 with the **WRIT** command. 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. The user can, however, assign his or her own name to NUNIT2 (see description of **SAVE** command) and change the writing mode to formatted. The **WRITE** command, on the other hand, does not allow user-specification of file names and is written in unformatted mode.

Through the **SAVE** and **WRITE** commands, the user can select the variables to be archived and their frequency of output. 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.

Table 3-6. Field Variables Obtainable in Tabular Format.
(sheet 1 of 2)

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
8	POR	n_D	Diffusive porosity
9	VOL	V	Volume of computational cell
10	RR	R	Thermal buoyancy
11	ALPHA	S_s	Storage term; depends on which equation was solved last
12	FO	--	Value of the state variable at the previous time step; depends on which equation (P, t, or C) was solved last
13	FCX	--	X-direction convective flux related to a variable (P, T, C); depends on which equation was solved last
14	FCY	--	Y-direction convective flux related to a variable (P, T, C); depends on which equation was solved last
15	FCZ	--	Z-direction convective flux related to a variable (P, T, C); depends on which equation was solved last
16	AFX	--	X-face area of computational cell
17	AFY	--	Y-face area of computational cell
18	AFZ	--	Z-face area of computational cell
19	FDX	--	X-direction diffusive flux related to a variable (P, T, C); depends on which equation was solved last

Table 3-6. Field Variables Obtainable in Tabular Format.
(sheet 2 of 2)

Output order	Fortran name	Mathematical symbol	Description
20	FDY	--	Y-direction diffusive flux related to a variable (P, T, C); depends on which equation was solved last
21	FDZ	--	Z-direction diffusive flux related to a variable (P, T, C); depends on which equation was solved last
22	IZ	--	Zone number of the computational cell

3.7 SEQUENTIAL CONTROL OF DATA DURING SIMULATIONS

In the PORMC 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 3-1) 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 3-4 by a letter 'C' in the column headed 'Type'.

For stochastic problems, the solution sequence specified initially is followed in all the realizations. This is done by storing the input file on NUNIT5 (file name MONTEIN) for use in every realization. File MONTEIN is deleted when the **END** command is encountered.

An illustration of the specifications for a two-segment calculation sequence is given in Table 3-7. In this illustration, the output requirements for both the archive file and the tabular output are changed after 50 time steps. In Table 3-7, keywords are shown in boldface type for emphasis only; in actual practice, standard-face type must be used.

An example problem is presented in Appendix B. Details of the structure of each input command of Table 3-1 are given in Chapter 4.0.

3.8 SUMMARY

The PORMC computer code is composed of 118 subroutines. The AFLOW subroutine controls the flow of information between subroutines. Storage is allocated in the main subroutine, PORMC. 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-two field variables are present in PORMC; they use most of the storage.

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.

Table 3-7. 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, realizations = 50
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., eff por = 0.4, total por = 0.5, diff por = 0.5
HYDRAulic properties are STOCHastic
/   prop  dist type  mean   std dev   min    max      comment
   Ss      0      0.1     0       0.1    0.1    / deterministic
   Kx     -1      3        0        0      0      / same as Ky
   Ky      5     -3.4    -2.3    -4.5   -1.0   / lognormal
   Kz      5     -2.1    -1.8    -3.5   -0.5   / lognormal
/   cross correlations
/   Ss      Kx      Ky      Kz
   Ss          0      0      0
   Kx          0      0      0
   Ky          0      0      0
   for zones 1 to 1 in steps of 1
/
/***** Comment: Start of first segment of calculations
SOLVE for 50 years in time step of 1.0 year
/
OUTPut for variables P and T
WRITe 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
WRITe variables U, V, W, P, T and C
/
END

```

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.

All input data, output requirements, and control information are provided to PORMC 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.

4.0 DETAILED DESCRIPTION OF PORMC KEYWORD COMMANDS

The sequence of numeric and other data that follow a keyword is described in this chapter. The notation of Section 3.6 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 is 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, they must be typed in the sequence N_1 , N_2 , N_3 , N_4 , 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.

Two numerical indexes are associated with each of the stochastic quantities in PORMC. The quantities that can be stochastic and their corresponding indexes are shown in Table 4-1. The group index is used to specify cross-correlations among the members of that group. The number index is used to specify autocorrelation and few other parameters; this will become apparent from the command descriptions provided later.

When the code user has decided to treat one or more of the quantities listed in Table 4-1 as stochastic, he or she has to assign probability distributions to them. Nine possible options are available for assigning probability distributions in PORMC. Once a distribution is chosen, appropriate statistics indicated in Table 4-2 must be specified. The numeric indexes for various distributions are also indicated in Table 4-2.

In addition to the marginal PDFs shown in Table 4-2, various types of pair-wise correlations between the stochastic variables also can be specified. The simplest type of correlation structure is one in which all variables are statistically independent; i.e., correlation is zero. The other extreme is when two variables are fully (linearly) correlated. In this case, if the value of one of these variables, A , is known, the value of variable B , which is fully correlated with A , is given by

$$B = a + b A \quad (4.0-1)$$

where a and b are deterministic constants. This type of correlation is allowed between any two variables listed in Table 4-1.

Nonzero cross-correlation is allowed between parameters of the same property group listed in Table 4-1. With four parameters in a group, the cross-correlation matrix for these groups appears as shown in Figure 4-1. Because correlation matrixes are symmetric (also positive definite), only the upper triangular part is shown in Figure 4-1. The six locations marked with x are the correlation coefficients that need to be defined by the user. In the

Table 4-1. Number Indexes for Stochastic Properties.

Property	Property group name	Property group index	Property number index
Specific storage	Hydraulic	1	1
Hydraulic conductivity in x-direction	Hydraulic	1	2
Hydraulic conductivity in y-direction	Hydraulic	1	3
Hydraulic conductivity in z-direction	Hydraulic	1	4
Specific heat	Thermal	2	5
Thermal conductivity in x-direction	Thermal	2	6
Thermal conductivity in y-direction	Thermal	2	7
Thermal conductivity in z-direction	Thermal	2	8
Partition coefficient	Transport	3	9
Molecular diffusion Coefficient	Transport	3	10
Longitudinal Dispersivity	Transport	3	11
Transverse Dispersivity	Transport	3	12
Bulk density	Soil/Rock	4	13
Effective porosity	Soil/Rock	4	14
Total porosity	Soil/Rock	4	15
Diffusive porosity	Soil/Rock	4	16
Air entry pressure or van Genuchten's α	Unsaturated	5	17
van Genuchten's exponent n	Unsaturated	5	18
Gardner's exponent	Unsaturated	5	19
Unsaturated property scaling parameter	Unsaturated	5	20
Fluid source term	Source	6	21
Heat source term	Source	6	22
Species source term	Source	6	23

Table 4-2. Parameters of Specifying Probability Distribution Function of a Variable.

Distribution of P	Transformed variable	Numeric index	Descriptive parameters			
			First	Second	Third	Fourth
Constant	None	0	Value of P	None	None	None
Uniform	None	1	Lower limit of P	Upper limit of P	None	None
Log Uniform (base 10)	$Q = \log_{10}P$	2	Lower limit of Q	Upper limit of Q	None	None
Log Uniform (base e)	$Q = \log_e P$	3	Lower limit of Q	Upper limit of Q	None	None
Normal	None	4	Mean of P	Standard deviation of P	Lower limit of P	Upper limit of P
Log Normal (base 10)	$Q = \log_{10}P$	5	Mean of Q	Standard deviation of Q	Lower limit of P	Upper limit of P
Log Normal (base e)	$Q = \log_e P$	6	Mean of Q	Standard deviation of Q	Lower limit of P	Upper limit of P
Exponential	None	7	1/ Mean of P	None	None	None
Empirical	None	8	None	None	None	None

Figure 4-1. Cross-Correlation Matrix for Properties in a Group.

	P1	P2	P3	P4
P1	1	x	x	x
P2		1	x	x
P3			1	x
P4				1

fifth property group in Table 4-1, the exponent of the Gardner or exponential relation is not expected to be cross-correlated with either the parameters of the van Genuchten or the Brooks and Corey characteristic curves. Therefore, only two parameters can be cross-correlated in this group. Hence, for this group only one cross-correlation coefficient needs to be specified.

Finally, the spatial autocorrelation of a limited number of properties may be specified. A property may be spatially correlated within a zone or layer. No interlayer spatial correlation is allowed. In other words, zones or layers are declared based on the understanding that their properties are statistically independent. Also, all spatial correlations are assumed to be homogeneous, that is the correlation between a property at two points is dependent on the distance between them and not on their absolute position. However, statistical anisotropy is allowed; i.e., the correlation structure may depend on coordinate direction.

If there are N nodes in a zone (or layer) in which a property P is autocorrelated, the storage required for the correlation matrix is $[N \times (N+1) / 2]$. Obviously, depending on the number of nodes over which a property is autocorrelated, these correlation matrixes can become very large, which is the reason for limiting the number of autocorrelated variables.

The spatial correlation is assumed to be represented by a continuous function described by model semivariograms. Four forms common in geostatistics are used in PORMC. These are the linear, exponential, spherical, and Gaussian models.

Detailed description of commands follows. Commands are arranged in alphabetical order.

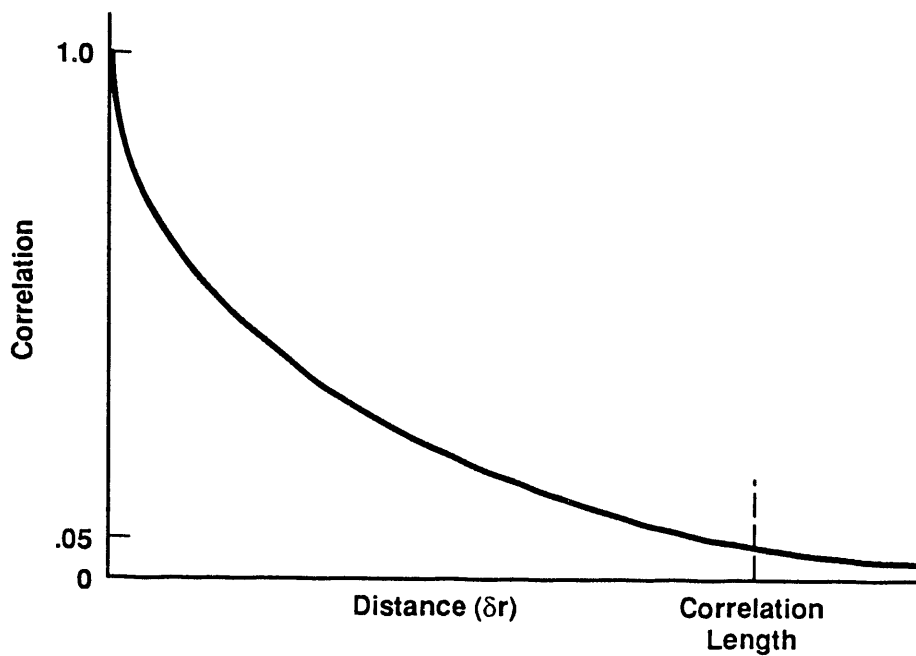
4.1 AUTOCORRELATION SPECIFICATION COMMAND

4.1.1 Purpose

The purpose is to read spatial- (or auto-) covariance (or correlations) data of a stochastic variable. The spatial correlation structure is defined through one of the four commonly accepted functional forms described below. These functional forms use the concept of a correlation length, which is illustrated in Figure 4-2. The spatial correlation is assumed to be homogeneous; i.e., it depends on spatial separation between locations and not on absolute locations. In other words, values of a stochastic quantity at two locations separated by δr have the same covariance irrespective of the actual locations in space. Geometric anisotropy, however, is allowed. This is done by specifying the correlation lengths to be dependent on coordinate directions.

PORMC assumes that second-order stationarity exists (i.e., the mean and variance are constant over the domain of interest). See Section 2.11.1 for more information.

Figure 4-2. Concept of a Correlation Length.



H9106030.1

4.1.2 Syntax

Ten numeric fields are associated with this command as explained below.

AUTO {N1, N2, ..., N10} {LINE | EXPO | SPHE | GAUS}

LINE | EXPO | SPHE | GAUS: One of the four character strings LINEar, EXPONential, SPHERical, or GAUSSian must be provided to indicate the type of covariance function applicable to the spatially correlated variable under specification.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	$\geq 1 \leq 20$	None	The numerical index of the stochastic variable for which covariance is being specified. The numerical indexes for various possible stochastic variables are shown in Table 4-1. The source terms (variable numbers 21, 22, and 23) are not allowed to have covariances.
N2	Any	None	Range [distance (h)] for the linear model (see Figure 2-10). For other models, this value should be 0.
N3	> 0	None	The sample variance of the random variable.
N4	≥ 0	0	The nugget effect for the random variable.
N5	> 0	None	Correlation length in x-direction.
N6	> 0	None	Correlation length in y-direction.
N7	> 0	None	Correlation length in z-direction.
N8	1 to LZN	1	The starting zone number to which this specification applies.
N9	$\geq N8$ $\leq LZN$	1	The last zone number to which this specification applies.
N10	1 to LZN	1	The interval in the zone number designation. The specification will be effective for N8 to N9 at increments of N10, in the manner of a FORTRAN DO loop.

4.1.3 Comments

Because the covariance matrixes can become very large, only a limited number of random variables in a limited number of zones (or layers) can be spatially correlated. Dimension parameters LAVAR and LAZN determine the maximum number of autocorrelated variables allowed and the maximum number of zones in which that variable can be spatially correlated. Dimension parameter

LANOD puts an upper limit on the number of nodes in any one of these zones. The current settings for these dimension parameters are LAVAR = 4, LAZN = 3, LANOD = 100. These dimensions can be changed to suit a particular problem.

The variance specified with this command must agree with the variance (standard deviation) specified when marginal probability distributions are specified with other commands.

4.1.4 Examples

AUTO rv = 2 (KX), range=0, var=2.0, nug=0, corx=20,cory=10,corz=18.5 for zones 1 to 5 in steps of 2 EXPO.

4.2 BALANCE CALCULATION COMMAND

4.2.1 Purpose

The purpose is to check how well material and energy balance is maintained during the course of calculations. The **BALANCE** command causes the calculation of material and/or energy fluxes crossing the six surfaces of a user-specified rectangular region. The change of material and/or energy within the same region is also calculated.

4.2.2 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 {P | T | C}, ['fname'], [FORM | UNFO], [N1, N2, ..., N8]

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

'fname': A character expression that specifies the file name to which the balance information is written. 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. The default name of this file is assumed to be **FLUXBAL**.

FORM or UNFO: The character expression 'FORMatted' or 'UNFOrmatted' defines the nature of the data format in the restart file. If this specification is omitted, the file is assumed to be formatted.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	2 IMAX	2	The starting I-node index for flux computations.
N2	2 JMAX	2	The starting J-node index for flux computations.

Numeric field	Numeric value	Default value	Remarks and explanations
N3	2 KMAX	2	The starting K-node index for flux computations
N4	2 IMAX	IMAX	The ending I-node index for flux computations
N5	2 JMAX	JMAX	The ending J-node index for flux computations
N6	2 KMAX	KMAX	The ending K-node index for flux computations
N7	>0	1	The frequency (in terms of the number of time steps) at which the balance information is printed to the output file; if a BALANCE command exists in the input stream, the balance information is also printed when the OUTPUT NOW command is encountered. See comments below for more information.
N8	>0	1	The frequency (in terms of number of realizations) at which the balance information is printed; for example, N8 = 2 will cause the balance information printed for realization number 2, 4, ... etc.

4.2.3 Comments

Output produced by the use of the **FLUX** command is also written in the same file. If both the **FLUX** and **BALANCE** commands are in the same file, the file name should be specified on only one of these commands.

Because variable time steps are allowed in PORMC (see **SOLVE** command), it may not always be possible to match the frequency of printing (N7 above) with a particular time of interest. Many users find it useful to obtain the balance (and the flux, if **FLUX** command exists) information at the same time as other information on dependent variables. To serve this purpose, balance (and flux) information is automatically written to the user-named or **FLUXBAL** file whenever the user gives the **OUTPUT NOW** command. To get just this output, the user should specify a large value for N7; e.g., N7 = 32000. If N7 is, for example, 10, the balance (and flux, if **FLUX** command exists) information will be written every 10 time steps. In addition, it will also be written at the time **OUTPUT NOW** is encountered.

Balance and flux information is printed in a tabular form as shown in Appendix B. The **ILO**, **IHI**, **JLO**, **JHI**, **KLO**, and **KHI** define the subregion on which the balance calculations are performed. Note that when **ILO** = **IHI**, the subregion collapses into a **YZ** plane. The **XY** and **ZX** planes are similarly identified. The instantaneous diffusive and convective fluxes, the cumulative (in time) diffusive and convective fluxes, and the total (diffusive + convective) fluxes through each plane bounding the subregion are printed. In addition, the instantaneous change in storage and the decay (if balance of a radioactive species is requested) are also printed.

The flux and balance information is produced for every realization.

4.2.4 Examples

BALANCE calculations for T /entire region, every time step
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
BALANCE for P: frequency = 32000 /print only when other output is asked

4.3 BOUNDARY CONDITION COMMAND

4.3.1 Purpose

The purpose is to specify boundary conditions at the external boundaries of the domain of interest. As explained in Section 2.7.5, the user may choose from three types of boundary conditions (Dirichlet, Neumann, and mixed). The general form of the boundary condition is

$$-a\delta F/\delta N = b(F - F_0) + c \quad (4.3-1)$$

where

F = the dependent variable (C, P or T)

N = the coordinate x (or r), y (or θ), or z
(whichever is normal to the boundary)

a, b, c, F_0 = constants.

The boundary conditions are assumed to be deterministic in nature.

4.3.2 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 {P | T | C}, {N1}, [N2, N3, ..., N13]

P | T | C: One of the character strings P, T, or C. 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 4-3 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.
	3		The x-y plane at K=KMAX. The outward normal at boundary is along the positive direction of z.
N2	0	0	Index for type of boundary conditions.
	0		Dirichlet boundary condition ($a = c = 0$, $b = 1$ in Equation 4.3-1) is specified at a boundary node.
	1		Dirichlet boundary condition is specified at the wall of a boundary cell (see Figure 2-2).
	2		Neumann boundary condition ($b = 0$ in Equation 4.3-1) is specified at the wall of the boundary cell.
	3		Mixed boundary condition at the wall of a boundary cell ($c = 0$ in Equation 4.3-1).
	4		Seepage boundary condition at the wall of a boundary cell ($a = 1$, $b = c = 0$ if $F < F_o$; $a = c = 0$, $b = 1$ otherwise). Applicable to pressure equation only.
N3	Any	0	Value of variable (F_o of Equation 4.3-1) for a Dirichlet or seepage boundary, flux (the term c of Equation 4.3-1) for a Neumann boundary, and equilibrium value of a variable (F_o of Equation 4.3-1) 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_o are the same as those for F ; units for flux are those of fluid velocity, heat, and mass for P, T, and C, respectively.

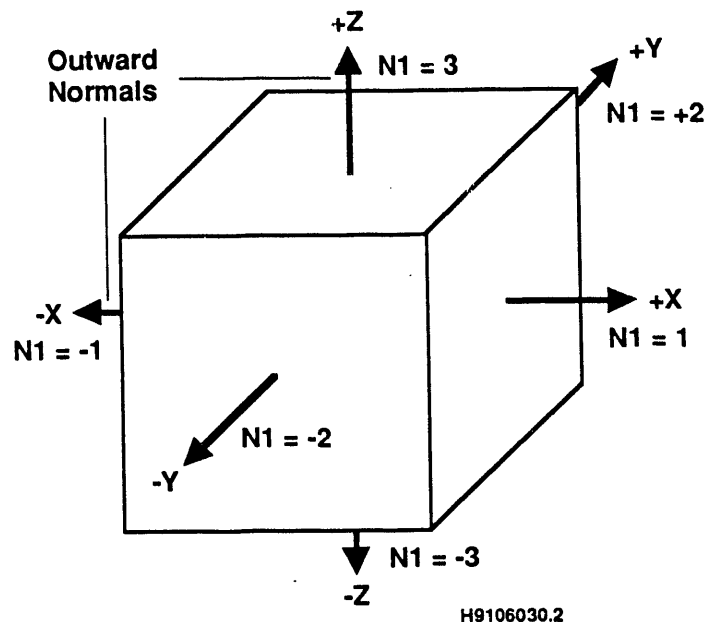
Numeric field	Numeric value	Default value	Remarks and explanations
N4	Any	0	The term 'b' is the heat or mass transfer coefficient of Equation 4.3-1, if N2 = 3; otherwise, this input is ignored. However, a value must be explicitly specified if any of the numeric fields, N5 through N10, are not zero. Units 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) indexes 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) indexes of boundary plane. The numerical values must be such that N8 ≥ N5, N9 ≥ N6, and N10 ≥ 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 Equation 4.3-1) according to the equation: $\text{boundary value} = N3 + N11 \cdot x + N12 \cdot y + N13 \cdot z$ <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>

4.3.3 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 4-3. 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.

This specification applies to time-independent boundary conditions. By using multiple SOLVE commands (see SOLVE command), the user may alter boundary conditions in time.

Figure 4-3. Illustration of Boundary Index Notation.



4.3.4 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 Neumann 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
```

4.4 CHARACTERISTIC CURVES COMMAND

4.4.1 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; however, only the functional form can be stochastic. The following functional relationships are available (for definition of symbols and more discussion, see Section 2.7.3).

- The van Genuchten (1978) Soil-Moisture Retention Relations:

$$\theta^* = [1 + (\alpha \Psi)^n]^{-m}, h < 0 \quad (4.4-1a)$$

$$\theta^* = 1, h \geq 0 \quad (4.4-1b)$$

$$m = (1-a/n) \quad (4.4-1c)$$

The value of a in Equation 4.4-1c depends on whether Mualam's (a = 1) or Burdine's (a = 2) theory is used to estimate the relative conductivity. The respective relative conductivity relations are as follows:

$$k_r = \theta^{*a} [1 - (1 - \theta^{*1/m})^m]^2 \quad (4.4-2a)$$

or

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m] \quad (4.4-2b)$$

- Brooks and Corey (1966) Soil-Moisture Retention Relations:

$$\theta^* = (\Psi/\Psi^*)^{-\beta}, \Psi < -\Psi^* \quad (4.4-3a)$$

$$\theta^* = 1, \Psi \geq -\Psi^* \quad (4.4-3b)$$

and the relations for relative conductivity corresponding to Mualam and Burdine theories are, respectively,

$$k_r = \theta^{*(5/2 + 2/\beta)} \quad (4.4-4a)$$

or

$$k_r = \theta^{3 + 2/\beta}. \quad (4.4-4b)$$

- Gardner's (or Exponential) Relation for k_r :

$$k_r = \exp(-\gamma \Psi) \quad (4.4-5)$$

The van Genuchten moisture-retention relations are used in conjunction with Equation 4.4-5.

- Use of scaling theory:

Scaling factors are defined through the use of similitude theory (Sposito and Jury 1985) that can be used to obtain the characteristic curves at any point in a similar medium as follows:

$$\Psi(\theta) = \Psi^*(\theta^*) / \chi \quad (4.4-6a)$$

$$k_r = \kappa^2 k_r^* \quad (4.4-6b)$$

where θ^* and k_r^* are the scaled-mean hydraulic functions and χ and κ are the scaling factors. In PORMC, κ is assumed to be a linear function of χ , i.e.,

$$\kappa = a + b \chi. \quad (4.4-6c)$$

The scaling factors vary in space. Use of scaling theory may be useful for stochastic simulations.

- Tabular characteristic curves:

The fifth 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. However, the tabular option cannot be used for specifying stochastic properties.

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

4.4.2 Syntax

When all properties are deterministic

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

COND: 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, N1 = number of data sets in the table; and (3) if properties are specified as functions, N1 = α , Equation 4.4-1, if van Genuchten (1978) relations are selected; and N1 = Ψ^* for Brooks and Corey (1966) relations of Equation 4.4-3. The units of α are reciprocal of Ψ and that of Ψ^* must be the same as that of Ψ .
N2	0	See remarks	If FOR command is not used and properties are in a table, 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, 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 Equation 4.4-1 or β of Equation 4.4-3 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. If properties are specified as functions, N3 = exponent of the Gardner or exponential relation.

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 must be specified as zero.
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	0	None	Continuation of tabular values until property specification is complete.

Syntax when one or more of the properties are stochastic

CHAR {N1,N2, ..., N26}, [N27, N28, ..., Nn], [COND], [STOC], [SCAL]

COND: The action of modifier **COND**uctivity has been explained in Section 4.4.

STOC: The second character string associated with this command is **STOC**hastic or blanks. By including **STOC**hastic on this command, the user can specify stochastic properties. As indicated above, the option of reading soil-moisture characteristic curves in the form of a table is not available with the **STOC**hastic modifier. Even when only one of the parameters associated with the **CHAR**acteristic command is stochastic, the modifier **STOC**hastic must be used.

SCAL: The third character string is SCALE or blanks. The presence of SCALE in this command indicates that the characteristic curves will be scaled according to the theory given first by Miller and Miller (1956).

Numeric field	Numeric value	Default value	Remarks and explanations
N1	≤ 8	0	<p>Type of probability distribution for van Genuchten's α (Equation 4.4-1a) or Brooks and Corey's Ψ^* (Equation 4.4-3a). N1 takes on values from less than 0 (e.g., N1 = -1) to 8. Probability distribution types represented by various values of N1 are described in Table 4-2.</p> <p>Assigning a negative value to N1 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N2 (see below) specifies the other variable for which complete probabilistic description must be provided through its appropriate keywords.</p>
N2	> 0	None	<p>For N1 < 0, N2 is the index number of property with which van Genuchten's α or Brooks and Corey's Ψ^* is perfectly correlated. The numeric indexes used for specifying the property with which α or Ψ^* may be fully correlated are described in Table 4-1.</p> <p>If $0 \leq N1 \leq 7$, N2 = the first parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>For N1 = 8, N2 = number of data pairs in the empirical frequency table that will be used to specify the probability distribution.</p> <p>A value for N2, even though not significant, must be provided if any numeric field subsequent to N2 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N3	Any	None	<p>For $N1 < 0$, $N3 =$ coefficient a of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, $N3 =$ the second parameter of the probability distribution specified by $N1$. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>$N3$ is not used if $N1 = 8$.</p> <p>A value for $N3$, even though not used, must be provided if any numeric field subsequent to $N3$ is nonzero.</p>
N4	Any	None	<p>For $N1 < 0$, $N4 =$ coefficient b of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, $N4 =$ the third parameter of the probability distribution specified by $N1$. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the left (lowest) truncation point for the probability distribution. If the distribution is not to be truncated on the left, the user must set $N4 = -999$.</p> <p>$N4$ is not used if $N1 = 8$.</p> <p>A value for $N4$, even though not used, must be provided if any numeric field subsequent to $N4$ is nonzero.</p>
N5	Any	None	<p>$N5$ has no significance when $N1 < 0$ or $N1 = 8$. When $0 \leq N1 \leq 7$, $N5 =$ the fourth parameter of the probability distribution specified by $N1$. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter indicates the right (upper) truncation point of the probability distribution. If the distribution is not to be truncated on the right, the user must set $N5 = -999$.</p> <p>A value for $N5$, even though not significant, must be provided if any numeric field subsequent to $N4$ is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N6	≤ 8	0	Type of probability distribution for van Genuchten's n (Equation 4.4-1a) or Brooks and Corey's β (Equation 4.4-3a). N6 takes on values from less than 0 (e.g., $N6 = -1$) to 8. Probability distribution types represented by various values of N6 are described in Table 4-2. Assigning a negative value to N6 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N7 (see below) specifies the other variable for which complete probabilistic description must be provided through its appropriate keywords.
N7 to N10	Any	None	Information about van Genuchten's n or Brooks and Corey's β in the manner described for N2 to N5.
N11 to N15	Any	None	Statistical data about the exponent γ (Equation 4.4-5) of the Gardner or Exponential relation for relative conductivity. The manner of specification is the same as that for N1 to N5.
N16 to N20	Any	None	Statistical data about the scaling factor (χ of Equation 4.3-6a) in the manner of N1 to N5. This data is ignored in the absence of modifier SCALE. However, some numerical values must be provided if any subsequent value is going to be nonzero.
N21	>-1 $<+1$	0	Correlation coefficient between van Genuchten's α and n or Brooks and Corey's Ψ^* and β . $N21 = \pm 1$ means perfect correlation, which is indicated by assigning a negative value to either N1 or N6.
N22	Any	None	The factor a of Equation 4.4-6c.
N23	Any	None	The factor b of Equation 4.4-6c.
N24 to N26	1 to LZN 1	1	N24 to N26 select the zones to which N1 through N23 apply. Their interpretation is identical to N1, N2, and N3, respectively, of the FOR command. If these values are omitted, the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, the input is assumed to apply to zone number 1. Numerical values must be provided if values subsequent to N23 are nonzero.

Numeric field	Numeric value	Default value	Remarks and explanations
N27	Any	None	First value in the table of empirical distribution. This table has two columns. The first column contains values of the random variable. The second column has the corresponding cumulative relative frequencies. The table is arranged in terms of ascending cumulative relative frequencies; i.e., the smallest cumulative relative frequency is listed first. N27, therefore, is the first value of the random variable.
N28	>0	None	Relative frequency associated with the value N27 above.
N29 to Nn	Any	None	Subsequent values in the empirical distribution above in the manner of N27 and N28 above.

4.4.3 Comments

This command works in conjunction with the **UNSA**turated and **FOR** commands. The saturation fraction, Ψ , 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 **UNSA**turated command). It should be noted that the **UNSA**turated command must precede the **CHAR**acteristic command.

The syntax given in Section 4.4.2 to specify stochastic properties can also be used to specify deterministic properties. This can be done by selecting the probability distribution type 0, which signifies that the particular property is constant or deterministic.

The units of van Genuchten's α are $1/L$, where L is the length unit and those of Ψ^* in the Brooks and Corey equation are L .

As many empirical probability tables can be read as there are random variables. **LUD** is the parameter that is used to dimension the array for storing these empirical tables. It denotes the maximum number of sets (value of the random variable, cumulative relative frequency). Currently, its value is set at 100, meaning that each random variable can have up to 100 sets defining the probability distribution.

The user should also be aware that the parameter **LVALUE** (the maximum number of values following a keyword) may be affected. In addition, if more than one parameter in a group is to be specified in tabular format, the tables must appear sequentially, following all other input for that group.

4.4.4 Examples

/The following two examples are for deterministic properties

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.)

/Examples below are for stochastic properties

CHAR alpha: PDF=4(normal), mean=1.87, std=1.0, low=0, hi=2.5, van n:

PDF=1(uniform), low=0.2, hi=3.2, 0,0, Gardner 0,0,0,0,0 xcor=.6,
0,0,0,0,0 for zones 1 to 6 in steps of 2

CHAR air entry: PDF=0(constant), val=2.0, 0,0,0, beta: PDF=8(empirical),
5,0,0,0, gama=0,0,0,0,0 xcor=0(independent) 0,0,0,0,0 for zone 3 to 3
in steps of 1 PDF table is (.1,.2),(.15,.3),(.6,.4),(.8,.6),(.9,.99)

4.5 CONVERGENCE CRITERIA COMMAND

4.5.1 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 2.10). 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.

4.5.2 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: $R_1 = \sum Ax - b \leq N_2 \quad (4.5-1)$ 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 $R_2 = \max (1 - F_p^{n+1} / F_p^n) \leq N_2 \quad (4.5-2)$ 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 Equation 4.5-1 or Equation 4.5-2.
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, its variations are ignored. This input is ignored if N1 = 1.

4.5.3 Comments

This command is used in two ways. If the steady-state mode of solution is invoked by the SOLVE command, the criteria of this command are used to check convergence of the steady-state. However, if a transient solution is invoked, 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.

4.5.4 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

4.5.5 Status

Convergence option 1 (specified by N1 above) for this command is not currently active in Version 1.0 of PORMC.

4.6 CYLINDRICAL GEOMETRY COMMAND

4.6.1 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.

4.6.2 Syntax

No numerical value is interpreted with this command.

CYLI

4.6.3 Comments

Cartesian geometry is the default. Hence, either a **CYL**indrical 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 nonnegative. This restriction implies that

$$r_i > 0; i = 2, 3, \dots, \text{IMAX}. \quad (4.6-1a)$$

r_1 may be less than zero, but it must satisfy

$$r_1 \geq -r_2. \quad (4.6-1b)$$

Equation 4.6-1b 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 $-r_2$ such that the first element boundary in the r-direction is located at $r = 0$.

4.6.4 Examples

CYLindrical geometry for this problem

4.7 DATUM SPECIFICATION COMMAND

4.7.1 Purpose

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

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

4.7.2 Syntax

DATU {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.

4.7.3 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.

4.7.4 Examples

DATUm zstar = 0.0, maxpsi = 1.E20, minkr = 1.E-20

4.8 DEBUG COMMAND

4.8.1 Purpose

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

4.8.2 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, 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 the following explains.

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

4.8.3 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.

4.8.4 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
```

4.8.5 Status

This command is not fully operational in all installations of PORMC.

4.9 DENSITY FUNCTION COMMAND

4.9.1 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 2.7.1).

4.9.2 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 $\rho = \rho^* [(T_c - T)/(T_c - T^*)]^A. \quad (4.9-1)$
	2		Density changes according to the equation $\rho = A_1 + A_2 T + A_3 T^2 + A_4 T^3. \quad (4.9-2)$
	3		Density changes according to the equation $\rho = \rho^* [1 + A_5(T^* - T) + A_6(C^* - C)]. \quad (4.9-3)$
N2	Any	0	Reference temperature, T^* ; ignored if Equation 4.9-2 is used.
N3	Any	0.2	Coefficient A (Equation 4.9-1) or A_1 (Equation 4.9-2) or A_5 (Equation 4.9-3); the default value is appropriate when fluid is water and Equation 4.9-2 is to be used.
N4	Any	374.15	Coefficient T_c , A_2 , or C^* ; the default value is appropriate when the fluid is water and Equation 4.9-2 is to be used.
N5	Any	0	Coefficient A_3 or A_6 .
N6	Any	0	Coefficient A_4 .
N7	0	0	The effect of $\delta T/\delta t$ is ignored in computing the pressure source term (see Equation 2.1-3).
	1		The effect of $\delta T/\delta t$ is retained.

4.9.3 Comments

The **DENS**ity command provides for a coupling between the pressure and temperature equations. It triggers the consideration of temperature-dependence of hydraulic conductivity, incorporation of thermal buoyancy in the pressure equation, and if opted, the incorporation of the $\delta T/\delta t$ term in the pressure equation.

4.9.4 Examples

```

DENSity type 1 $ Use equation 4.9-1 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

```

4.10 DISABLE EQUATION COMMAND

4.10.1 Purpose

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

4.10.2 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.

4.10.3 Examples

DISAble P equation
DISAble T and C equations

4.11 END OF DATA COMMAND

4.11.1 Purpose

The purpose is to signify the end of a problem.

4.11.2 Syntax

No numeric values are supplied with this command.

END

4.11.3 Comments

This command signifies the end of problem specification. In contrast to PORFLO-3, the deterministic analog of PORMC, multiple problems cannot be specified in the PORMC input file. 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.

4.11.4 Examples

END

4.12 FIXED DEPENDENT VARIABLE COMMAND

4.12.1 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 the **FIXED** 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.

4.12.2 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 N6.

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.

4.12.3 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.

4.12.4 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)

4.13 FLUID PROPERTIES COMMAND

4.13.1 Purpose

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

4.13.2 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.

4.13.3 Comments

These fluid properties are employed only if the default mode of property specification (see **PROPerTy** command) by weighted averages of components (e.g., water and rock) is active. The default values are in kilogram, meter, or second units. In this case, the effective (or equivalent) properties of the soil (or rock) (see Equation 2.1-13) 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.

4.13.4 Examples

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

4.14 FLUX CALCULATION COMMAND

4.14.1 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.

4.14.2 Syntax

The flux plane is specified by the indexes 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. Only the frequency on the first **FLUX** command is effective.

```
FLUX {P | T | C}, {XY | YX | YZ | ZY | ZX | XZ}, ['fname'],
      [FORM | UNFO], [N1, N2, N3, N4, N5, N6, N7, N8]
```

- C or P or T: 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.
- 'fname': A character expression that specifies the file name to which the flux information is written. 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. The default name of this file is assumed to be **FLUXBAL**.
- FORM
or
UNFO: The character expression 'FORMatted' or 'UNFOrmatted' defines the nature of the data in the restart file. If this specification is omitted, the file is assumed to be formatted.

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 the number of time steps) at which the flux information is printed to the output file. If a FLUX command exists in the input stream, the flux information is also printed when the OUTPUT NOW command is encountered. See the following comments for more information.
N8	>0	1	The frequency (in terms of the number of realizations) at which the flux is printed to the output file.

4.14.3 Comments

Output produced by the use of the **BALANCE** command is also written in the same file. If both the **FLUX** and **BALANCE** commands are used, the file name should be specified on only one of these commands.

Because variable time steps are allowed in PORMC (see **SOLVE** command), it may not be always possible to match the frequency of printing (N7 above) with a particular time of interest. Many users find it useful to obtain the flux (and the balance, if **BALANCE** command exists) information at the same time as other information on dependent variables. To serve this purpose, flux (and balance) information is automatically written to the user named or **FLUXBAL** file whenever the user gives the **OUTPUT NOW** command. To get just this output, the user should specify a large value for N7, e.g., N7 = 32000. If N7 is 10, for example, then the flux (and balance, if **BALANCE** command exists) information will be written every 10 time steps. In addition, it will also be written at the time **OUTPUT NOW** is encountered.

Fluxes across up to 20 planes may simultaneously be monitored in Version 1.0 of PORMC. 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, the first value will prevail (also see previous comments).

Flux and balance information is printed in a tabular form as shown previously in Figure 4-2. The instantaneous diffusive and convective fluxes,

the cumulative (in time) diffusive and convective fluxes and the total (diffusive + convective) fluxes through each plane are printed.

The flux and balance information is produced for every realization.

4.14.4 Examples

FLUX of P (fluid) through an XY plane defined by (2,2,2) to (8,9,2), every 5 time steps

FLUX of P through YZ plane (2,2,2) to (2,11,15), write on 'flux.dat' in FORMatted mode every 20 time steps

FLUX of C (species) through ZX plane (2,5,8) to (7,5,19) every 32000 time steps

4.15 FOR MATERIAL TYPE COMMAND

4.15.1 Purpose

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

4.15.2 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.
N2	N1 LZN	1	The highest zone number to which property specification applies. If N2 is not specified, 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, it is taken to be 1.

4.15.3 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, 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 of the properties of that zone.

4.15.4 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

4.16 GRID SPECIFICATION COMMAND

4.16.1 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.

4.16.2 Syntax

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

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

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	3	The number of grid nodes in the z-direction.
N4	>0	1	The number of Monte Carlo realizations desired--a value for N4 must be provided if any value after N4 is nonzero.
N5	>1 <2147483646	2567293	Seed for generating random numbers.
N6	> $-\pi/2$ < $\pi/2$	0	Angle subtended by bedding planes with the x-axis; positive counterclockwise.
N7	> $-\pi/2$ < $\pi/2$	0	Angle subtended by bedding planes with the y-axis; positive counterclockwise.

4.16.3 Comments

The first 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). The fourth numeric field provides the number of Monte Carlo realizations to be obtained. A value of zero for N4 means only one realization is required.

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 indexes. Due care must therefore be taken that, in the input of data, no reference is made to grid node indexes 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.

4.16.4 Examples

GRID use default values and single realization
GRID is 31 by 25 by 12, number of realizations = 50
GRID 10 X 20 X 13, realizations = 5, seed = 25679312
GRID 3 X 3 X 165, realizations = 10, seed = 324567892, xdip=-.15, ydip=0

4.17 HALF-LIFE SPECIFICATION COMMAND

4.17.1 Purpose

The purpose is to specify the half-life of radioactive decay or chemical reaction rate for the species under consideration. R_c of Equation 2.3-4 is computed from the half-life as given in Equation 4.17-1 below.

The actual rate of decay, R_c of Equation 2.3-4, for a species, C, is calculated from the relation:

$$R_c = 0.69314718 / \lambda \quad (4.17-1)$$

where λ is the half-life of radioactive decay or chemical reaction for the species and 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.

4.17.2 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, λ , of radioactive decay or chemical reaction for the species under consideration. The default value ensures that no decay occurs, provided that the simulation time is much smaller than 1 E+20 time units.

4.17.3 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

4.18 HISTORY OUTPUT COMMAND

4.18.1 Purpose

The purpose is to specify and control graphical and tabular output of time history for variables shown in Table 3-6 at specified nodes.

4.18.2 Syntax

HIST [character string], [TABLEs], ['fname'], [FORM | UNFO],
{N1, N2, N3}, [N4, N5,, 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, a character string beginning with "TABL" must be specified somewhere on the command line.

'fname': A character expression that specifies the file name to which the flux information is written. 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. The default name of this file is assumed to be **TIMEHIS**.

FORM
or
UNFO: The character expression 'FORMatted' or 'UNFOrmatted' defines the nature of the data in the TIMEHIS file. If this specification is omitted, the file is assumed to be formatted.

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 indexes of the second 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., time steps. A value of 0 is interpreted to be equal to 1.
Nn+1	>0	1	Realization frequency at which the time history is to be obtained.

4.18.3 Comments

The time-history plot file is generated on unit number NUNIT3. Printer plots of history data are generated at the end of hardcopy output file.

4.18.4 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

4.19 HYDRAULIC PROPERTIES COMMAND

4.19.1 Purpose

The purpose is to specify the hydraulic properties of the host porous matrix, or those of the planar or linear features. This input must be provided if the pressure equation is to be solved.

4.19.2 Syntax

Syntax when all properties are deterministic

LZN is a dimension parameter (maximum number of zones allowed) 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> $S_s = S_s^* (\rho / \rho^*). \quad (4.19-1)$ <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> $K_x = k_r K_x^* (\rho \mu^* / \rho^* \mu) \quad (4.19-2)$ <p>where K_x^* is a reference value of the saturated hydraulic conductivity 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 N2 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 N2 field, as described above.</p>

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

Syntax when one or more of the properties are stochastic

HYDR [STOC], {N1, N2, ..., N26}, [N27,N28,N29], [N30,N31, ..., Nn]

STOC: The character string associated with this command is STOChastic or blanks. By including STOChastic on this command, the user can specify stochastic hydraulic properties. Even when only one of the parameters associated with the HYDRaumatic properties command is stochastic, the modifier STOChastic must be used.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	≤ 8	0	Type of probability distribution for specific storativity S_s of Equation 4.19-1. N1 takes on values from less than 0 (e.g., N1 = -1) to 8. Probability distribution types represented by various values of N1 are described in Table 4-2. Assigning a negative value to N1 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N2 (see below) specifies the other variable for which complete probabilistic description must be provided through its appropriate keywords.

Numeric field	Numeric value	Default value	Remarks and explanations
N2	>0	None	<p>For $N1 < 0$, N2 is the index number of property with which S_s is perfectly correlated. The numeric indexes used for specifying the property with which S_s may be fully correlated are described in Table 4-1.</p> <p>If $0 \leq N1 \leq 7$, N2 = the first parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>For $N1 = 8$, N2 = number of data pairs in the empirical frequency table that will be used to specify the probability distribution.</p> <p>A value for N2, even though not significant, must be provided if any numeric field subsequent to N2 is nonzero.</p>
N3	Any	None	<p>For $N1 < 0$, N3 = coefficient a of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, N3 = the second parameter of the probability distribution indicated by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>N3 is not used if $N1 = 8$.</p> <p>A value for N3, even though not used, must be provided, if any numeric field subsequent to N3 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N4	Any	None	<p>For $N1 < 0$, $N4 =$ coefficient b of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, $N4 =$ the third parameter of the probability distribution specified by $N1$. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the left (lower) truncation point for the probability distribution. If the distribution is not to be truncated on the left, the user must set $N4 = .999$.</p> <p>$N4$ is not used if $N1 = 8$.</p> <p>A value for $N4$, even though not used, must be provided, if any numeric field subsequent to $N4$ is nonzero.</p>
N5	Any	None	<p>$N5$ has no significance when $N1 < 0$ or $N1 = 8$. When $0 \leq N1 \leq 7$, $N5 =$ the fourth parameter of the probability distribution specified by $N1$. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the right (upper) truncation point for the probability distribution. If the distribution is not to be truncated on the right, the user must set $N5 = -999$.</p> <p>A value for $N5$, even though not significant, must be provided if any numeric field subsequent to $N5$ is nonzero.</p>
N6	≤ 8	0	<p>Type of probability distribution for reference value of the saturated hydraulic conductivity, K_x^* of Equation 4.19-2. $N6$ takes on values from less than 0 (e.g., $N6 = -1$) to 8. Probability distribution types represented by various values of $N6$ are described in Table 4-2.</p> <p>Assigning a negative value to $N6$ directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. $N7$ (see below) specifies the other variable for which a complete probabilistic description must be provided through its appropriate keywords.</p>

Numeric field	Numeric value	Default value	Remarks and explanations																									
N7 to N10	Any	None	Information about K_x^* in the manner described for N2 to N5.																									
N11 to N15	Any	None	Statistical data about the reference value of the y-direction saturated hydraulic conductivity, K_y^* . The manner of specification is the same as for N1 to N5 above.																									
N16 to N20	>-1	0	Statistic data about the reference value of the z-direction saturated hydraulic conductivity, K_z^* . The manner of specification is the same as for N1 to N5 above.																									
N21 to N26	Any	None	<p>Cross-correlation between the four variables of this property group (Group No. 1 of Table 4-1). The six values to be read are marked by crosses in the following correlation matrix.</p> <table style="margin-left: auto; margin-right: auto;"> <tr> <td></td> <td>S_s</td> <td>K_x</td> <td>K_y</td> <td>K_z</td> </tr> <tr> <td>S_s</td> <td></td> <td>x</td> <td>x</td> <td>x</td> </tr> <tr> <td>K_x</td> <td></td> <td></td> <td>x</td> <td>x</td> </tr> <tr> <td>K_y</td> <td></td> <td></td> <td></td> <td>x</td> </tr> <tr> <td>K_z</td> <td></td> <td></td> <td></td> <td></td> </tr> </table>		S_s	K_x	K_y	K_z	S_s		x	x	x	K_x			x	x	K_y				x	K_z				
	S_s	K_x	K_y	K_z																								
S_s		x	x	x																								
K_x			x	x																								
K_y				x																								
K_z																												
N27 to N29	1 to LZN	1	<p>N27 to N29 select the zones to which N1 through N4 apply. Their interpretation is identical to N1, N2, and N3, respectively, of the FOR command. If these values are omitted, the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, the input is assumed to apply to zone number 1.</p> <p>Numerical values must be provided if values subsequent to N26 are nonzero.</p>																									
N30	Any	None	First value in the table of empirical distribution. This table has two columns: the first column contains values of the random variable, and the second column has the corresponding cumulative relative frequencies. The table is arranged in terms of ascending cumulative relative frequencies; i.e., the smallest cumulative relative frequency is listed first. N30, therefore, is the first value of the random variable.																									
N31	>0	None	Relative frequency associated with the value N30 above.																									

Numeric field	Numeric value	Default value	Remarks and explanations
N32	Any	None	Subsequent values in the empirical Nn distribution above in the manner of N30 and N31 above.

4.19.3 Comments

As many empirical probability tables can be read as there are random variables. LUD is the parameter that is used to dimension the array for storing these empirical tables. It denotes the maximum number of sets (value of the random variable, cumulative relative frequency). Currently its value is set at 100, which means that each random variable can have up to 100 sets defining the probability distribution.

The user should also be aware that the parameter LVALUE (the maximum number of values following a keyword) may be affected. In addition, if more than one parameter in a group is to be specified in tabular format, the tables must appear sequentially, following all other input for that group.

The syntax given in Section 4.19.2 to specify stochastic properties can also be used to specify deterministic properties. This can be done by selecting the probability distribution type 0, which signifies that the particular property is constant or deterministic.

4.19.4 Examples

The following examples depict the hydraulic property specification when all the hydraulic properties are deterministic.

```
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
```

Following are examples when one or more of the hydraulic properties are stochastic.

```
HYDRaulic properties: STOChastic
/ prop      dist type    mean  std   min   max
  Ss         0           .01   0     0     0 / deterministic
  Kx         5          -.3   .1    -1    -.004 /lognormal
  Ky        -1           2     0     1     0 / perfectly cor with Kx
  Kz        -1           2     0     .1    0 / perfectly cor with Kx
/ cross-correlation / perfect correlation is not to be read in matrix
/ below
/           Ss         Kx         Ky         Kz
  Ss         0           0           0
  Kx         0           0           0
  Ky         0           0           0
```

this specification applies to zone 1 to 10 in steps of 5 / zones 1, 6

HYDRaulic properties: STOChastic

Ss 8 (tabular) 15,0,0,0 Kx 0 (fixed) 1,0,0,0 Ky 0 (fixed) 1,0,0,0
 Kz 0 (fixed) .1,0,0,0, no cross correlation 0,0,0,0,0,0 for zone 1,1,1

/	Ss	prob
	.001	.01
	.008	.02
	.009	.1
	.01	.25
	.02	.38
	.03	.427
	.035	.5
	.04	.6
	.043	.65
	.076	.76
	.077	.80
	.0776	.90
	.078	.95
	.0785	.98
	.079	.9999

4.20 INITIAL CONDITION COMMAND

4.20.1 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

$$F(I,J,K) = F_0 + a \cdot X(I) + b \cdot Y(J) + c \cdot Z(K) \quad (4.20-1)$$

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, 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.

4.20.2 Syntax

A maximum of LVALUE (currently LVALUE = 150) numeric fields can be interpreted by this command. LVALUE is dimension parameter, which would have to be changed if more numerical fields are to be interpreted in a command. The INITIAL command may be repeated as many times as necessary to complete the specification.

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

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 4.20-1 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.

Numeric field	Numeric value	Default value	Remarks and explanations
N4	1 KMAX	1	The starting K-grid node index of the subregion.
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 4.20-1.
		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 4.20-1, if $N8 \leq 1$. 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 4.20-1, if $N8 \leq 1$. If $N8=2$, this factor is taken to be the initial value of the variable at the second node in the subregion (node with indexes 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 4.20-1, if $N8 \leq 1$. If $N8=2$, N11 is the initial value of the variable at the third node in the subregion.
N12	Any	0	The values of the fourth 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			

4.20.3 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, the input is assumed to apply to all of the flow field.

4.20.4 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); mode =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

4.21 INTEGRATION PROFILE COMMAND

4.21.1 Purpose

The purpose is to select a 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 2.8). The default option is the hybrid scheme, which employs the central difference scheme for low grid Peclet numbers and upwinding for high Peclet numbers.

4.21.2 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.

4.21.3 Comments

The default option should be adequate for most applications. However, if the local grid Peclet number (see Section 2.8) significantly exceeds a value of 10, the exponential scheme may be desirable.

4.21.4 Examples

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

4.22 MATRIX SOLUTION METHOD COMMAND

4.22.1 Purpose

The purpose is to select the manner of solution of the matrix of equations. Five options, Alternating Direction Implicit (ADI), Cholesky Decomposition, Gaussian Elimination, Point Successive Over-Relaxation (PSOR), and Reduced System Conjugate-Gradient (RSCG) are available (see Section 2.9).

4.22.2 Syntax

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

direction: 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 indexes. 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, more than one MATRix command should be used.

Option	Meaning
ADI	Matrix is solved by the Alternating Direction Implicit method. <u>This is the default option.</u>
SOR	Matrix is solved by the Point Successive Over-Relaxation Method.
GAUS	Matrix is solved by Gaussian Elimination.
CHOL	Matrix is solved by Cholesky Decomposition.
RSCG	Matrix is solved by the Reduced System Conjugate-Gradient 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.

4.22.3 Examples

MATRix sweeps in X direction only
MATRix sweeps in X and Y directions: F: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-4

4.23 OUTPUT TABLES COMMAND

4.23.1 Purpose

The purpose is to select the field arrays (see Table 3-6) to be written to the output file unit IWR (see Table 3-2), and to specify the manner and frequency of output.

4.23.2 Syntax

OUTP [character strings], [XY | XZ | YZ], [NARRow | WIDE], [NOW],
[N1, N2, N3, ... N25]

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 3-6 for which the output is desired (see Section 3.6 for further information).

XY | XZ | YZ: 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	\geq	See below	The frequency index (time steps) for tabular output. The output is obtained every N1 time steps; for example, a specification of N1=10 will lead to output at the 10th, 20th, 30th, etc., time steps. By default, tabular output is obtained automatically at the end of simulations for all active variables.
N2	≥ 1	1	The frequency index (realizations) for tabular output. The output is obtained every N2 realizations. By default, tabular output is obtained for every successful (i.e., converged) realization.

Numeric field	Numeric value	Default value	Remarks and explanations
N3 to N25	$0 \leq N \leq 23$	0	The index number(s) of the input property(ies) for which summary statistics are to be printed in the output file. By default, summary statistics are printed for all properties that are identified as being stochastic.

4.23.3 Comments

If an **OUTPUT** command is specified without any of the attributes given in the syntax above, the output of field arrays is completely suppressed. If no **OUTPUT** command is specified, 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 PORMC is used. Successive **OUTPUT** commands may be employed to accommodate changing output requirements at various stages of simulation.

OUTPUT NOW also leads to the archiving of fluxes (if **FLUX** command exists) and mass and energy balances (if **BALANCE** command is included). This output, however, is written in a different file than the IWR file (see **FLUX** and **BALANCE** commands).

4.23.4 Examples

OUTPUT: U, V, W in **NARROW** tabular format
OUTPUT: U, V, C, and P in **WIDE** tabular format **NOW**, every 5 realizations
OUTPUT: U, V, C, P, and **THETA** by XZ planes in **WIDE** tabular format **NOW**
OUTPUT: U, V, P and T in **NARROW** format **NOW** and every 20 steps every 2 realizations
OUTPUT tables for V, W, P, and **THETA** by YZ planes every 15 steps
OUTPUT for none of the variables
OUTPUT P, **THETA** **NOW** every 1 step, every 1 realization, summary stats only for properties 3, 17, and 18

4.24 PAUSE COMMAND

4.24.1 Purpose

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

4.24.2 Syntax

This command supports no numeric fields.

PAUS

4.24.3 Comments

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

4.24.4 Examples

PAUSE and await operator action.

4.25 PROPERTY CALCULATION COMMAND

4.25.1 Purpose

This command has a dual purpose. 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 2.2 and 2.3). By default, fluid and matrix properties are provided separately and the effective properties are calculated internally in the code. However, the **PROP**erty command, used in conjunction with the **THER**mal and **TRAN**sport commands, provides an option to directly read 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 **HYDR**aulic, **THER**mal, **TRAN**sport, and **UNSA**turated 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 **PROP**erty command, the user can provide instructions to use harmonic, geometric, or arithmetic mean of the nodal values for the cell interface. Geometric mean is the default mode.

4.25.2 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 **PROP**erty specification applies.

EFFEctive: If the modifier **EFFEctive** is encountered on the **PROP** command, it is assumed that the properties read through the **THER**mal and **TRAN**sport 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 **EFFEctive** is not encountered, the properties read by the **THER**mal and **TRAN**sport 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 upwind (or upstream) of the interface.

4.25.3 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·K)], and the input value of N1 of the TRANsport command is assumed to be the partition coefficient, k_d . However, if the EFFective modifier on this command is encountered, 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/(m³·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.

Because 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 Geometric mean. If this option is acceptable, 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.

4.25.4 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

4.26 QUIT COMMAND

4.26.1 Purpose

The purpose is to indicate the end of instructions and completion of all problems.

4.26.2 Syntax

QUIT

4.26.3 Comments

This command is identical to the **END** command.

4.26.4 Examples

QUIT

4.27 R-COORDINATE COMMAND

4.27.1 Purpose

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

4.27.2 Syntax

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

4.27.3 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, 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

$$N_1 \geq -N_2; \quad N_i > 0 : i = 2, 3, \dots, \text{IMAX}. \quad (4.27-1)$$

For problems in which the first cell (boundary between nodes at I=1 and I=2) is to be the axis of symmetry, N_1 should be equal to $-N_2$, such that the first element boundary in the r-direction is located at $r=0$.

4.27.4 Examples

See X command.

4.28 READ RESTART FILE COMMAND

4.28.1 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.

4.28.2 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, 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, the first set is read from the archive file. A data set in this context consists of several records, as explained in Section 3.6.

4.28.3 Examples

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

4.29 REFERENCE NODE COMMAND

4.29.1 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, W, and TH. In addition, the convergence rate or residuals are also printed.

4.29.2 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.

4.29.3 Comments

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

4.29.4 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

4.30 RELAXATION FACTOR COMMAND

4.30.1 Purpose

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

4.30.2 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		

4.30.3 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, a value less than unity may help obtain a stable solution. Alternatively, if the convergence rate is too slow, a value greater than unity may result in more rapid convergence. A value less than 0 or greater than 2 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 textbooks (Varga 1962).

4.30.4 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

4.31 ROCK PROPERTIES COMMAND

4.31.1 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.

4.31.2 Syntax

Syntax when all the properties are deterministic

LZN is a dimension parameter denoting the maximum number of zones allowed.

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

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>0	1	The density of dry, solid component, ρ_s
N2	0 1	1	The effective (or flow) porosity, n_E . $n_E \leq n_D \leq n_T$
N3	0 1	1	The total porosity, n_T . $n_E \leq n_D \leq n_T$
N4	0 1	1	The connected (or diffusive) porosity, n_D . $n_E \leq n_D \leq n_T$
N5 N7	1 LZN	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, the input is assumed to apply to the zones specified by any previous FOR command. If no FOR command was previously specified, the input is assumed to apply to zone number 1.

Syntax when one or more of the properties are stochastic

ROCK [STOC], {N1, N2, ..., N26}, [N27,N28,N29], [N30,N31, ..., Nn]

STOC: The character string associated with this command is STOChastic or blanks. By including STOChastic on this command, the user can specify stochastic hydraulic properties. Even when only one of the parameters associated with the ROCK properties command is stochastic, the modifier STOChastic must be used.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	≤8	0	<p>Type of probability distribution for rock density ρ_s. N1 takes on values from less than 0 (e.g., N1 = -1) to 8. Probability distribution types represented by various values of N1 are described in Table 4-2.</p> <p>A negative value for N1 is interpreted to mean that ρ_s is perfectly correlated with some other variable. It directs the program to omit sampling of this stochastic variable and obtain its values from the associated correlated variable. N2 (see below) specifies the other variable with which this variable is perfectly correlated.</p>
N2	>0	None	<p>For N1 < 0, N2 is the index number of property with which ρ_s is perfectly correlated. The numeric indexes used for specifying the property with which ρ_s may be fully correlated are described in Table 4-1.</p> <p>If $0 \leq N1 \leq 7$, N2 = the first parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>For N1 = 8, N2 = number of data pairs in the empirical frequency table that will be used to specify the probability distribution.</p> <p>A value for N2, even though not significant, must be provided if any numeric field subsequent to N2 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N3	Any	None	<p>For $N1 < 0$, N3 = coefficient a of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, N3 = the second parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>N3 is not used if $N1 = 8$.</p> <p>A value for N3, even though not used, must be provided if any numeric field subsequent to N3 is nonzero.</p>
N4	Any	None	<p>For $N1 < 0$, N4 = coefficient b of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, N4 = the third parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the left (lower) truncation point for the probability distribution. If the distribution is not to be truncated on the left, the user must set $N4 = -999$.</p> <p>N4 is not used if $N1 = 8$.</p> <p>A value for N4, even though not used, must be provided if any numeric field subsequent to N4 is nonzero.</p>
N5	Any	None	<p>N5 has no significance when $N1 < 0$ or $N1 = 8$. When $0 \leq N1 \leq 7$, N5 = the fourth parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the right (upper) truncation point for the probability distribution. If the distribution is not to be truncated on the right, the user must set $N5 = -999$. A value for N5, even though not significant, must be provided if any numeric field subsequent to N5 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations																									
N6	≤8	0	<p>Type of probability distribution for the effective porosity n_E, N6 takes on values from less than 0 (e.g., N6 = -1) to 8. Probability distribution types represented by various values of N6 are described in Table 4-2.</p> <p>Assigning a negative value to N6 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N7 (see below) specifies the other variable with which this variable is correlated.</p>																									
N7 to N10	Any	None	Information about effective porosity in the manner described for N2 to N5 above.																									
N11 to N15	Any	None	Statistical data about the total porosity, n_T . The manner of specification is the same as for N1 to N5 above.																									
N16 to N20	>-1	0	Statistical data about diffusivity porosity, n_D . The manner of specification is the same as for N1 to N5 above.																									
N21 to N26	Any	None	<p>Cross-correlation between the four variables of this property group (Group 4 of Table 4-1). The six values to be read are marked by crosses in the following correlation matrix.</p> <table style="margin-left: auto; margin-right: auto;"> <tr> <td></td> <td>ρ_s</td> <td>n_E</td> <td>n_T</td> <td>n_D</td> </tr> <tr> <td>n_s</td> <td></td> <td>x</td> <td>x</td> <td>x</td> </tr> <tr> <td>n_E</td> <td></td> <td></td> <td>x</td> <td>x</td> </tr> <tr> <td>n_T</td> <td></td> <td></td> <td></td> <td>x</td> </tr> <tr> <td>n_D</td> <td></td> <td></td> <td></td> <td></td> </tr> </table>		ρ_s	n_E	n_T	n_D	n_s		x	x	x	n_E			x	x	n_T				x	n_D				
	ρ_s	n_E	n_T	n_D																								
n_s		x	x	x																								
n_E			x	x																								
n_T				x																								
n_D																												
N27 to N29	1 to LZN	1	<p>N27 to N29 select the zones to which N1 through N4 apply. Their interpretation is identical to N1, N2, and N3, respectively, of the FOR command. If these values are omitted, the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, the input is assumed to apply to zone number 1.</p> <p>Numerical values must be provided if values subsequent to N29 are nonzero.</p>																									

Numeric field	Numeric value	Default value	Remarks and explanations
N30	Any	None	First value in the table of empirical distribution. This table has two columns: the first column contains values of the random variable, and the second column has the corresponding cumulative relative frequencies. The table is arranged in terms of ascending cumulative relative frequencies; i.e., the smallest cumulative relative frequency is listed first. N30, therefore, is the first value of the random variable.
N31	>0	None	Relative frequency associated with the value N30 above.
N32 to Nn	Any	None	Subsequent values in the empirical distribution above in the manner of N30 and N31 above.

4.31.3 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, the porosity input is used only for computing the dispersion coefficient; the density input is ignored.

When porosities are deterministic, these should be specified such that $n_E \leq n_D \leq n_T$. For stochastic porosities, all samples may not satisfy this relationship unless proper correlation is specified. For such samples strict equality is enforced. For example, if in a sample $n_E > n_D$, then n_E is set equal to n_D . For unsaturated flow problems, $n_D - n_E$ is taken as the residual moisture. n_D and n_E may be specified as perfectly correlated if the value of the residual moisture is deterministic as indicated in one of the following examples.

As many empirical probability tables can be read as there are random variables. LUD is the parameter that is used to dimension the array for storing these empirical tables. It denotes the maximum number of sets (value of the random variable, cumulative relative frequency). Currently, its value is set at 100, meaning that each random variable can have up to 100 sets defining the probability distribution.

The user should also be aware that the parameter LVALUE (the maximum number of values following a keyword) may be affected. In addition, if more than one parameter in a group is to be specified in tabular format, the tables must appear sequentially, following all other input for that group.

The syntax given in Section 4.31.2 to specify stochastic properties can also be used to specify deterministic properties. This can be done by selecting the probability distribution type 0, which signifies that the particular property is constant or deterministic.

4.31.4 Examples

The following are examples for specifying deterministic rock properties.

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

The following are examples when one or more of the rock properties are stochastic.

```
ROCK properties: STOChastic
/ prop      dist type    mean    std    min    max
  rho       0           .01     0     0     0 / deterministic
  eff por   4           .3      .1    .15   .45 /normal
  tot por   -1          15     0     1     0 / = dif por
  dif por   -1          14     .05   1     0 / res moist=.05
/ cross-correlation / perfect correlation is not to be read in matrix
/ below
/          rho          nE          nT          nD
  rho      0            0            0            0
  nE       0            0            0            0
  nD       0            0            0            0
  this specification applies to zone 1 to 10 in steps of 5 / zones 1, 6
```

```
ROCK properties: STOChastic
rho 8 (tabular) 8,0,0,0 nE -1 (cor to nD) 16,0,0,0
nT -1 (cor to nD) 16,0,0,0 nD 8 (tabular)
5,0,0,0, no cross correlation 0,0,0,0,0 for zone
1,1,1
```

```
/          rho          prob
  2000      .01
  2050      .02
  2090      .1
  2110      .25
  2200      .38
  2250      .427
  2300      .8
  2400      .99
/          nD          prob
  .1         .05
  .13        .15
  .19        .2
  .25        .5
  .27        .7
```

4.32 SAVE OUTPUT COMMAND

4.32.1 Purpose

The purpose is to write the output to restart, plot, and archive files. This command should be used only when either a deterministic problem is being solved or only one realization of a stochastic problem is desired. For stochastic problems, the corresponding command is **WRITE**.

4.32.2 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 3-6 for which the output is desired (see Section 3.6 for additional information) to be written in the files.
- '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).
- fmt: The character expression '**FORMatted**' or '**UNFORMatted**' 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.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1	See below	The time-step frequency index for output. 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.

4.32.3 Comments

If the **SAVE** command is specified without any attributes, writing of the field arrays to the archive file is completely suppressed. If no **SAVE** command is specified, 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.

This command should not be used for stochastic problems where multiple realizations are to be saved. For such problems, the command **WRITE** should be used instead.

4.32.4 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
```

4.33 SCALE INPUT COMMAND

4.33.1 Purpose

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

$$Q_{in} = a \cdot Q + b \quad (4.33-1)$$

where

Q_{in} = the internal representation of a variable

Q = the value specified by the user

a, b = user-specified constants.

4.33.2 Syntax

SCAL [N1, N2]

Numeric field	Numeric value	Default value	Remarks and explanations
N1	Any	1	The multiplier, a, of Equation 4.33-1. It is automatically set to 1 at the end of each application.
N2	Any	0	Addend, b, of Equation 4.33-1. It is automatically set to 0 at the end of each application.

4.33.3 Comments

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

4.33.4 Examples

SCALE multiply by 3.3 and add 10

SCALE multiply by 0.3048

4.34 SCREEN WRITE COMMAND

4.34.1 Purpose

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

4.34.2 Syntax

SCRE

4.34.3 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.

4.34.4 Examples

SCREen echo for diagnostic output

4.35 SOIL PROPERTIES COMMAND

4.35.1 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. This command is identical to the **ROCK** command.

4.35.2 Syntax

The syntax depends on whether the properties are deterministic or stochastic. See the **ROCK** command.

4.35.3 Comments

This command is identical to the **ROCK** command.

4.35.4 Examples

See the **ROCK** command.

4.36 SOLVE EQUATIONS COMMAND

4.36.1 Purpose

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

4.36.2 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, 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, the 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 the case of a 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, 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 3.5) 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 SOLV 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.

Numeric field	Numeric value	Default value	Remarks and explanations
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.

4.36.3 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 3-7.

4.36.4 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

4.37 SOURCE SPECIFICATION COMMAND

4.37.1 Purpose

The purpose is to specify location, type, and magnitude of the sources (or sinks) for fluid, heat, or chemical species. Either deterministic or stochastic sources can be specified.

4.37.2 Syntax

SOUR {P | T | C}, [EXPO], [VOLU], [SOLU], [STOC], {N1, N2}, [N3, ..., Nn]

P | T | C: One of the character strings P, T, C. It denotes a corresponding variable in Table 3-6 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, the source is assumed to be specified as an exponential decay function made up of one or more components according to the equation:

$$S_f = \sum_{n=1}^N s_n \exp(-f_n t), \quad (4.37-1)$$

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, 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, 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.

STOC:

The default is a deterministic source. If the character string STOChastic is present in this command, the source is interpreted as stochastic. Stochastic source cannot be specified as a (time, source strength) table. A time-dependent stochastic source can be developed by using multiple SOLVE commands.

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; i.e., it must have previously appeared on a ZONE command. The cumulative number of zones for all SCURce commands must not exceed the specified value of the LSZ dimension parameter (see Section 3.4).
N2	0	0	In the absence of STOChastic modifier, N2 = number of sets (either time - release rate sets if a table is being specified or $s_n - f_n$ sets of Equation 4.37-1) of values that will follow. The cumulative number of sets for all SOURce commands must not exceed the specified value of the LSO dimension parameter (see Section 3.4). in the presence of a STOChastic modifier, N2 = number of sets in the probability distribution function table if $N6 < 0$; otherwise, this value is ignored. However, a value for N2 must be provided if any of the subsequent values are nonzero.
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 4.37-1, if the EXPO modifier is present.

Numeric field	Numeric value	Default value	Remarks and explanations
N4	Any	0	<p>In the absence of SOLU, N4 = the strength of source [or the first parameter (Table 4-2) of the probability distribution specified by N6, if STOC is present] or s_n of Equation 4.37-1.</p> <p>When SOLU is present (applicable to source for C only), N4 = inventory of the source. The inventory is assumed to be deterministic even when the source is stochastic. The strength may be scaled according to Equation 4.33-1 by the SCALE command.</p>
N5	Any	0	<p>The saturation limit (or solubility) of the species, if SOLU is present. If STOC is also present, N5 = first parameter (Table 4-2) of the probability distribution of solubility. The type of distribution is specified by N6.</p> <p>In the absence of STOC and SOLU, N5 = next value (similar to N3) in the source table.</p>
N6	Any	None	<p>In the absence of STOC and SOLU, N6 = next value (similar to N4) in the source table.</p> <p>In the presence of STOC, N6 = type of probability distribution for source strength or solubility (if SOLU is also present). N6 takes on values from less than 1 to 8. Probability distribution types represented by various values of N1 are described in Table 4-2.</p>
N7	Any	None	<p>In the absence of STOC and SOLU, N7 = next value (similar to N3) in the source table.</p> <p>In the presence of STOC, N7 = the second parameter of the probability distribution specified by N6. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p>
N8	Any	None	<p>When STOC is present, N8 = the third parameter of the probability distribution specified by N6. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>In the absence of STOC, N8 = next value (similar to N4) in the source table.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N9	Any	None	When STOC is present, N9 = the fourth parameter of the probability distribution specified by N6. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. In the absence of STOC, N9 = next value (similar to N3) in the source table.
N10	Any	None	If STOC is present, N10 = first value in the table of empirical distribution. This table has two columns. The first column contains values of the random variable. The second column has the corresponding cumulative relative frequencies. The table is arranged in terms of ascending cumulative relative frequencies; i.e., the smallest cumulative relative frequency is listed first. N10 is the first value of the random variable. In the absence of STOC, N10 = next value (similar to N4) in the source table.
N11	Any	None	If STOC is present, N11 = relative frequency corresponding to N10 above. In the absence of STOC, it is the next value in the source table.
N12 to Nn	Any	None	Subsequent values in the empirical distribution table or deterministic source-term table in the manner of N10 and N11 above.

4.37.3 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.

4.37.4 Examples

The following are examples of deterministic source specification.

SOURCE for P: zone 1; # sets = 1: time=0., value=100 cubic ft/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

The following are examples when sources are stochastic.

SOUR for P in zone 1 is STOChastic

sets = 1, start time = 0, mean value = 100, solu = 0, dist = 4
(normal), std = 10, lower limit = 50, upper limit = 120

SOURce of C in zone 5 is SOLUbility limited and STOChastic

pdf sets = 10, start time = 2, inventory = 50, mean solubility = 1.5
dist = 8 (tabular), std = 0, lower limit = 0, upper limit = 0,
pdf table is:

/	solubility	cum prob
	.5	.15
	.6	.2
	.8	.25
	1.0	.28
	1.3	.35
	1.5	.5
	2.0	.6
	2.5	.8
	4.5	.9
	7.5	1.0

4.38 SUBDOMAIN COMMAND

4.38.1 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.

4.38.2 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 the 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.

4.38.3 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.

4.38.4 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.

4.39 THERMAL PROPERTIES COMMAND

4.39.1 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. Thermal properties may be deterministic or stochastic.

4.39.2 Syntax

Syntax when all the properties are deterministic

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 2.2) of material. By default, N1 is taken to be specific heat of solids, c_s ; however, if the PROPER ty command is present, 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 2.2) of material. By default, N2 is taken to be the thermal conductivity of the solids, k_s ; however, if the PROPER ty command is present, 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, the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, the input is assumed to apply to zone number 1.

Syntax when one or more of the properties are stochastic

THER [STOC], {N1, N2, ..., N26}, [N27,N28,N29], [N30,N31, ..., Nn]

STOC: The character string associated with this command is STOChastic or blanks. By including STOChastic on this command, the user can specify stochastic hydraulic properties. Even when only one of the parameters associated with the THERmal Properties command is stochastic, the modifier STOChastic must be used.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	≤8	0	<p>Type of probability distribution for specific heat. N1 takes on values from less than 0 (e.g., N1 = -1) to 8. Probability distribution types represented by various values of N1 are described in Table 4-2.</p> <p>Assigning a negative value to N1 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N2 (see below) specifies the other variable for which complete probabilistic description must be provided through its appropriate keywords.</p>
N2	>0	None	<p>For N1 <0, N2 is the index number of property with which specific heat is perfectly correlated. The numeric indexes used for specifying the property with which it may be fully correlated are described in Table 4-1.</p> <p>If $0 \leq N1 \leq 7$, N2 = the first parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>For N1 = 8, N2 = number of data pairs in the empirical frequency table that will be used to specify the probability distribution.</p> <p>A value for N2, even though not significant, must be provided if any numeric field subsequent to N2 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N3	Any	None	<p>For $N1 < 0$, N3 = coefficient a of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, N3 = the second parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>N3 is not used if $N1 = 8$.</p> <p>A value for N3, even though not used, must be provided if any numeric field subsequent to N3 is nonzero.</p>
N4	Any	None	<p>For $N1 < 0$, N4 = coefficient b of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, N4 = the third parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the left (lower) truncation point for the probability distribution. If the distribution is not to be truncated on the left, the user must set $N4 = -999$.</p> <p>N4 is not used if $N1 = 8$.</p> <p>A value of N4, even though not used, must be provided if any numeric field subsequent to N4 is nonzero.</p>
N5	Any	None	<p>N5 has no significance when $N1 < 0$ or $N1 = 8$. When $0 \leq N1 \leq 7$, N5 = the fourth parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the right (upper) truncation point for the probability distribution. If the distribution is not to be truncated on the right, the user must set $N5 = -999$.</p> <p>A value for N5, even though not significant, must be provided if any numeric field subsequent to N5 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations																									
N6	≤8	0	Type of probability distribution for the x-direction thermal conductivity. N6 takes on values from less than 0 (e.g., N6 = -1) to 8. Probability distribution types represented by various values of N6 are described in Table 4-2. Assigning a negative value to N6 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N7 (see below) specifies the other variable for which complete probabilistic description must be provided through its appropriate keywords.																									
N7 to N10	Any	None	Information about x-direction thermal conductivity in the manner described for N2 to N5.																									
N11 to N15	Any	None	Statistical data about the y-direction thermal conductivity. The manner of specification is the same as for N1 to N5 above.																									
N16 to N20	>-1	0	Statistical data about the z-direction thermal conductivity. The manner of specification is the same as for N1 to N5 above.																									
N21 to N26	Any	None	Cross-correlation between the four variables of this property group (group No. 2 of Table 4-1). The six values to be read are marked by crosses in the following correlation matrix. <div style="text-align: center;"> <table> <tr> <td></td> <td>C_e</td> <td>K_{Tx}</td> <td>K_{Ty}</td> <td>K_{Tz}</td> </tr> <tr> <td>C_e</td> <td></td> <td>x</td> <td>x</td> <td>x</td> </tr> <tr> <td>K_{Tx}</td> <td></td> <td></td> <td>x</td> <td>x</td> </tr> <tr> <td>K_{Ty}</td> <td></td> <td></td> <td></td> <td>x</td> </tr> <tr> <td>K_{Tz}</td> <td></td> <td></td> <td></td> <td></td> </tr> </table> </div>		C_e	K_{Tx}	K_{Ty}	K_{Tz}	C_e		x	x	x	K_{Tx}			x	x	K_{Ty}				x	K_{Tz}				
	C_e	K_{Tx}	K_{Ty}	K_{Tz}																								
C_e		x	x	x																								
K_{Tx}			x	x																								
K_{Ty}				x																								
K_{Tz}																												
N27 to N29	1 to LZN	1	N27 to N29 select the zones to which N1 through N4 apply. Their interpretation is identical to N1, N2, and N3, respectively, of the FOR command. If these values are omitted, the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, the input is assumed to apply to zone number 1. Numerical values must be provided if values subsequent to N29 are nonzero.																									

Numeric field	Numeric value	Default value	Remarks and explanations
N30	Any	None	First value in the table of empirical distribution. This table has two columns: the first column contains values of the random variable; the second column has the corresponding cumulative relative frequencies. The table is arranged in terms of ascending cumulative relative frequencies; i.e., the smallest cumulative relative frequency is listed first. N30, therefore, is the first value of the random variable.
N31	>0	None	Relative frequency associated with the value N30 above.
N32 to Nn	Any	None	Subsequent values in the empirical distribution above in the manner of N30 and N31 above.

4.39.3 Comments

As many empirical probability tables can be read as there are random variables. LUD is the parameter that is used to dimension the array for storing these empirical tables. It denotes the maximum number of sets (value of the random variable, cumulative relative frequency). Currently, its value is set at 100, which means that each random variable can have up to 100 sets defining the probability distribution.

The user should also be aware that the parameter LVALUE (the maximum number of values following a keyword) may be affected. In addition, if more than one parameter in a group is to be specified in tabular format, the tables must appear sequentially, following all other input for that group.

The syntax given in Section 4.39.2 to specify stochastic properties can also be used to specify deterministic properties. This can be done by selecting the probability distribution type 0, which signifies that the particular property is constant or deterministic.

For stochastic simulations, the longitudinal and transverse dispersivities (α_L , α_T) are set to zero in the code.

4.39.4 Examples

The following examples depict the thermal property specification when all the thermal properties are deterministic.

```

THERmal specific heat = 1, conductivity = 45. dispersivity: 3, 1.5
THERmal properties cp=26, kt=45 alphas=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

```

The following examples depict when one or more of the thermal properties are stochastic.

THERmal properties are **STOChastic**

```

/ prop      dist type    mean    std    min    max
  Ce         0         .01     0      0      0 / deterministic
  KTx        5        -.3     .1     -1    -.004 /lognormal
  KTy        -1         2      0      1      0 / perfectly cor with KTx
  KTz        -1         2      0      .1     0 / perfectly cor with KTx
/ cross-correlation / perfect correlation is not to be read in matrix
/ below
/          Ce          KTx          KTy          KTz
          Ce          0            0            0
          KTx          0            0            0
          KTy          0            0            0
          KTz          0            0            0

```

this specification applies to zone 1 to 10 in steps of 5 / zones 1, 6

THERmal properties are **STOChastic**

```

sp heat Ce has tabular (type 8) dist, 6 sets in pdf table 0, 0, 0
thermal cond KTx is fixed (type 0) val = 1, 0, 0, 0
thermal cond KTy is also fixed (type 0) val = .5, 0, 0, 0
thermal cond KTz is also fixed (type 0) val = .1, 0, 0, 0
no cross correlation 0, 0, 0, 0, 0, 0 for zone 1,1,1
/ pdf table for sp heat is
/      Sp          prob
      .001         .01
      .008         .02
      .009         .1
      .01          .25
      .02          .38
      .03          .427

```

4.40 THETA COORDINATE COMMAND

4.40.1 Purpose

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

4.40.2 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, the input values are taken to be in degrees.

4.40.3 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.)

4.40.4 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

4.41 TIME COMMAND

4.41.1 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.

4.41.2 Syntax

TIME {N1}

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

4.41.3 Examples

TIME = 50 years at start of simulations

4.42 TITLE SPECIFICATION COMMAND

4.42.1 Purpose

The purpose is to specify the problem title.

4.42.2 Syntax

TITL followed by character information.

4.42.3 Comments

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

4.42.4 Examples

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

4.43 TRANSPORT PROPERTIES COMMAND

4.43.1 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.

4.43.2 Syntax

Syntax when all the transport properties are deterministic

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 PROP erty command is present, 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 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, the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, the input is assumed to apply to zone number 1.

Syntax when one or more of the properties are stochastic

TRAN [STOC], {N1, N2, ..., N26}, [N27,N28,N29], [N30,N31, ..., Nn]

STOC: The character string associated with this command is STOChastic or blanks. By including STOChastic on this command, the user can specify stochastic hydraulic properties. Even when only one of the parameters associated with the TRANsport properties command is stochastic, the modifier STOChastic must be used.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	≤8	0	<p>Type of probability distribution for partition coefficient. N1 takes on values from less than 0 (e.g., N1 = -1) to 8. Probability distribution types represented by various values of N1 are described in Table 4-2.</p> <p>Assigning a negative value to N1 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N2 (see below) specifies the other variable for which complete probabilistic description must be provided through its appropriate keywords.</p>
N2	>0	None	<p>For N1 < 0, N2 = the index number of property with which partition coefficient is perfectly correlated. The numeric indexes used for specifying the property with which it may be fully correlated are described in Table 4-1.</p> <p>If $0 \leq N1 \leq 7$, N2 = the first parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>For N1 = 8, N2 = the number of data pairs in the empirical frequency table that will be used to specify the probability distribution.</p> <p>A value for N2, even though not significant, must be provided if any numeric field subsequent to N2 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations
N3	Any	None	<p>For $N1 < 0$, N3 = coefficient a of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, N3 = the second parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2.</p> <p>N3 is not used if $N1 = 8$.</p> <p>A value for N3, even though not used, must be provided if any numeric field subsequent to N3 is nonzero.</p>
N4	Any	None	<p>For $N1 < 0$, N4 = coefficient b of Equation 4.0-1, which describes the perfect linear correlation between two variables.</p> <p>When $0 \leq N1 \leq 7$, N4 = the third parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the left (lower) truncation point for the probability distribution. If the distribution is not to be truncated on the left, the user must set $N4 = -999$.</p> <p>N4 is not used if $N1 = 8$.</p> <p>A value for N4, even though not used, must be provided if any numeric field subsequent to N4 is nonzero.</p>
N5	Any	None	<p>N5 has no significance when $N1 < 0$ or $N1 = 8$. When $0 \leq N1 \leq 7$, N5 = the fourth parameter of the probability distribution specified by N1. The nature of this parameter depends on the type of probability distribution and is described in Table 4-2. When specified, this parameter provides the right (upper) truncation point for the probability distribution. If the distribution is not to be truncated on the right, the user must set $N5 = -999$.</p> <p>A value for N5, even though not significant, must be provided if any numeric field subsequent to N5 is nonzero.</p>

Numeric field	Numeric value	Default value	Remarks and explanations																									
N6	≤ 8	0	<p>Type of probability distribution for the molecular diffusion coefficient. N6 takes on values from less than 0 (e.g., N6 = -1) to 8. Probability distribution types represented by various values of N6 are described in Table 4-2.</p> <p>Assigning a negative value to N6 directs the program to omit sampling of this stochastic variable because it is perfectly correlated with another variable. N7 (see below) specifies the other variable for which complete probabilistic description must be provided through its appropriate keywords.</p>																									
N7 to N10	Any	None	Information about molecular diffusion coefficient in the manner described for N2 to N5.																									
N11 to N15	Any	None	Statistical data about the longitudinal dispersivity. The manner of specification is the same as for N1 to N5 above.																									
N16 to N20	Any	0	Statistical data about the transverse dispersivity. The manner of specification is the same as for N1 to N5 above.																									
N21 to N26	Any	None	<p>Cross-correlation between the four variables of this property group (Group 3 of Table 4-1). The six values to be read are marked by crosses in the following correlation matrix.</p> <table style="margin-left: auto; margin-right: auto;"> <tr> <td></td> <td>k_d</td> <td>α_M</td> <td>α_l</td> <td>α_t</td> </tr> <tr> <td>k_d</td> <td></td> <td>x</td> <td>x</td> <td>x</td> </tr> <tr> <td>α_M</td> <td></td> <td></td> <td>x</td> <td>x</td> </tr> <tr> <td>α_l</td> <td></td> <td></td> <td></td> <td>x</td> </tr> <tr> <td>α_t</td> <td></td> <td></td> <td></td> <td></td> </tr> </table>		k_d	α_M	α_l	α_t	k_d		x	x	x	α_M			x	x	α_l				x	α_t				
	k_d	α_M	α_l	α_t																								
k_d		x	x	x																								
α_M			x	x																								
α_l				x																								
α_t																												

Numeric field	Numeric value	Default value	Remarks and explanations
N27 to N29	1 to LZN	1	N27 to N29 select the zones to which N1 through N4 apply. Their interpretation is identical to N1, N2, and N3, respectively, of the FOR command. If these values are omitted, the input is assumed to apply to the zones specified by any previous FOR command; if no FOR command was previously specified, the input is assumed to apply to zone number 1. Numerical values must be provided if values subsequent to N29 are nonzero.
N30	Any	None	First value in the table of empirical distribution. This table has two columns: the first column contains values of the random variable; the second column has the corresponding cumulative relative frequencies. The table is arranged in terms of ascending relative frequencies; i.e., the smallest cumulative relative frequency is listed first. N30, therefore, is the first value of the random variable.
N31	>0	None	Relative frequency associated with the value N30 above.
N32 to Nn	Any	None	Subsequent values in the empirical distribution above in the manner of N30 and N31 above.

4.43.3 Comments

As many empirical probability tables can be read as there are random variables. LUD is the parameter that is used to dimension the array for storing these empirical tables. It denotes the maximum number of sets (value of the random variable, cumulative relative frequency). Currently its value is set at 100, which means that each random variable can have up to 100 sets defining the probability distribution.

The user should also be aware that the parameter LVALUE (the maximum number of values following a keyword) may be affected. In addition, if more than one parameter in a group is to be specified in tabular format, the tables must appear sequentially, following all other input for that group.

The syntax given in Section 4.43.2 to specify stochastic properties can also be used to specify deterministic properties. This can be done by selecting the probability distribution type 0, which signifies that the particular property is constant or deterministic.

4.43.4 Examples

The following examples depict the transport property specification when all the thermal properties are deterministic.

TRANsport properties: kd=1, Dm=5.24, alpha L=10, alpha T=1
 TRAN: Kd=0, dm=1 E-03, L=10, T=1, for ZONE 1
 TRANsport Kd=1.1 E-03, dm=0., L=10, T=1, for zones 1 to 5
 TRANsport Rd=21, dm=0., L=10, T=1, for ZONE 1 to 5 in step 2

The following examples depict when one or more of the transport properties are stochastic.

TRANsport properties are STOChastic

```

/ prop      dist type      mean      std      min      max
  Kd         0         .01         0         0         0 / deterministic
  D          5        -.3          .1        -1        -.004 /lognormal
  disl       4         2          1         .5         3 / normal
  disy      -1        12         0         .1         0 / perf cor with disl
/ cross-correlation / perfect correlation is not to be read in matrix
/ below
/          Kd          D          disl          dist
      Kd          0          0          0
      D           0          0          0
      disl        0          0          0
  
```

this specification applies to zone 1 to 1 in steps of 1.

TRANsport properties are STOChastic

```

part coeff has normal (type 4) dist, mean=2, std=1, min=0, max=3
mol diff coef is det (type 0) val = .0001, 0, 0, 0
long disp has empirical dist (type 8), sets =10, 0, 0, 0
tran disp is perfectly corr (-1) with long disp (var 15), a=0, b=1, 0
cross correlation 0, 0, 0, 0, 0, 0 for zone 1,1,1
/ pdf table for long disp is
/
  
```

```

      disl      prob
      1         .01
      3         .02
      4         .1
      5         .25
      7         .38
      8         .427
     10         .8
     13         .85
     15         .93
     20         1.0
  
```

4.44 TRAVEL TIME COMMAND

4.44.1 Purpose

The purpose is to provide input for calculation of travel time of fluid particles in the velocity field obtained by solving the pressure equation. The starting locations of particles and their termination characteristics can be specified by this command. Currently a maximum of 10 particles can be tracked. As many TRAVel commands are needed as there are particles to be tracked.

4.44.2 Syntax

TRAV [XY | YX | YZ | ZY | ZX | XZ], [SATU], {N1, N2, N3, N4, N5}

XY | YX: Travel time is to be calculated from starting location to an XY plane located at a Z-distance given by N4 (see below).

YZ | ZY: Travel time is to be calculated from starting location to a YZ plane located at an X-distance given by N4 (see below).

ZX | XZ: Travel time is to be calculated from starting location to a ZX plane located at a Y-distance given by N4 (see below).

SATU: Travel time is to be calculated until the particle enters a saturated zone.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	>X ₁	None	X coordinate of particle starting location.
N2	>Y ₁	None	Y coordinate of particle starting location.
N3	>Z ₁	None	Z coordinate of particle starting location.
N4	>0	None	The location of XY, YZ, or ZX particle stopping plane, if one of these character strings is present. If none of the character strings denoting a plane is present, N4 = distance for which travel time is to be calculated. N4 is ignored if SATU is present on this command; however, some numerical value must be provided for N4 if N5 is nonzero.

Numeric field	Numeric value	Default value	Remarks and explanations
N5	≥ 0	0	The time at which the particle travel is to begin; only applicable to transient problems.

4.44.3 Comments

Often travel time to a particular boundary, such as a river, is of interest. Because such a boundary will usually be represented by a plane in the model, specification of a particle-stopping location as a XY, YZ, or ZX plane facilitates this calculation. In this case, the actual distance traveled by the particle to reach the stopping plane is not specified. In the case in which no stopping plane is specified, the travel time is calculated until the actual distance traveled by the particle is equal to the specified value. The stopping location is a priori unknown in this case.

In a transient problem, if $N5 > 0$, the particle travel calculation starts in a time step when $t \geq N5$. Diagnostic messages are printed if a particle stops before reaching the specified end location.

4.44.4 Examples

TRAVel time from (10,20.5,-30.1) to an XY plane at $z = -60$
 TRAVel time from (30.5,43.2,10) to SATU (water table); start time = 1 yr
 TRAVel time (40.3, 132.7, -3.5), travel distance = 50 m, start time = 0

4.45 UNSATURATED PROPERTIES COMMAND

4.45.1 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 2.7.3).

4.45.2 Syntax

UNSA [TABU], [HEAD], [VAN | BROO | EXPO], [BURD | MUAL],
[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, the conductivity characteristic is taken to be specified as tabulated values of Ψ relative to k_r .

VAN and MUAL: The unsaturated properties are calculated according to van Genuchten - Mualem formulae. These formulae are as follows:

$$\theta^* = [1 + (\alpha \Psi)^n]^{-m}, \quad h < 0 \quad (4.45-1a)$$

$$\theta^* = 1, \quad h \geq 0 \quad (4.45-1b)$$

$$m = (1 - 1/n) \quad (4.45-1c)$$

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m]^2. \quad (4.45-1d)$$

VAN and BURD: The unsaturated properties are calculated according to van Genuchten - Burdine formulae. For relative saturation, these formulae are as follows:

$$\theta^* = [1 + (\alpha \Psi)^n]^{-m}, h < 0 \quad (4.45-2a)$$

$$\theta^* = 1, h \geq 0 \quad (4.45-2b)$$

$$m = (1 - 2/n) \quad (4.45-2c)$$

$$k_r = \theta^{*2} [1 - (1 - \theta^{*1/m})^m]. \quad (4.45-2d)$$

BROO and MUAL: The unsaturated properties are calculated according to the Brooks and Corey - Mualam relations. These formulae are as follows:

$$\theta^* = (\Psi/\Psi^*)^{-\beta}, \Psi < -\Psi^* \quad (4.45-3a)$$

$$\theta^* = 1, \Psi \geq -\Psi^* \quad (4.45-3b)$$

$$k_r = \theta^{*(5/2 + 2/\beta)}. \quad (4.45-3c)$$

BROO and BURD: The unsaturated properties are calculated according to the Brooks and Corey - Burdine relations. These formulae are as follows:

$$\theta^* = (\Psi/\Psi^*)^{-\beta}, \Psi < -\Psi^* \quad (4.45-4a)$$

$$\theta^* = 1, \Psi \geq -\Psi^* \quad (4.45-4b)$$

$$k_r = \theta^{*(3+2/\beta)}. \quad (4.45-4c)$$

EXPO: The relative saturation is calculated according to van Genuchten - Mualem formulae, but the relative permeability is calculated according to the exponential (Gardner's) relation. These formulae are as follows:

$$\theta^* = [1 + (\alpha \Psi)^n]^{-m}, h < 0 \quad (4.45-5a)$$

$$\theta^* = 1, h \geq 0 \quad (4.45-5b)$$

$$m = (1 - 1/n) \quad (4.45-5c)$$

$$k_r = \exp(-\gamma\Psi). \quad (4.45-5d)$$

Numeric field	Numeric value	Default value	Remarks and explanations
N1 to 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, N1 to N3 need not be specified.

4.45.3 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.

4.45.4 Examples

UNSAaturated properties in TABUlated form for zone 2 to 6 in steps of 2

UNSAaturated prop: TABUlated form; HEAD versus relative K specification

UNSAaturated prop: VAN genuchten with BURDine theory

UNSAaturated BROOKs and Corey with MUALEm theory

4.46 USER IDENTIFICATION COMMAND

4.46.1 Purpose

The purpose is to specify user identification for purposes of archiving.

4.46.2 Syntax

USER followed by character information

4.46.3 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.

4.46.4 Examples

USER John Doe
USER 5C380

4.47 VISCOSITY FUNCTIONS COMMAND

4.47.1 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 HYDRauiC command).

4.47.2 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 $\mu = B_1 \exp[B_2/(T+\alpha)]. \quad (4.47-1)$
	2		Viscosity changes according to the equation $\mu = B_3 + B_4T + B_5T^2 + B_6T^3. \quad (4.47-2)$
	3		Viscosity changes according to the equation $\mu = \mu^* \exp[B_7(T^*-T) - B_8(T^*-T)^2]. \quad (4.47-3)$
N2	Any	0	The reference temperature, T^* , at which the reference viscosity is μ^* (Equation 4.47-3).
N3	Any	See remarks	The coefficient B_2 of Equation 4.47-1, B_3 of Equation 4.47-2, or B_7 of Equation 4.47-3. Default value is 1436 if N1=1; otherwise, it is zero.
N4	Any	See remarks	The coefficient α of Equation 4.47-1, B_4 of Equation 4.47-2, or B_8 of Equation 4.47-3. Default value is 273.15 if N1=1; otherwise, it is zero.
N5	Any	0	The coefficient B_5 of Equation 4.47-2; this input is ignored for all other choices of N1.
N6	Any	0	The coefficient B_6 of Equation 4.47-2; this input is ignored for all other choices of N1.

4.47.3 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

4.48 WINDOW OUTPUT COMMAND

4.48.1 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) indexes.

4.48.2 Syntax

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

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1 I MAX	1	The starting I-node index of the subdomain.
N2	1 J MAX	1	The starting J-node index of the subdomain.
N3	1 K MAX	1	The starting K-node index of the subdomain.
N4	N1 I MAX	I MAX	The ending I-node index of the subdomain.
N5	N2 J MAX	J MAX	The ending J-node index of the subdomain.
N6	N3 K MAX	K MAX	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.

4.48.3 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.

4.48.4 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

4.49 WRITE STOCHASTIC PLOT FILES COMMAND

4.49.1 Purpose

The purpose is to write in appropriate files the output for the purpose of restart, plot, and archive. Depending on the number of realizations, the output of stochastic problems can be very large. The **WRITE** command opens a separate file for each output variable and writes to it.

4.49.2 Syntax

WRIT [character strings], [FORM | UNFO], [NOW], [N1, N2]

character string: One or more of the strings of characters U, V, W, P, T, and THET. Each character string represents a corresponding variable in Table 3-6 for which the output is desired (see Section 3.6 for additional information) to be written in the files. The output is written in files named STOCH.x where x is a numeral that depends on the character string. x = 1, 2, 3, 4, 5, 6, and 7 for U, V, W, P, T, C, and THETA, respectively.

FORM | UNFO: The character expression 'FORMatted' or 'UNFOrmatted' defines the format of the data on the archive file. By default, the file is assumed to be unformatted.

NOW: The archive output is produced immediately.

Numeric field	Numeric value	Default value	Remarks and explanations
N1	1	See below	The time-step frequency index for output. 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.
N2	>0	1	The realization frequency index for output. The output is written every N2 realizations. Thus, if N2 = 5, output will be written for the 5th, 10, 15th, etc., realizations.

4.49.3 Comments

If the **WRIT** command is specified without any attributes, writing of the field arrays to the archive file is completely suppressed. If no **WRIT** command is specified, 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.

As many output files are created as there are number of variables to be written.

4.49.4 Examples

```
WRITE U, N, W on file 'DEMO.PLT' in FORMatted mode
WRITE U, N, P, THETA, and C every 100 time steps and every 2 realizations
WRITE W, P, and C NOW
WRITE U, T, and C NOW and every 20 steps
WRITE none of the variables
```

4.50 X-COORDINATE COMMAND

4.50.1 Purpose

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

4.50.2 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.
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.

4.50.3 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

4.51 Y-COORDINATE COMMAND

4.51.1 Purpose

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

4.51.2 Syntax

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

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

4.51.3 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.

4.51.4 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

4.52 Z-COORDINATE COMMAND

4.52.1 Purpose

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

4.52.2 Syntax

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

4.52.3 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.

4.52.4 Examples

See the X command.

4.53 ZONE SPECIFICATION COMMAND

4.53.1 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 and fixed values of variables.

4.53.2 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	1LZN	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	1KMAX	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.
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.

4.53.3 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

$$\text{Area} = (\pi/4) \cdot (D^2 - d^2). \quad (4.53-1)$$

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

4.53.4 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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APPENDIX A

DESCRIPTION OF FREE-FORMAT COMMAND LANGUAGE

The user interface with PORMC is through the FREEFORM command language developed by Analytic & Computational Research, Inc. (Runchal 1987). 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 American National Standard 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 following sections.

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 is 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 lowercase.
- 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+, and A&B. are all valid examples of a keyword. The keyword specifications of ABCD, abcd, ABCDEFGH, AbCd123, and ABCDxxxxxxxxxxxx (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, and .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 uppercase (E). 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.) maybe represented as (3*30. or 3*3.0E+1); embedded separators or nonnumeric 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, and 1*1.23E02 are all equivalent.

The strings 1ABC, 11X11, 1+2, 11., and 1+1.E1 are all invalid numeric specifications. In the first three, nonnumeric 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 sign (=), the colon (:), the semicolon (;), the apostrophe ('), the left parenthesis '(', and the right parenthesis ')'. '.

Examples:

The sequence of characters, ';;:)', =====, '=', and (;) are all valid separator fields. However, the characters (a) or (l) 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 'l' 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 REFERENCE

Runchal, A. K., 1987, "Theory and Application of the PORFLOW Model for Analysis of Coupled Fluid Flow, Heat and Radionuclide Transport in Porous Media," in *Coupled Processes Associated with Nuclear Waste Repositories*, Academic Press, New York, New York, pp. 495-516.

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APPENDIX B

ILLUSTRATIVE PROBLEM

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APPENDIX B

ILLUSTRATIVE PROBLEM

1.0 PROBLEM INPUT

Data for the following problem is drawn from a field experiment conducted in a shallow trench at Las Cruces, New Mexico. This problem is set up as a one-dimensional infiltration problem with saturated hydraulic conductivity, van Genuchten parameters, and porosity as random variables. This problem, with 50 realizations, took approximately 4.5 h of central processing unit time on the Hanford Cray¹ X-MP/EA232 computer.

This problem could also be set up as a two- or three-dimensional problem. However, Monte Carlo simulation of multidimensional problems require considerably more central processing unit time. Even though the data for the following problem is drawn from a field experiment, it is not presented here as a verification of the PORMC model. Such verification will require a more careful formulation of the problem.

The set of input instructions is given below.

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TITLE: ONE-D TRANSIENT PROBLEM - LAS CRUCES FIELD EXPERIMENT
/-----
/ REF: DATA FROM NMSU 06/89 DATA PREPARED BY SIGNE WURSTNER
/-----
USER: BSAGAR
GRID: 3 by 3 by 162 realizations = 50, seed=85631
X coordinates: type 3 (uniform), min=0, max=1, ratio=1
Y coordinates: type 3 (uniform), min=0, max=1, ratio=1
Z coordinates: type 3 (uniform), min=-8.025, max=0.025, ratio=1
/-----
D.TUM: 0., maximum tension: 1.E30, minimum relative k: 10e-20
/-----
ZONE 1 from (1,1,1) TO (3,3,162)
/-----
FOR zone 1
HYDRaulic saturated properties are STOCHastic:
/ storativity equal to eff porosity
storativity: -1 perfect corr with por 14 0 1 0
Kx          : -1 perfect corr with Kz 4 0 1 0
Ky          : -1 perfect corr with Kz 4 0 1 0
Kz          : 8 (tabular pdf, see table below) 35 sets -999 -999 -999
corr        : 0 0 0 0 0 0
zone 1 to zone 1 in steps of 1
/ Program: CDFTLB Version:1.0 User: Signe Wurstner Run ID: 9002270850.1
/ Cumulative Probability Table for Kz
1.40000E-02 0.00000
9.95000E-02 0.01000
1.11000E-01 0.01500
1.39000E-01 0.02000
1.48375E-01 0.02500
1.77250E-01 0.03000
1.95000E-01 0.04000
2.27500E-01 0.05000

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¹Cray is a trademark of Cray Research Inc., Minneapolis, Minnesota.

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3.14875E-01 0.07500
3.74000E-01 0.10000
4.90750E-01 0.15000
6.20000E-01 0.20000
8.35750E-01 0.25000
1.06850E+00 0.30000
1.57375E+00 0.35000
2.11700E+00 0.40000
2.76200E+00 0.45000
3.68350E+00 0.50000
4.51075E+00 0.55000
5.33100E+00 0.60000
6.04250E+00 0.65000
7.04200E+00 0.70000
7.77200E+00 0.75000
8.79800E+00 0.80000
9.70150E+00 0.85000
1.09460E+01 0.90000
1.21231E+01 0.92500
1.35650E+01 0.95000
1.42220E+01 0.96000
1.53335E+01 0.97000
1.70963E+01 0.97500
1.81425E+01 0.98000
2.17477E+01 0.98500
2.58765E+01 0.99000
6.73060E+01 1.00000
/
SOIL properties are STOCHastic:
/variable distribution value
rho: 0 (constant) 1.66 0 0 0
/ eff por = wcs - wcr
/set diffusive and total porosity equal to effective porosity
eff por: 8(tabular) 35 sets (see below for table) -999 -999 -999
tot por: -1 14 0 1 0
diff por: -1 14 0 1 0
corr : 0 0 0 0 0 0
for zone 1 to 1 in steps of 1
/ Program: CDFTLB Version:1.0 User: Signe Wurstner Run ID: 900221154233
/ Cumulative Probability Table for effective porosity
/
value prob
1.2000E-01 0.0000
1.4064E-01 0.0100
1.4400E-01 0.0150
1.4628E-01 0.0200
1.5090E-01 0.0250
1.6200E-01 0.0300
1.6656E-01 0.0400
1.7120E-01 0.0500
1.8130E-01 0.0750
1.8600E-01 0.1000
1.9260E-01 0.1500
2.0360E-01 0.2000
2.0900E-01 0.2500
2.1500E-01 0.3000
2.1900E-01 0.3500
2.2260E-01 0.4000
2.2700E-01 0.4500
2.3200E-01 0.5000
2.3600E-01 0.5500
2.4040E-01 0.6000
2.4600E-01 0.6500
2.5200E-01 0.7000
2.5800E-01 0.7500
2.6400E-01 0.8000
2.7100E-01 0.8500
2.7800E-01 0.9000
2.8600E-01 0.9250
2.9180E-01 0.9500
2.9544E-01 0.9600
3.0108E-01 0.9700
3.0290E-01 0.9750
3.0572E-01 0.9800
3.1308E-01 0.9850
3.1800E-01 0.9900
4.5200E-01 1.0000

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/
UNSATURATED conductivity VAN with MUAL
CHARacteristics are STOChastic
alpha      8  35 sets  -999 -999 -999
n          8  35 sets  -999 -999 -999
lamda     0  0        0  0  0 (not required)
ualfa     0  0        0  0  0
corr      0
ualfaA    0  0
for zone 1 to zone 1 in steps of 1
/
/ Program: CDFTLB  Version:1.0  User: Signe Wurstner  Run ID: 900221154233
/ Cumulative Probability Table for alpha
/
      value      prob
6.1000E-01      0.0000
1.0564E+00      0.0100
1.1722E+00      0.0150
1.2256E+00      0.0200
1.2860E+00      0.0250
1.3600E+00      0.0300
1.5368E+00      0.0400
1.6420E+00      0.0500
1.8400E+00      0.0750
2.0380E+00      0.1000
2.3880E+00      0.1500
2.6580E+00      0.2000
2.9700E+00      0.2500
3.2100E+00      0.3000
3.4400E+00      0.3500
3.6860E+00      0.4000
3.9500E+00      0.4500
4.0900E+00      0.5000
4.4200E+00      0.5500
4.6800E+00      0.6000
4.9480E+00      0.6500
5.3680E+00      0.7000
5.8000E+00      0.7500
6.4660E+00      0.8000
7.2260E+00      0.8500
8.4000E+00      0.9000
9.3980E+00      0.9250
1.0484E+01      0.9500
1.1428E+01      0.9600
1.2836E+01      0.9700
1.4840E+01      0.9750
1.6597E+01      0.9800
2.3295E+01      0.9850
3.1908E+01      0.9900
1.5012E+02      1.0000
/
/ Program: CDFTLB  Version:1.0  User: Signe Wurstner  Run ID: 900221154233
/ Cumulative Probability Table for n
/
      value      prob
1.3031E+00      0.0000
1.3237E+00      0.0100
1.3376E+00      0.0150
1.3440E+00      0.0200
1.3591E+00      0.0250
1.3737E+00      0.0300
1.3806E+00      0.0400
1.3897E+00      0.0500
1.4073E+00      0.0750
1.4235E+00      0.1000
1.4499E+00      0.1500
1.4777E+00      0.2000
1.5002E+00      0.2500
1.5206E+00      0.3000
1.5355E+00      0.3500
1.5550E+00      0.4000
1.5811E+00      0.4500
1.6009E+00      0.5000
1.6300E+00      0.5500
1.6445E+00      0.6000
1.6699E+00      0.6500
1.7011E+00      0.7000
1.7311E+00      0.7500

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1.7706E+00	0.8000
1.8086E+00	0.8500
1.8942E+00	0.9000
1.9572E+00	0.9250
2.0705E+00	0.9500
2.1541E+00	0.9600
2.2493E+00	0.9700
2.2995E+00	0.9750
2.3267E+00	0.9800
2.3731E+00	0.9850
2.5534E+00	0.9900
4.3825E+00	1.0000

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/-----
/-----
PROPERTY at cell faces: use GEOMETRIC mean of nodal values
INITIAL conditions: P=-100.0 from (1,1,1) to (3,3,162); mode=1, 0,0,1
BOUNDARY cond for P: -1(left), type=2(flux), flux=0
BOUNDARY cond for P: +1(right), type=2(flux), flux=0
BOUNDARY cond for P: -2(front), type=2(flux), flux=0
BOUNDARY cond for P: +2(back), type=2(flux), flux=0
BOUNDARY cond for P: -3(bottom), type=2(flux), flux=0
BOUNDARY cond for P: +3(top), type=2(flux), flux=-0.0179 m per d (recharge)
/-----
/MATRIX solution method for P: ADI, sweeps=1,
MATRIX solution method for P: RSCG, maxit=100, conv crit=5E-11
CONVERGENCE criteria for P: option 2, acceptable error=.0001, maxit=100
DISABLE T and C equations
REFERENCE node: (2,2,155) every 10 time steps
WINDOW for output (2,2,100) TO (2,2,162) in steps of 1,1,1
/SCREEN echo
FLUX for P through XY plane (1,1,161) to (3,3,161) every 100 time steps
FLUX for P through XY plane (1,1,160) to (3,3,160)
FLUX for P through XY plane (1,1,159) to (3,3,159)
FLUX for P through XY plane (1,1,158) to (3,3,158)
FLUX for P through XY plane (1,1,157) to (3,3,157)
FLUX for P through XY plane (1,1,156) to (3,3,156)
FLUX for P through XY plane (1,1,155) to (3,3,155)
FLUX for P through XY plane (1,1,154) to (3,3,154)
FLUX for P through XY plane (1,1,153) to (3,3,153)
OUTPUT in XZ plane
SOLVE in transient mode for 30 days, dt=0.0003, dtmagnf=1.05, max dt= 0.10
WRITE W, P, Theta in XZ plane NOW
OUTPUT: W, P, THETA in XZ plane NOW
END

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2.0 PROBLEM OUTPUT

Five output files were produced by the above input instructions. These were as follows.

1. PROB.OUT : Hardcopy output containing tables for every realization.
2. FLUXBAL. : Output on fluxes through specified planes in the flow field.
3. STOCH.3 : Plot file containing vertical velocities.
4. STOCH.4 : Plot file containing hydraulic heads.
5. STOCH.7 : Plot file containing relative saturations.

Parts of only the first two of these files are presented below as the sample output. Only parts are presented because the complete files are very large in size and would take too much space in this manual. The smaller FLUXBAL. is presented first, followed by PROB.OUT.

2.1 FLUX OUTPUT

Flux output of only the first two realizations is shown as an example.

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER											1 AT TIME	7.830E-01	+++++
ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX		
2	2	2	2	161	161	-4.121E-11	0.000E+00	-4.121E-11	-1.726E-11	0.000E+00	-1.726E-11		
2	2	2	2	160	160	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12		
+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER											1 AT TIME	1.009E+01	+++++
ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX		
2	2	2	2	161	161	-5.085E-10	0.000E+00	-5.085E-10	-2.597E-09	0.000E+00	-2.597E-09		
2	2	2	2	160	160	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11		
+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER											1 AT TIME	2.009E+01	+++++
ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX		
2	2	2	2	161	161	-1.346E-09	0.000E+00	-1.346E-09	-1.129E-08	0.000E+00	-1.129E-08		
2	2	2	2	160	160	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		
2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11		

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+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 1 AT TIME 3.000E+01 +++++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-3.096E-09	0.000E+00	-3.096E-09	-3.233E-08	0.000E+00	-3.233E-08
2	2	2	2	160	160	-1.891E-12	0.000E+00	-1.891E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 7.830E-01 +++++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.494E-03	0.000E+00	-4.494E-03	-2.098E-03	0.000E+00	-2.098E-03
2	2	2	2	160	160	-4.903E-03	0.000E+00	-4.903E-03	-6.602E-04	0.000E+00	-6.602E-04
2	2	2	2	159	159	-5.899E-05	0.000E+00	-5.899E-05	-3.852E-06	0.000E+00	-3.852E-06
2	2	2	2	158	158	-2.148E-08	0.000E+00	-2.148E-08	-1.524E-09	0.000E+00	-1.524E-09
2	2	2	2	157	157	-1.651E-10	0.000E+00	-1.651E-10	-1.808E-10	0.000E+00	-1.808E-10
2	2	2	2	156	156	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10
2	2	2	2	155	155	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10
2	2	2	2	154	154	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10
2	2	2	2	153	153	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 1.009E+01 +++++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.474E-03	0.000E+00	-4.474E-03	-4.348E-02	0.000E+00	-4.348E-02
2	2	2	2	160	160	-4.472E-03	0.000E+00	-4.472E-03	-4.167E-02	0.000E+00	-4.167E-02
2	2	2	2	159	159	-4.470E-03	0.000E+00	-4.470E-03	-3.974E-02	0.000E+00	-3.974E-02
2	2	2	2	158	158	-4.468E-03	0.000E+00	-4.468E-03	-3.769E-02	0.000E+00	-3.769E-02
2	2	2	2	157	157	-4.465E-03	0.000E+00	-4.465E-03	-3.552E-02	0.000E+00	-3.552E-02
2	2	2	2	156	156	-4.460E-03	0.000E+00	-4.460E-03	-3.325E-02	0.000E+00	-3.325E-02
2	2	2	2	155	155	-4.455E-03	0.000E+00	-4.455E-03	-3.099E-02	0.000E+00	-3.099E-02
2	2	2	2	154	154	-4.447E-03	0.000E+00	-4.447E-03	-2.875E-02	0.000E+00	-2.875E-02
2	2	2	2	153	153	-4.438E-03	0.000E+00	-4.438E-03	-2.651E-02	0.000E+00	-2.651E-02

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 2.009E+01 +++++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.475E-03	0.000E+00	-4.475E-03	-8.823E-02	0.000E+00	-8.823E-02
2	2	2	2	160	160	-4.475E-03	0.000E+00	-4.475E-03	-8.641E-02	0.000E+00	-8.641E-02
2	2	2	2	159	159	-4.475E-03	0.000E+00	-4.475E-03	-8.448E-02	0.000E+00	-8.448E-02
2	2	2	2	158	158	-4.475E-03	0.000E+00	-4.475E-03	-8.242E-02	0.000E+00	-8.242E-02
2	2	2	2	157	157	-4.475E-03	0.000E+00	-4.475E-03	-8.025E-02	0.000E+00	-8.025E-02
2	2	2	2	156	156	-4.475E-03	0.000E+00	-4.475E-03	-7.798E-02	0.000E+00	-7.798E-02
2	2	2	2	155	155	-4.475E-03	0.000E+00	-4.475E-03	-7.570E-02	0.000E+00	-7.570E-02
2	2	2	2	154	154	-4.475E-03	0.000E+00	-4.475E-03	-7.344E-02	0.000E+00	-7.344E-02
2	2	2	2	153	153	-4.475E-03	0.000E+00	-4.475E-03	-7.119E-02	0.000E+00	-7.119E-02

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 3.000E+01 +++++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.475E-03	0.000E+00	-4.475E-03	-1.326E-01	0.000E+00	-1.326E-01
2	2	2	2	160	160	-4.475E-03	0.000E+00	-4.475E-03	-1.308E-01	0.000E+00	-1.308E-01
2	2	2	2	159	159	-4.475E-03	0.000E+00	-4.475E-03	-1.288E-01	0.000E+00	-1.288E-01
2	2	2	2	158	158	-4.475E-03	0.000E+00	-4.475E-03	-1.268E-01	0.000E+00	-1.268E-01
2	2	2	2	157	157	-4.475E-03	0.000E+00	-4.475E-03	-1.246E-01	0.000E+00	-1.246E-01
2	2	2	2	156	156	-4.475E-03	0.000E+00	-4.475E-03	-1.223E-01	0.000E+00	-1.223E-01
2	2	2	2	155	155	-4.475E-03	0.000E+00	-4.475E-03	-1.201E-01	0.000E+00	-1.201E-01
2	2	2	2	154	154	-4.475E-03	0.000E+00	-4.475E-03	-1.178E-01	0.000E+00	-1.178E-01
2	2	2	2	153	153	-4.475E-03	0.000E+00	-4.475E-03	-1.155E-01	0.000E+00	-1.155E-01

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 3 AT TIME 7.830E-01 +++++

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 1 AT TIME 7.830E-01 +++++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.121E-11	0.000E+00	-4.121E-11	-1.726E-11	0.000E+00	-1.726E-11
2	2	2	2	160	160	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12

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2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-1.480E-12	0.000E+00	-1.480E-12

+++----- FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 1 AT TIME 1.009E+01 -----+++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-5.085E-10	0.000E+00	-5.085E-10	-2.597E-09	0.000E+00	-2.597E-09
2	2	2	2	160	160	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11
2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-1.907E-11	0.000E+00	-1.907E-11

+++----- FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 1 AT TIME 2.009E+01 -----+++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-1.346E-09	0.000E+00	-1.346E-09	-1.129E-08	0.000E+00	-1.129E-08
2	2	2	2	160	160	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11
2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-3.797E-11	0.000E+00	-3.797E-11

+++----- FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 1 AT TIME 3.000E+01 -----+++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-3.096E-09	0.000E+00	-3.096E-09	-3.233E-08	0.000E+00	-3.233E-08
2	2	2	2	160	160	-1.891E-12	0.000E+00	-1.891E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	159	159	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	158	158	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	157	157	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	156	156	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	155	155	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	154	154	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11
2	2	2	2	153	153	-1.890E-12	0.000E+00	-1.890E-12	-5.671E-11	0.000E+00	-5.671E-11

+++----- FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 7.830E-01 -----+++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.494E-03	0.000E+00	-4.494E-03	-2.098E-03	0.000E+00	-2.098E-03
2	2	2	2	160	160	-4.903E-03	0.000E+00	-4.903E-03	-6.602E-04	0.000E+00	-6.602E-04
2	2	2	2	159	159	-5.899E-05	0.000E+00	-5.899E-05	-3.852E-06	0.000E+00	-3.852E-06
2	2	2	2	158	158	-2.148E-08	0.000E+00	-2.148E-08	-1.524E-09	0.000E+00	-1.524E-09
2	2	2	2	157	157	-1.651E-10	0.000E+00	-1.651E-10	-1.808E-10	0.000E+00	-1.808E-10
2	2	2	2	156	156	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10
2	2	2	2	155	155	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10
2	2	2	2	154	154	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10
2	2	2	2	153	153	-1.579E-10	0.000E+00	-1.579E-10	-1.804E-10	0.000E+00	-1.804E-10

+++----- FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 1.009E+01 -----+++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.474E-03	0.000E+00	-4.474E-03	-4.348E-02	0.000E+00	-4.348E-02
2	2	2	2	160	160	-4.472E-03	0.000E+00	-4.472E-03	-4.167E-02	0.000E+00	-4.167E-02
2	2	2	2	159	159	-4.470E-03	0.000E+00	-4.470E-03	-3.974E-02	0.000E+00	-3.974E-02
2	2	2	2	158	158	-4.468E-03	0.000E+00	-4.468E-03	-3.769E-02	0.000E+00	-3.769E-02
2	2	2	2	157	157	-4.465E-03	0.000E+00	-4.465E-03	-3.552E-02	0.000E+00	-3.552E-02
2	2	2	2	156	156	-4.460E-03	0.000E+00	-4.460E-03	-3.325E-02	0.000E+00	-3.325E-02
2	2	2	2	155	155	-4.455E-03	0.000E+00	-4.455E-03	-3.099E-02	0.000E+00	-3.099E-02
2	2	2	2	154	154	-4.447E-03	0.000E+00	-4.447E-03	-2.875E-02	0.000E+00	-2.875E-02
2	2	2	2	153	153	-4.438E-03	0.000E+00	-4.438E-03	-2.651E-02	0.000E+00	-2.651E-02

+++----- FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 2.009E+01 -----+++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.475E-03	0.000E+00	-4.475E-03	-8.823E-02	0.000E+00	-8.823E-02
2	2	2	2	160	160	-4.475E-03	0.000E+00	-4.475E-03	-8.641E-02	0.000E+00	-8.641E-02
2	2	2	2	159	159	-4.475E-03	0.000E+00	-4.475E-03	-8.448E-02	0.000E+00	-8.448E-02

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2	2	2	2	158	158	-4.475E-03	0.000E+00	-4.475E-03	-8.242E-02	0.000E+00	-8.242E-02
2	2	2	2	157	157	-4.475E-03	0.000E+00	-4.475E-03	-8.025E-02	0.000E+00	-8.025E-02
2	2	2	2	156	156	-4.475E-03	0.000E+00	-4.475E-03	-7.798E-02	0.000E+00	-7.798E-02
2	2	2	2	155	155	-4.475E-03	0.000E+00	-4.475E-03	-7.570E-02	0.000E+00	-7.570E-02
2	2	2	2	154	154	-4.475E-03	0.000E+00	-4.475E-03	-7.344E-02	0.000E+00	-7.344E-02
2	2	2	2	153	153	-4.475E-03	0.000E+00	-4.475E-03	-7.119E-02	0.000E+00	-7.119E-02

+++++ FLUX CALCULATIONS FOR VARIABLE # 1 FOR REALIZATION NUMBER 2 AT TIME 3.000E+01 +++++

ILO	IHI	JLO	JHI	KLO	KHI	CONV INST FLUX	DIFF INST FLUX	TOTAL INST FLUX	CONV CUM FLUX	DIFF CUM FLUX	TOTAL CUM FLUX
2	2	2	2	161	161	-4.475E-03	0.000E+00	-4.475E-03	-1.326E-01	0.000E+00	-1.326E-01
2	2	2	2	160	160	-4.475E-03	0.000E+00	-4.475E-03	-1.308E-01	0.000E+00	-1.308E-01
2	2	2	2	159	159	-4.475E-03	0.000E+00	-4.475E-03	-1.288E-01	0.000E+00	-1.288E-01
2	2	2	2	158	158	-4.475E-03	0.000E+00	-4.475E-03	-1.268E-01	0.000E+00	-1.268E-01
2	2	2	2	157	157	-4.475E-03	0.000E+00	-4.475E-03	-1.246E-01	0.000E+00	-1.246E-01
2	2	2	2	156	156	-4.475E-03	0.000E+00	-4.475E-03	-1.223E-01	0.000E+00	-1.223E-01
2	2	2	2	155	155	-4.475E-03	0.000E+00	-4.475E-03	-1.201E-01	0.000E+00	-1.201E-01
2	2	2	2	154	154	-4.475E-03	0.000E+00	-4.475E-03	-1.178E-01	0.000E+00	-1.178E-01
2	2	2	2	153	153	-4.475E-03	0.000E+00	-4.475E-03	-1.155E-01	0.000E+00	-1.155E-01

2.2 TABULAR OUTPUT

As previously mentioned, output of only a few realizations is presented.

```

PPPPP   OOOO   RRRRR   MM   MM   CCCCC
P  P  O  O  R  R  M  M  M  M  C
P  P  O  O  R  R  M  M  M  M  C
PPPPP   O  O  RRRRR   M  M  M  C
P  P  O  O  R  R  M  M  M  C
P  P  O  O  R  R  M  M  M  C
P  P  OOOO  R  R  M  M  M  CCCCC
    
```

VERSION 1.0:.001

This Run Made on 3/20/1991 at 19:14:49

I.D. = 320911914

```

::      OOO N N EEEEE   DDDD   TTTT #### AAA N N SSS III EEEEE N N TTTT
::      O O NM N E      D D      T # # A A NM N S   I E NN N T
::      O O NM N EEEEE  ----- D D      T #### AAAAA N N N SSS I EEEE N N N T
::      O O N NM E      D D      T # # A A N NM S   S I E N NN T
::      OOO N N EEEEE   DDDD   T # # A A N N SSS III EEEEE N N T
    
```

```

PPPP #### OOO BBBB L EEEEE M M L AAA SSS CCC #### U U CCC EEEEE SSS
P P # # O O B B L E MM MM L A A S C C # # U U C C E S
PPPP #### O O BBBB L EEEE M M M ----- L AAAAA SSS C #### U U C EEEE SSS
P # # O O B B L E M M M L A A S C C # # U U C C E S
P # # OOO BBBB LLLL EEEEE M M LLLL A A SSS CCC # # UUU CCC EEEEE SSS
    
```

```

FFFF III EEEEE L DDDD EEEEE X X PPPP EEEEE #### III M M EEEEE N N TTTT
F I E L D D E X X P P E # # I MM MM E NN N T
FFFF I EEEE L D D EEEE X PPPP EEEE #### I M M M EEEE NN N T
F I E L D D E X X P E # # I M M E NN N T
F III EEEEE LLLL DDDD EEEEE X X P EEEEE # # III M M EEEEE N N T
    
```

Results from this code are based on the use of unverified software and are not for use in license related applications.

1

THIS OUTPUT IS PRODUCED BY THE COMPUTATIONAL MODEL

----- P O R M C -----

FOR TRANSIENT OR STEADY STATE STOCHASTIC 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

VERSION 1.0: DATED: 22 OCT 1989

DATE OF RUN: 3/20/1991 - TIME OF RUN: 19:14:49

RECORD OF INPUT DATA STREAM

** RECORD NO. 1 KEYWORD ***** TITLE: ONE-D TRANSIENT PROBLEM - LAS CRUCES FIELD EXPERIMENT
** RECORD NO. 2 COMMENT ***** /-----
** RECORD NO. 3 COMMENT ***** / REF: DATA FROM NMSU 06/89 DATA PREPARED BY SIGNE WURSTNER
** RECORD NO. 4 COMMENT ***** /-----
** RECORD NO. 5 KEYWORD ***** USER: BSAGAR
** RECORD NO. 6 KEYWORD ***** GRID: 3 by 3 by 162 realizations = 50, seed=85631

=====> UNIT 8 OPEN FOR I/O IN UNFORMATTED MODE; FILE NAME: montein

** RECORD NO. 7 KEYWORD ***** X coordinates: type 3 (uniform), min=0, max=1, ratio=1
** RECORD NO. 8 KEYWORD ***** Y coordinates: type 3 (uniform), min=0, max=1, ratio=1
** RECORD NO. 9 KEYWORD ***** Z coordinates: type 3 (uniform), min=-8.025, max=0.025, ratio=1
** RECORD NO. 10 COMMENT ***** /-----
** RECORD NO. 11 KEYWORD ***** DATUM: 0., maximum tension: 1.E30, minimum relative k: 10e-20
** RECORD NO. 12 COMMENT ***** /-----
** RECORD NO. 13 KEYWORD ***** ZONE 1 from (1,1,1) to (3,3,162)
** RECORD NO. 14 COMMENT ***** /-----
** RECORD NO. 15 KEYWORD ***** FOR zone 1
** RECORD NO. 16 KEYWORD ***** HYDRAULIC saturated properties are STOCHASTIC:
** RECORD NO. 17 COMMENT ***** / storativity equal to eff porosity
** RECORD NO. 18 CONTINUATION ** storativity: -1 perfect corr with por 14 0 1 0
** RECORD NO. 19 CONTINUATION ** Kx : -1 perfect corr with Kz 4 0 1 0
** RECORD NO. 20 CONTINUATION ** Ky : -1 perfect corr with Kz 4 0 1 0
** RECORD NO. 21 CONTINUATION ** Kz : 8 (tabular pdf, see table below) 35 sets -999 -999 -999
** RECORD NO. 22 CONTINUATION ** corr : 0 0 0 0 0 0
** RECORD NO. 23 CONTINUATION ** zone 1 to zone 1 in steps of 1
** RECORD NO. 24 COMMENT ***** / Program: CDFTLB Version:1.0 User: Signe Wurstner Run ID: 900227085021
** RECORD NO. 25 COMMENT ***** / Cumulative Probability Table for Kz
** RECORD NO. 26 CONTINUATION ** 1.40000E-02 0.00000
** RECORD NO. 27 CONTINUATION ** 9.95000E-02 0.01000
** RECORD NO. 28 CONTINUATION ** 1.11000E-01 0.01500
** RECORD NO. 29 CONTINUATION ** 1.39000E-01 0.02000
** RECORD NO. 30 CONTINUATION ** 1.48375E-01 0.02500
** RECORD NO. 31 CONTINUATION ** 1.77250E-01 0.03000
** RECORD NO. 32 CONTINUATION ** 1.95000E-01 0.04000
** RECORD NO. 33 CONTINUATION ** 2.27500E-01 0.05000
** RECORD NO. 34 CONTINUATION ** 3.14875E-01 0.07500
** RECORD NO. 35 CONTINUATION ** 3.74000E-01 0.10000

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** RECORD NO. 36 CONTINUATION ** 4.90750E-01 0.15000
** RECORD NO. 37 CONTINUATION ** 6.20000E-01 0.20000
** RECORD NO. 38 CONTINUATION ** 8.35750E-01 0.25000
** RECORD NO. 39 CONTINUATION ** 1.06850E+00 0.30000
** RECORD NO. 40 CONTINUATION ** 1.57375E+00 0.35000
** RECORD NO. 41 CONTINUATION ** 2.11700E+00 0.40000
** RECORD NO. 42 CONTINUATION ** 2.76200E+00 0.45000
** RECORD NO. 43 CONTINUATION ** 3.68350E+00 0.50000
** RECORD NO. 44 CONTINUATION ** 4.51075E+00 0.55000
** RECORD NO. 45 CONTINUATION ** 5.33100E+00 0.60000
** RECORD NO. 46 CONTINUATION ** 6.04250E+00 0.65000
** RECORD NO. 47 CONTINUATION ** 7.04200E+00 0.70000
** RECORD NO. 48 CONTINUATION ** 7.77200E+00 0.75000
** RECORD NO. 49 CONTINUATION ** 8.79800E+00 0.80000
** RECORD NO. 50 CONTINUATION ** 9.70150E+00 0.85000
** RECORD NO. 51 CONTINUATION ** 1.09460E+01 0.90000
** RECORD NO. 52 CONTINUATION ** 1.21231E+01 0.92500
** RECORD NO. 53 CONTINUATION ** 1.35650E+01 0.95000
** RECORD NO. 54 CONTINUATION ** 1.42220E+01 0.96000
** RECORD NO. 55 CONTINUATION ** 1.53335E+01 0.97000
** RECORD NO. 56 CONTINUATION ** 1.70963E+01 0.97500
** RECORD NO. 57 CONTINUATION ** 1.81425E+01 0.98000
** RECORD NO. 58 CONTINUATION ** 2.17477E+01 0.98500
** RECORD NO. 59 CONTINUATION ** 2.58765E+01 0.99000
** RECORD NO. 60 CONTINUATION ** 6.73060E+01 1.00000
** RECORD NO. 61 COMMENT ***** /
** RECORD NO. 62 KEYWORD ***** SOIL properties are STOCHastic:
** RECORD NO. 63 COMMENT ***** /variable distribution value
** RECORD NO. 64 CONTINUATION ** rho: 0 (constant) 1.66 0 0 0
** RECORD NO. 65 COMMENT ***** / eff por = wcs - wcr
** RECORD NO. 66 COMMENT ***** /set diffusive and total porosity equal to effective porosity
** RECORD NO. 67 CONTINUATION ** eff por: 8(tabular) 35 sets (see below for table) -999 -999 -999
** RECORD NO. 68 CONTINUATION ** tot por: -1 14 0 1 0
** RECORD NO. 69 CONTINUATION ** diff por: -1 14 0 1 0
** RECORD NO. 70 CONTINUATION ** corr : 0 0 0 0 0 0
** RECORD NO. 71 CONTINUATION ** for zone 1 to 1 in steps of 1
** RECORD NO. 72 COMMENT ***** / Program: CDFTLB Version:1.0 User: Signe Wurstner Run ID: 900221154233
** RECORD NO. 73 COMMENT ***** / Cumulative Probability Table for effective porosity
** RECORD NO. 74 COMMENT ***** /
** RECORD NO. 75 CONTINUATION ** value prob
** RECORD NO. 76 CONTINUATION ** 1.2000E-01 0.0000
** RECORD NO. 77 CONTINUATION ** 1.4064E-01 0.0100
** RECORD NO. 78 CONTINUATION ** 1.4400E-01 0.0150
** RECORD NO. 79 CONTINUATION ** 1.4628E-01 0.0200
** RECORD NO. 80 CONTINUATION ** 1.5090E-01 0.0250
** RECORD NO. 81 CONTINUATION ** 1.6200E-01 0.0300
** RECORD NO. 82 CONTINUATION ** 1.6656E-01 0.0400
** RECORD NO. 83 CONTINUATION ** 1.7120E-01 0.0500
** RECORD NO. 84 CONTINUATION ** 1.8130E-01 0.0750
** RECORD NO. 85 CONTINUATION ** 1.8600E-01 0.1000
** RECORD NO. 86 CONTINUATION ** 1.9260E-01 0.1500
** RECORD NO. 87 CONTINUATION ** 2.0360E-01 0.2000
** RECORD NO. 88 CONTINUATION ** 2.0900E-01 0.2500
** RECORD NO. 89 CONTINUATION ** 2.1500E-01 0.3000
** RECORD NO. 90 CONTINUATION ** 2.1900E-01 0.3500
** RECORD NO. 91 CONTINUATION ** 2.2260E-01 0.4000
** RECORD NO. 92 CONTINUATION ** 2.2700E-01 0.4500
** RECORD NO. 93 CONTINUATION ** 2.3200E-01 0.5000
** RECORD NO. 94 CONTINUATION ** 2.3600E-01 0.5500
** RECORD NO. 95 CONTINUATION ** 2.4040E-01 0.6000
** RECORD NO. 96 CONTINUATION ** 2.4600E-01 0.6500
** RECORD NO. 97 CONTINUATION ** 2.5200E-01 0.7000
** RECORD NO. 98 CONTINUATION ** 2.5800E-01 0.7500
** RECORD NO. 99 CONTINUATION ** 2.6400E-01 0.8000
** RECORD NO. 100 CONTINUATION ** 2.7100E-01 0.8500
** RECORD NO. 101 CONTINUATION ** 2.7800E-01 0.9000
** RECORD NO. 102 CONTINUATION ** 2.8600E-01 0.9250
** RECORD NO. 103 CONTINUATION ** 2.9180E-01 0.9500
** RECORD NO. 104 CONTINUATION ** 2.9544E-01 0.9600
** RECORD NO. 105 CONTINUATION ** 3.0108E-01 0.9700
** RECORD NO. 106 CONTINUATION ** 3.0290E-01 0.9750
** RECORD NO. 107 CONTINUATION ** 3.0572E-01 0.9800
** RECORD NO. 108 CONTINUATION ** 3.1308E-01 0.9850
** RECORD NO. 109 CONTINUATION ** 3.1800E-01 0.9900
** RECORD NO. 110 CONTINUATION ** 4.5200E-01 1.0000
** RECORD NO. 111 COMMENT ***** /
** RECORD NO. 111 KEYWORD ***** UNSATURATED conductivity VAN with MUAL

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** RECORD NO.112 KEYWORD ***** CHARACTERISTICS are STOchastic
** RECORD NO.113 CONTINUATION ** alpha      8  35 sets -999 -999 -999
** RECORD NO.114 CONTINUATION ** n         8  35 sets -999 -999 -999
** RECORD NO.115 CONTINUATION ** lamda     0  0         0  0  0 (not required)
** RECORD NO.116 CONTINUATION ** ualfa    0  0         0  0  0
** RECORD NO.117 CONTINUATION ** corr     0
** RECORD NO.118 CONTINUATION ** ualfaA   0  0
** RECORD NO.119 CONTINUATION ** for zone 1 to zone 1 in steps of 1
** RECORD NO.120 COMMENT ***** /
** RECORD NO.121 COMMENT ***** / Program: CDFTLB  Version:1.0  User: Signe Wurstner  Run ID: 900221154233
** RECORD NO.122 COMMENT ***** / Cumulative Probability Table for alpha
** RECORD NO.123 COMMENT ***** /
** RECORD NO.124 CONTINUATION **          value      prob
** RECORD NO.125 CONTINUATION **          6.1000E-01    0.0000
** RECORD NO.126 CONTINUATION **          1.0564E+00    0.0100
** RECORD NO.127 CONTINUATION **          1.1722E+00    0.0150
** RECORD NO.128 CONTINUATION **          1.2256E+00    0.0200
** RECORD NO.129 CONTINUATION **          1.2860E+00    0.0250
** RECORD NO.130 CONTINUATION **          1.3600E+00    0.0300
** RECORD NO.131 CONTINUATION **          1.5368E+00    0.0400
** RECORD NO.132 CONTINUATION **          1.6420E+00    0.0500
** RECORD NO.133 CONTINUATION **          1.8400E+00    0.0750
** RECORD NO.134 CONTINUATION **          2.0380E+00    0.1000
** RECORD NO.135 CONTINUATION **          2.3880E+00    0.1500
** RECORD NO.136 CONTINUATION **          2.6580E+00    0.2000
** RECORD NO.137 CONTINUATION **          2.9700E+00    0.2500
** RECORD NO.138 CONTINUATION **          3.2100E+00    0.3000
** RECORD NO.139 CONTINUATION **          3.4400E+00    0.3500
** RECORD NO.140 CONTINUATION **          3.6860E+00    0.4000
** RECORD NO.141 CONTINUATION **          3.9500E+00    0.4500
** RECORD NO.142 CONTINUATION **          4.0900E+00    0.5000
** RECORD NO.143 CONTINUATION **          4.4200E+00    0.5500
** RECORD NO.144 CONTINUATION **          4.6800E+00    0.6000
** RECORD NO.145 CONTINUATION **          4.9480E+00    0.6500
** RECORD NO.146 CONTINUATION **          5.3680E+00    0.7000
** RECORD NO.147 CONTINUATION **          5.8000E+00    0.7500
** RECORD NO.148 CONTINUATION **          6.4660E+00    0.8000
** RECORD NO.149 CONTINUATION **          7.2260E+00    0.8500
** RECORD NO.150 CONTINUATION **          8.4000E+00    0.9000
** RECORD NO.151 CONTINUATION **          9.3980E+00    0.9250
** RECORD NO.152 CONTINUATION **          1.0484E+01    0.9500
** RECORD NO.153 CONTINUATION **          1.1428E+01    0.9600
** RECORD NO.154 CONTINUATION **          1.2836E+01    0.9700
** RECORD NO.155 CONTINUATION **          1.4840E+01    0.9750
** RECORD NO.156 CONTINUATION **          1.6597E+01    0.9800
** RECORD NO.157 CONTINUATION **          2.3295E+01    0.9850
** RECORD NO.158 CONTINUATION **          3.1908E+01    0.9900
** RECORD NO.159 COMMENT ***** /
** RECORD NO.160 COMMENT ***** / Program: CDFTLB  Version:1.0  User: Signe Wurstner  Run ID: 900221154233
** RECORD NO.161 COMMENT ***** / Cumulative Probability Table for n
** RECORD NO.162 COMMENT ***** /
** RECORD NO.163 CONTINUATION **          value      prob
** RECORD NO.164 CONTINUATION **          1.3031E+00    0.0000
** RECORD NO.165 CONTINUATION **          1.3237E+00    0.0100
** RECORD NO.166 CONTINUATION **          1.3376E+00    0.0150
** RECORD NO.167 CONTINUATION **          1.3440E+00    0.0200
** RECORD NO.168 CONTINUATION **          1.3591E+00    0.0250
** RECORD NO.169 CONTINUATION **          1.3737E+00    0.0300
** RECORD NO.170 CONTINUATION **          1.3806E+00    0.0400
** RECORD NO.171 CONTINUATION **          1.3897E+00    0.0500
** RECORD NO.172 CONTINUATION **          1.4073E+00    0.0750
** RECORD NO.173 CONTINUATION **          1.4235E+00    0.1000
** RECORD NO.174 CONTINUATION **          1.4499E+00    0.1500
** RECORD NO.175 CONTINUATION **          1.4777E+00    0.2000
** RECORD NO.176 CONTINUATION **          1.5002E+00    0.2500
** RECORD NO.177 CONTINUATION **          1.5206E+00    0.3000
** RECORD NO.178 CONTINUATION **          1.5355E+00    0.3500
** RECORD NO.179 CONTINUATION **          1.5550E+00    0.4000
** RECORD NO.180 CONTINUATION **          1.5811E+00    0.4500
** RECORD NO.181 CONTINUATION **          1.6009E+00    0.5000
** RECORD NO.182 CONTINUATION **          1.6300E+00    0.5500
** RECORD NO.183 CONTINUATION **          1.6445E+00    0.6000
** RECORD NO.184 CONTINUATION **          1.6699E+00    0.6500
** RECORD NO.185 CONTINUATION **          1.7011E+00    0.7000
** RECORD NO.186 CONTINUATION **          1.7311E+00    0.7500
** RECORD NO.187 CONTINUATION **          1.7706E+00    0.8000
** RECORD NO.188 CONTINUATION **          1.8086E+00    0.8500

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** RECORD NO.188 CONTINUATION **          1.8942E+00    0.9000
** RECORD NO.189 CONTINUATION **          1.9572E+00    0.9250
** RECORD NO.190 CONTINUATION **          2.0705E+00    0.9500
** RECORD NO.191 CONTINUATION **          2.1541E+00    0.9600
** RECORD NO.192 CONTINUATION **          2.2493E+00    0.9700
** RECORD NO.193 CONTINUATION **          2.2995E+00    0.9750
** RECORD NO.194 CONTINUATION **          2.3267E+00    0.9800
** RECORD NO.195 CONTINUATION **          2.3731E+00    0.9850
** RECORD NO.196 CONTINUATION **          2.5534E+00    0.9900
** RECORD NO.197 CONTINUATION **          4.3825E+00    1.0000
** RECORD NO.198 COMMENT ***** /-----
** RECORD NO.199 COMMENT ***** /-----
** RECORD NO.200 KEYWORD ***** PROPERTY at cell faces: use GEOMETRIC mean of nodal values
** RECORD NO.201 KEYWORD ***** INITIAL conditions: P=-100.0 from (1,1,1) to (3,3,162); mode=1, 0,0,1
** RECORD NO.202 KEYWORD ***** BOUNDARY cond for P: -1(left), type=2(flux), flux=0
** RECORD NO.203 KEYWORD ***** BOUNDARY cond for P: +1(right), type=2(flux), flux=0
** RECORD NO.204 KEYWORD ***** BOUNDARY cond for P: -2(front), type=2(flux), flux=0
** RECORD NO.205 KEYWORD ***** BOUNDARY cond for P: +2(back), type=2(flux), flux=0
** RECORD NO.206 KEYWORD ***** BOUNDARY cond for P: -3(bottom), type=2(flux), flux=0
** RECORD NO.207 KEYWORD ***** BOUNDARY cond for P: +3(top), type=2(flux), flux=-0.0179 m per d (recharge)
** RECORD NO.208 COMMENT ***** /-----
** RECORD NO.209 COMMENT ***** /MATRIX solution method for P: ADI, sweeps=1,
** RECORD NO.210 KEYWORD ***** MATRIX solution method for P: RSCG, maxit=100, conv crit=5E-11
** RECORD NO.211 KEYWORD ***** CONVERGENCE criteria for P: option 2, acceptable error=.0001, maxit=100
** RECORD NO.212 KEYWORD ***** DISABLE T and C equations
** RECORD NO.213 KEYWORD ***** REFERENCE node: (2,2,155) every 10 time steps
** RECORD NO.214 KEYWORD ***** WINDOW for output (2,2,100) TO (2,2,162) in steps of 1,1,1
** RECORD NO.215 COMMENT ***** /SCREEN echo
** RECORD NO.216 KEYWORD ***** FLUX for P through XY plane (1,1,161) to (3,3,161) every 100 time steps
** RECORD NO.217 KEYWORD ***** FLUX for P through XY plane (1,1,160) to (3,3,160)
** RECORD NO.218 KEYWORD ***** FLUX for P through XY plane (1,1,159) to (3,3,159)
** RECORD NO.219 KEYWORD ***** FLUX for P through XY plane (1,1,158) to (3,3,158)
** RECORD NO.220 KEYWORD ***** FLUX for P through XY plane (1,1,157) to (3,3,157)
** RECORD NO.221 KEYWORD ***** FLUX for P through XY plane (1,1,156) to (3,3,156)
** RECORD NO.222 KEYWORD ***** FLUX for P through XY plane (1,1,155) to (3,3,155)
** RECORD NO.223 KEYWORD ***** FLUX for P through XY plane (1,1,154) to (3,3,154)
** RECORD NO.224 KEYWORD ***** FLUX for P through XY plane (1,1,153) to (3,3,153)
** RECORD NO.225 KEYWORD ***** OUTPUT in XZ plane
** RECORD NO.226 KEYWORD ***** SOLVE in transient mode for 30 days, dt=0.0003, dtmagnf=1.05,
** RECORD NO.227 CONTINUATION **          max dt= 0.10
** RECORD NO.228 KEYWORD ***** WRITE W, P, Theta in XZ plane in FORMatted mode NOW
** RECORD NO.229 KEYWORD ***** OUTPUT: W, P, THETA in XZ plane NOW
** RECORD NO.230 KEYWORD ***** END

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=====> UNIT 4 OPEN FOR I/O IN FORMATTED MODE; FILE NAME: fluxbal

1-----
ONE-D TRANSIENT PROBLEM - LAS CRUCES FIELD EXPERIMENT

```

GRID DIMENSIONS.....(IMAX,JMAX,KMAX) = 3 BY 3 BY162
MAXIMUM NUMBER OF NODES IN EACH 3-D ARRAY. = 1458
NUMBER OF THREE DIMENSIONAL FIELD ARRAYS.. = 23
FIELD LENGTH ALLOCATED FOR 3-D ARRAYS..... = 131.0 Kbyte
FIELD LENGTH ACTUALLY USED FOR 3-D ARRAYS. = 131.0 Kbyte

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X COORDINATE VALUES
=====
0.0000  0.5000  1.0000

```

```

Y COORDINATE VALUES
=====
0.0000  0.5000  1.0000

```

```

Z COORDINATE VALUES
=====
-8.0250 -7.9750 -7.9250 -7.8750 -7.8250 -7.7750 -7.7250 -7.6750

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-7.6250	-7.5750	-7.5250	-7.4750	-7.4250	-7.3750	-7.3250	-7.2750
-7.2250	-7.1750	-7.1250	-7.0750	-7.0250	-6.9750	-6.9250	-6.8750
-6.8250	-6.7750	-6.7250	-6.6750	-6.6250	-6.5750	-6.5250	-6.4750
-6.4250	-6.3750	-6.3250	-6.2750	-6.2250	-6.1750	-6.1250	-6.0750
-6.0250	-5.9750	-5.9250	-5.8750	-5.8250	-5.7750	-5.7250	-5.6750
-5.6250	-5.5750	-5.5250	-5.4750	-5.4250	-5.3750	-5.3250	-5.2750
-5.2250	-5.1750	-5.1250	-5.0750	-5.0250	-4.9750	-4.9250	-4.8750
-4.8250	-4.7750	-4.7250	-4.6750	-4.6250	-4.5750	-4.5250	-4.4750
-4.4250	-4.3750	-4.3250	-4.2750	-4.2250	-4.1750	-4.1250	-4.0750
-4.0250	-3.9750	-3.9250	-3.8750	-3.8250	-3.7750	-3.7250	-3.6750
-3.6250	-3.5750	-3.5250	-3.4750	-3.4250	-3.3750	-3.3250	-3.2750
-3.2250	-3.1750	-3.1250	-3.0750	-3.0250	-2.9750	-2.9250	-2.8750
-2.8250	-2.7750	-2.7250	-2.6750	-2.6250	-2.5750	-2.5250	-2.4750
-2.4250	-2.3750	-2.3250	-2.2750	-2.2250	-2.1750	-2.1250	-2.0750
-2.0250	-1.9750	-1.9250	-1.8750	-1.8250	-1.7750	-1.7250	-1.6750
-1.6250	-1.5750	-1.5250	-1.4750	-1.4250	-1.3750	-1.3250	-1.2750
-1.2250	-1.1750	-1.1250	-1.0750	-1.0250	-0.9750	-0.9250	-0.8750
-0.8250	-0.7750	-0.7250	-0.6750	-0.6250	-0.5750	-0.5250	-0.4750
-0.4250	-0.3750	-0.3250	-0.2750	-0.2250	-0.1750	-0.1250	-0.0750
-0.0250	0.0250						

ZONE IDENTIFIERS FOR THE FLOW FIELD

AT PLANE J = 2

=====

J=

162	111
161	111
160	111
159	111
158	111
157	111
156	111
155	111
154	111
153	111
152	111
151	111
150	111
149	111
148	111
147	111
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1 111
I= 123

BOUNDING INDICES FOR ACTIVE ZONES

=====
ZONE# LOWER BOUND UPPER BOUND
1 (1, 1, 1) (3, 3,162)

1- ONE-D TRANSIENT PROBLEM - LAS CRUCES FIELD EXPERIMENT

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 (T)... = 1
PROPERTY CALCULATION MODE (C)... = 1

START TIME = 0.000E+00
 CURRENT VALUE OF MAX. TIME = 3.000E+01
 STARTING TIME STEP = 3.000E-04
 TIME STEP INCREMENT FACTOR = 1.050E+00
 MAXIMUM TIME STEP = 1.000E-01
 TOTAL VOLUME OF FLUID IN FIELD.. = 5.390E-01

HYDRAULIC PROPERTIES OF POROUS MEDIA
 =====

ACTIVE ZONE #	SPECIFIC STORATIVITY	X-DIR. HYDRAULIC K	Y-DIR. HYDRAULIC K	Z-DIR. HYDRAULIC K
1	2.695E-01	7.561E+00	7.561E+00	7.561E+00

VALUES AT REFERENCE GRID NODE (2, 2,155)
 =====

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 = -1.003E+02
 THET- RELATIVE SATURATION LEVEL = 1.000E+00
 POR - MATRIX EFFECTIVE POROSITY. = 2.695E-01
 VOL - VOLUME OF GRID ELEMENTS... = 1.250E-02

DEPENDENT VARIABLE SPECIFICATIONS
 =====

VARIABLE	SYMBOL	SOLVE OPTION	INTEG. PROFILE	# OF SWEEPS	RELAX FACTOR
1	P	10	1	100	1.00

MATRIX SWEEP DIRECTIONS: X + Y + Z

*****STATISTICS OF INPUT SAMPLES*****

IZ/NODE	VARIABLE	DISTRIBUTION	N	MIN	MAX	AVG	MED	STD	COV	SKW
1	specific storativity	CORR	50	0.14E+00	0.39E+00	0.23E+00	0.23E+00	0.40E-01	0.17E+00	0.91E+00
1	X-dir hydraulic conducti	CORR	50	0.85E-01	0.28E+02	0.47E+01	0.36E+01	0.48E+01	0.10E+01	0.22E+01
1	Y-dir hydraulic conducti	CORR	50	0.85E-01	0.28E+02	0.47E+01	0.36E+01	0.48E+01	0.10E+01	0.22E+01
1	Z-dir hydraulic conducti	USER DEF	50	0.85E-01	0.28E+02	0.47E+01	0.36E+01	0.48E+01	0.10E+01	0.22E+01
1	density of solid materia	CONSTANT	50	0.17E+01	0.17E+01	0.17E+01	0.17E+01	0.00E+00	-0.99E+02	-0.99E+02
1	effective matrix porositi	USER DEF	50	0.14E+00	0.39E+00	0.23E+00	0.23E+00	0.40E-01	0.17E+00	0.91E+00
1	total matrix porosity	CORR	50	0.14E+00	0.39E+00	0.23E+00	0.23E+00	0.40E-01	0.17E+00	0.91E+00
1	diffusional matrix poros	CORR	50	0.14E+00	0.39E+00	0.23E+00	0.23E+00	0.40E-01	0.17E+00	0.91E+00
1	van Genuchten alpha/bub	USER DEF	50	0.12E+01	0.88E+02	0.61E+01	0.41E+01	0.12E+02	0.19E+01	0.65E+01
1	soil characteristic expo	USER DEF	50	0.14E+01	0.22E+01	0.16E+01	0.16E+01	0.17E+00	0.11E+00	0.95E+00
IZ/NODE	IVAR	NREAL	REALIZATION							
1	1									
		1	0.2695E+00							
		2	0.2619E+00							
		3	0.2249E+00							
		4	0.2629E+00							
		5	0.1845E+00							
		6	0.2294E+00							
		7	0.1821E+00							
		8	0.3942E+00							
		9	0.2374E+00							
		10	0.1767E+00							
		11	0.2298E+00							
		12	0.2114E+00							
		13	0.2187E+00							
		14	0.2260E+00							
		15	0.2326E+00							
		16	0.2381E+00							
		17	0.2347E+00							

18 0.2271E+00
 19 0.2442E+00
 20 0.2155E+00
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	43	0.2791E+00
	44	0.1717E+00
	45	0.2265E+00
	46	0.2239E+00
	47	0.2278E+00
	48	0.2097E+00
	49	0.2641E+00
1	50	0.2004E+00

17	1	0.4806E+01
	2	0.5783E+01
	3	0.4106E+01
	4	0.5739E+01
	5	0.4946E+01
	6	0.4467E+01
	7	0.2721E+01
	8	0.3765E+01
	9	0.5092E+01
	10	0.2535E+01
	11	0.3367E+01
	12	0.2985E+01
	13	0.1797E+01
	14	0.3856E+01
	15	0.4087E+01
	16	0.3149E+01
	17	0.4736E+01
	18	0.6157E+01
	19	0.4031E+01
	20	0.7048E+01
	21	0.5579E+01
	22	0.5903E+01
	23	0.1472E+01
	24	0.3012E+01
	25	0.2082E+01
	26	0.5278E+01
	27	0.3309E+01
	28	0.4722E+01
	29	0.8816E+02
	30	0.1237E+01
	31	0.3950E+01
	32	0.2011E+01
	33	0.3284E+01
	34	0.3220E+01
	35	0.3723E+01
	36	0.1016E+02
	37	0.3549E+01
	38	0.3700E+01
	39	0.2231E+01
	40	0.1222E+02
	41	0.5164E+01
	42	0.3530E+01
	43	0.2184E+01
	44	0.7145E+01
	45	0.2163E+01
	46	0.6743E+01
	47	0.7153E+01
	48	0.4983E+01
	49	0.8406E+01
	50	0.5620E+01

1	18	1	0.1947E+01
		2	0.1531E+01
		3	0.1807E+01
		4	0.1385E+01
		5	0.1413E+01
		6	0.1662E+01
		7	0.2212E+01
		8	0.1713E+01
		9	0.1524E+01
		10	0.1616E+01
		11	0.1485E+01
		12	0.1540E+01
		13	0.1530E+01
		14	0.1652E+01

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 39 0.1544E+01
 40 0.1803E+01
 41 0.2014E+01
 42 0.1427E+01
 43 0.1451E+01
 44 0.1872E+01
 45 0.1600E+01
 46 0.1748E+01
 47 0.1686E+01
 48 0.1576E+01
 49 0.1503E+01
 50 0.1582E+01

STEP NO.	TIME	[REFERENCE VALUES AT NODE (2, 2,155) FOR REALT NO. 1--]						[CONVERGENCE RATE / RESIDUALS]		
		U	V	W	P	T	C	TIMESTEP	REF. VAR.	INDEX
0	0.0000E+00	0.000E+00	0.000E+00	0.000E+00	-1.003E+02	1.000E+00	0.000E+00	2.8571E-04	2.000E-04	2.00
10	3.7734E-03	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	4.6540E-04	6.181E-06	0.618E-01
20	9.9198E-03	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	7.5809E-04	1.007E-05	0.101
30	1.9932E-02	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.2348E-03	1.640E-05	0.164
40	3.6240E-02	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	2.0114E-03	2.673E-05	0.267
50	6.2804E-02	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	3.2764E-03	4.355E-05	0.435
60	1.0608E-01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	5.3369E-03	7.098E-05	0.710
70	1.7656E-01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	8.6933E-03	2.842E-14	0.284E-09
80	2.9137E-01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.4160E-02	2.132E-14	0.213E-09
90	4.7838E-01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	2.3066E-02	2.132E-14	0.213E-09
100	7.8301E-01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	3.7572E-02	1.421E-14	0.142E-09
110	1.2792E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	6.1200E-02	1.421E-14	0.142E-09
120	2.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	9.9689E-02	2.842E-14	0.284E-09
130	3.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
140	4.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
150	5.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
160	6.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
170	7.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
180	8.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
190	9.0875E+00	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
200	1.0087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
210	1.1087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
220	1.2087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.132E-14	0.213E-09
230	1.3087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	7.105E-13	0.711E-08
240	1.4087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	7.958E-13	0.796E-08
250	1.5087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	8.953E-13	0.895E-08
260	1.6087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	1.016E-12	0.102E-07
270	1.7087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	1.123E-12	0.112E-07
280	1.8087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	1.279E-12	0.128E-07
290	1.9087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	1.414E-12	0.141E-07
300	2.0087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	1.570E-12	0.157E-07
310	2.1087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	1.748E-12	0.175E-07
320	2.2087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	1.933E-12	0.193E-07
330	2.3087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.160E-12	0.216E-07
340	2.4087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.416E-12	0.242E-07
350	2.5087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.657E-12	0.266E-07

360	2.6087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	2.963E-12	0.296E-07
370	2.7087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	3.276E-12	0.328E-07
380	2.8087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	3.610E-12	0.361E-07
390	2.9087E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.0000E-01	3.993E-12	0.399E-07
400	3.0000E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.2528E-02	8.527E-14	0.853E-09

=====> UNIT33 OPEN FOR I/O IN FORMATTED MODE; FILE NAME: stoch.3

=====> UNIT34 OPEN FOR I/O IN FORMATTED MODE; FILE NAME: stoch.4

=====> UNIT37 OPEN FOR I/O IN FORMATTED MODE; FILE NAME: stoch.7

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

CREATED BY PROGRAM : PORMC - VERSION 1.0: DATED: 22 OCT 1989
 DATA CREATED BY USER (ID) ... : BSAGAR - DATE OF ARCHIVED RECORDS : 3/20/1991
 TIME OF CREATION OF RECORDS . : 19:14:49
 TITLE (F THE ARCHIVED DATA SET: ONE-D TRANSIENT PROBLEM - LAS CRUCES FIELD EXPERIMENT
 SIMULATION TIME OF STORED DATA: 3.000E+01
 STEP NUMBER AT WHICH GENERATED: 400
 RUNNING COUNT OF TIME STEPS . : 400
 GRID DIMENSIONS OF STORED DATA: 3 BY 3 BY 162

----> WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT

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

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

CREATED BY PROGRAM : PORMC - VERSION 1.0: DATED: 22 OCT 1989
 DATA CREATED BY USER (ID) ... : BSAGAR - DATE OF ARCHIVED RECORDS : 3/20/1991
 TIME OF CREATION OF RECORDS . : 19:14:49
 TITLE OF THE ARCHIVED DATA SET: ONE-D TRANSIENT PROBLEM - LAS CRUCES FIELD EXPERIMENT
 SIMULATION TIME OF STORED DATA: 3.000E+01
 STEP NUMBER AT WHICH GENERATED: 400
 RUNNING COUNT OF TIME STEPS . : 400
 GRID DIMENSIONS OF STORED DATA: 3 BY 3 BY 162

----> WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD

<---- DATA SET NUMBER: 2 WRITTEN TO ARCHIVES ---->

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

CREATED BY PROGRAM : PORMC - VERSION 1.0: DATED: 22 OCT 1989
 DATA CREATED BY USER (ID) ... : BSAGAR - DATE OF ARCHIVED RECORDS : 3/20/1991
 TIME OF CREATION OF RECORDS . : 19:14:49
 TITLE OF THE ARCHIVED DATA SET: ONE-D TRANSIENT PROBLEM - LAS CRUCES FIELD EXPERIMENT
 SIMULATION TIME OF STORED DATA: 3.000E+01
 STEP NUMBER AT WHICH GENERATED: 400
 RUNNING COUNT OF TIME STEPS . : 400
 GRID DIMENSIONS OF STORED DATA: 3 BY 3 BY 162

----> WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 3 WRITTEN TO ARCHIVES ---->

400	3.0000E+01	0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.2528E-02	8.527E-14	0.853E-09
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-* REALIZATION 1W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -
 Z = K =
 0.000E+00 162 -1.79E-02
 -5.000E-02 161 -1.24E-08

-1.000E-01	160	-7.56E-12
-1.500E-01	159	-7.56E-12
-2.000E-01	158	-7.56E-12
-2.500E-01	157	-7.56E-12
-3.000E-01	156	-7.56E-12
-3.500E-01	155	-7.56E-12
-4.000E-01	154	-7.56E-12
-4.500E-01	153	-7.56E-12
-5.000E-01	152	-7.56E-12
-5.500E-01	151	-7.56E-12
-6.000E-01	150	-7.56E-12
-6.500E-01	149	-7.56E-12
-7.000E-01	148	-7.56E-12
-7.500E-01	147	-7.56E-12
-8.000E-01	146	-7.56E-12
-8.500E-01	145	-7.56E-12
-9.000E-01	144	-7.56E-12
-9.500E-01	143	-7.56E-12
-1.000E+00	142	-7.56E-12
-1.050E+00	141	-7.56E-12
-1.100E+00	140	-7.56E-12
-1.150E+00	139	-7.56E-12
-1.200E+00	138	-7.56E-12
-1.250E+00	137	-7.56E-12
-1.300E+00	136	-7.56E-12
-1.350E+00	135	-7.56E-12
-1.400E+00	134	-7.56E-12
-1.450E+00	133	-7.56E-12
-1.500E+00	132	-7.56E-12
-1.550E+00	131	-7.56E-12
-1.600E+00	130	-7.56E-12
-1.650E+00	129	-7.56E-12
-1.700E+00	128	-7.56E-12
-1.750E+00	127	-7.56E-12
-1.800E+00	126	-7.56E-12
-1.850E+00	125	-7.56E-12
-1.900E+00	124	-7.56E-12
-1.950E+00	123	-7.56E-12
-2.000E+00	122	-7.56E-12
-2.050E+00	121	-7.56E-12
-2.100E+00	120	-7.56E-12
-2.150E+00	119	-7.56E-12
-2.200E+00	118	-7.56E-12
-2.250E+00	117	-7.56E-12
-2.300E+00	116	-7.56E-12
-2.350E+00	115	-7.56E-12
-2.400E+00	114	-7.56E-12
-2.450E+00	113	-7.56E-12
-2.500E+00	112	-7.56E-12
-2.550E+00	111	-7.56E-12
-2.600E+00	110	-7.56E-12
-2.650E+00	109	-7.56E-12
-2.700E+00	108	-7.56E-12
-2.750E+00	107	-7.56E-12
-2.800E+00	106	-7.56E-12
-2.850E+00	105	-7.56E-12
-2.900E+00	104	-7.56E-12
-2.950E+00	103	-7.56E-12
-3.000E+00	102	-7.56E-12
-3.050E+00	101	-7.56E-12
-3.100E+00	100	-7.56E-12

I = 2
X = 5.00E-01

***- REALIZATION 1P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 ***

Z =	K =	
2.500E-02	162	-2.50E+00
-2.500E-02	161	-6.02E+01
-7.500E-02	160	-1.00E+02
-1.250E-01	159	-1.00E+02
-1.750E-01	158	-1.00E+02
-2.250E-01	157	-1.00E+02
-2.750E-01	156	-1.00E+02

-3.250E-01	155	-1.00E+02
-3.750E-01	154	-1.00E+02
-4.250E-01	153	-1.00E+02
-4.750E-01	152	-1.00E+02
-5.250E-01	151	-1.01E+02
-5.750E-01	150	-1.01E+02
-6.250E-01	149	-1.01E+02
-6.750E-01	148	-1.01E+02
-7.250E-01	147	-1.01E+02
-7.750E-01	146	-1.01E+02
-8.250E-01	145	-1.01E+02
-8.750E-01	144	-1.01E+02
-9.250E-01	143	-1.01E+02
-9.750E-01	142	-1.01E+02
-1.025E+00	141	-1.01E+02
-1.075E+00	140	-1.01E+02
-1.125E+00	139	-1.01E+02
-1.175E+00	138	-1.01E+02
-1.225E+00	137	-1.01E+02
-1.275E+00	136	-1.01E+02
-1.325E+00	135	-1.01E+02
-1.375E+00	134	-1.01E+02
-1.425E+00	133	-1.01E+02
-1.475E+00	132	-1.01E+02
-1.525E+00	131	-1.02E+02
-1.575E+00	130	-1.02E+02
-1.625E+00	129	-1.02E+02
-1.675E+00	128	-1.02E+02
-1.725E+00	127	-1.02E+02
-1.775E+00	126	-1.02E+02
-1.825E+00	125	-1.02E+02
-1.875E+00	124	-1.02E+02
-1.925E+00	123	-1.02E+02
-1.975E+00	122	-1.02E+02
-2.025E+00	121	-1.02E+02
-2.075E+00	120	-1.02E+02
-2.125E+00	119	-1.02E+02
-2.175E+00	118	-1.02E+02
-2.225E+00	117	-1.02E+02
-2.275E+00	116	-1.02E+02
-2.325E+00	115	-1.02E+02
-2.375E+00	114	-1.02E+02
-2.425E+00	113	-1.02E+02
-2.475E+00	112	-1.02E+02
-2.525E+00	111	-1.03E+02
-2.575E+00	110	-1.03E+02
-2.625E+00	109	-1.03E+02
-2.675E+00	108	-1.03E+02
-2.725E+00	107	-1.03E+02
-2.775E+00	106	-1.03E+02
-2.825E+00	105	-1.03E+02
-2.875E+00	104	-1.03E+02
-2.925E+00	103	-1.03E+02
-2.975E+00	102	-1.03E+02
-3.025E+00	101	-1.03E+02
-3.075E+00	100	-1.03E+02

I = 2
X = 5.00E-01

--* REALIZATION 1THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -*-*

Z =	K =	
2.500E-02	162	9.36E-02
-2.500E-02	161	4.67E-03
-7.500E-02	160	2.88E-03
-1.250E-01	59	2.88E-03
-1.750E-01	158	2.88E-03
-2.250E-01	157	2.88E-03
-2.750E-01	156	2.88E-03
-3.250E-01	155	2.88E-03
-3.750E-01	154	2.88E-03
-4.250E-01	153	2.88E-03
-4.750E-01	152	2.88E-03
-5.250E-01	151	2.88E-03

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-5.750E-01 150 2.88E-03
 -6.250E-01 149 2.88E-03
 -6.750E-01 148 2.88E-03
 -7.250E-01 147 2.88E-03
 -7.750E-01 146 2.88E-03
 -8.250E-01 145 2.88E-03
 -8.750E-01 144 2.88E-03
 -9.250E-01 143 2.88E-03
 -9.750E-01 142 2.88E-03
 -1.025E+00 141 2.88E-03
 -1.075E+00 140 2.88E-03
 -1.125E+00 139 2.88E-03
 -1.175E+00 138 2.88E-03
 -1.225E+00 137 2.88E-03
 -1.275E+00 136 2.88E-03
 -1.325E+00 135 2.88E-03
 -1.375E+00 134 2.88E-03
 -1.425E+00 133 2.88E-03
 -1.475E+00 132 2.88E-03
 -1.525E+00 131 2.88E-03
 -1.575E+00 130 2.88E-03
 -1.625E+00 129 2.88E-03
 -1.675E+00 128 2.88E-03
 -1.725E+00 127 2.88E-03
 -1.775E+00 126 2.88E-03
 -1.825E+00 125 2.88E-03
 -1.875E+00 124 2.88E-03
 -1.925E+00 123 2.88E-03
 -1.975E+00 122 2.88E-03
 -2.025E+00 121 2.88E-03
 -2.075E+00 120 2.88E-03
 -2.125E+00 119 2.88E-03
 -2.175E+00 118 2.88E-03
 -2.225E+00 117 2.88E-03
 -2.275E+00 116 2.88E-03
 -2.325E+00 115 2.88E-03
 -2.375E+00 114 2.88E-03
 -2.425E+00 113 2.88E-03
 -2.475E+00 112 2.88E-03
 -2.525E+00 111 2.88E-03
 -2.575E+00 110 2.88E-03
 -2.625E+00 109 2.88E-03
 -2.675E+00 108 2.88E-03
 -2.725E+00 107 2.88E-03
 -2.775E+00 106 2.88E-03
 -2.825E+00 105 2.88E-03
 -2.875E+00 104 2.88E-03
 -2.925E+00 103 2.88E-03
 -2.975E+00 102 2.88E-03
 -3.025E+00 101 2.88E-03
 -3.075E+00 100 2.88E-03

I = 2
 X = 5.00E-01

STEP	NO.	TIME	U	V	W	P	T	C	TIMESTEP	REF. VAR.	INDEX
400	3.0000E+01		0.000E+00	0.000E+00	-7.561E-12	-1.003E+02	2.884E-03	0.000E+00	1.2528E-02	8.527E-14	0.853E-09
[-REFERENCE VALUES AT NODE (2, 2,155) FOR REALI NO. 2-] [CONVERGENCE RATE / RESIDUALS]											
10	3.7734E-03		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	4.6540E-04	7.098E-05	0.710
20	9.9198E-03		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	7.5809E-04	1.116E-05	0.112
30	1.9932E-02		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	1.2348E-03	2.988E-05	0.299
40	3.6240E-02		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	2.0114E-03	6.388E-05	0.639
50	6.2804E-02		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	3.2764E-03	1.239E-05	0.124
60	1.0608E-01		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	5.3369E-03	2.017E-05	0.202
70	1.7656E-01		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	8.6933E-03	2.727E-05	0.273
80	2.9137E-01		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	1.4160E-02	7.712E-06	0.771E-01
90	4.7838E-01		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	2.3066E-02	5.659E-05	0.566
100	7.8301E-01		0.000E+00	0.000E+00	-6.318E-10	-1.003E+02	3.404E-02	0.000E+00	3.7572E-02	9.904E-05	0.990
110	1.2792E+00		0.000E+00	0.000E+00	-6.319E-10	-1.003E+02	3.404E-02	0.000E+00	6.1200E-02	9.942E-05	0.994
120	2.0875E+00		0.000E+00	0.000E+00	-2.429E-07	-8.562E+01	3.705E-02	0.000E+00	9.9689E-02	9.132E-05	0.913
130	3.0875E+00		0.000E+00	0.000E+00	-1.689E-02	-1.355E+00	3.791E-01	0.000E+00	1.0000E-01	5.728E-05	0.573

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140	4.0875E+00	0.000E+00	0.000E+00	-1.640E-02	-1.064E+00	4.459E-01	0.000E+00	1.0000E-01	8.987E-05	0.899
150	5.0875E+00	0.000E+00	0.000E+00	-1.691E-02	-9.671E-01	4.767E-01	0.000E+00	1.0000E-01	6.892E-05	0.689
160	6.0875E+00	0.000E+00	0.000E+00	-1.729E-02	-9.206E-01	4.937E-01	0.000E+00	1.0000E-01	9.530E-05	0.953
170	7.0875E+00	0.000E+00	0.000E+00	-1.753E-02	-8.956E-01	5.035E-01	0.000E+00	1.0000E-01	6.781E-05	0.678
180	8.0875E+00	0.000E+00	0.000E+00	-1.768E-02	-8.813E-01	5.094E-01	0.000E+00	1.0000E-01	8.476E-05	0.848
190	9.0875E+00	0.000E+00	0.000E+00	-1.777E-02	-8.729E-01	5.129E-01	0.000E+00	1.0000E-01	7.304E-05	0.730
200	1.0087E+01	0.000E+00	0.000E+00	-1.782E-02	-8.679E-01	5.150E-01	0.000E+00	1.0000E-01	6.423E-05	0.642
210	1.1087E+01	0.000E+00	0.000E+00	-1.785E-02	-8.649E-01	5.163E-01	0.000E+00	1.0000E-01	5.727E-05	0.573
220	1.2087E+01	0.000E+00	0.000E+00	-1.787E-02	-8.631E-01	5.171E-01	0.000E+00	1.0000E-01	5.155E-05	0.516
230	1.3087E+01	0.000E+00	0.000E+00	-1.788E-02	-8.620E-01	5.176E-01	0.000E+00	1.0000E-01	4.662E-05	0.466
240	1.4087E+01	0.000E+00	0.000E+00	-1.789E-02	-8.613E-01	5.179E-01	0.000E+00	1.0000E-01	4.244E-05	0.424
250	1.5087E+01	0.000E+00	0.000E+00	-1.789E-02	-8.609E-01	5.181E-01	0.000E+00	1.0000E-01	3.877E-05	0.388
260	1.6087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.606E-01	5.182E-01	0.000E+00	1.0000E-01	3.550E-05	0.355
270	1.7087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.605E-01	5.183E-01	0.000E+00	1.0000E-01	9.088E-05	0.909
280	1.8087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.604E-01	5.183E-01	0.000E+00	1.0000E-01	8.164E-05	0.816
290	1.9087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.183E-01	0.000E+00	1.0000E-01	7.353E-05	0.735
300	2.0087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.183E-01	0.000E+00	1.0000E-01	6.633E-05	0.663
310	2.1087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.183E-01	0.000E+00	1.0000E-01	5.996E-05	0.600
320	2.2087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.183E-01	0.000E+00	1.0000E-01	5.432E-05	0.543
330	2.3087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.184E-01	0.000E+00	1.0000E-01	4.935E-05	0.494
340	2.4087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.184E-01	0.000E+00	1.0000E-01	4.488E-05	0.449
350	2.5087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.184E-01	0.000E+00	1.0000E-01	4.092E-05	0.409
360	2.6087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.184E-01	0.000E+00	1.0000E-01	3.744E-05	0.374
370	2.7087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.184E-01	0.000E+00	1.0000E-01	3.436E-05	0.344
380	2.8087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.184E-01	0.000E+00	1.0000E-01	3.165E-05	0.317
390	2.9087E+01	0.000E+00	0.000E+00	-1.790E-02	-8.603E-01	5.184E-01	0.000E+00	1.0000E-01	2.926E-05	0.293
400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-8.602E-01	5.184E-01	0.000E+00	1.2528E-02	8.260E-05	0.826

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

----> WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT

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

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

----> WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD

<---- DATA SET NUMBER: 2 WRITTEN TO ARCHIVES ---->

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

----> WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 3 WRITTEN TO ARCHIVES ---->

400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-8.602E-01	5.184E-01	0.000E+00	1.2528E-02	8.260E-05	0.826
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-- REALIZATION 2W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -*-*

Z =	K =	
0.000E+00	162	-1.79E-02
-5.000E-02	161	-1.79E-02
-1.000E-01	160	-1.79E-02
-1.500E-01	159	-1.79E-02
-2.000E-01	158	-1.79E-02
-2.500E-01	157	-1.79E-02
-3.000E-01	156	-1.79E-02
-3.500E-01	155	-1.79E-02
-4.000E-01	154	-1.79E-02
-4.500E-01	153	-1.79E-02
-5.000E-01	152	-1.79E-02
-5.500E-01	151	-1.79E-02
-6.000E-01	150	-1.79E-02
-6.500E-01	149	-1.79E-02
-7.000E-01	148	-1.79E-02
-7.500E-01	147	-1.79E-02
-8.000E-01	146	-1.79E-02
-8.500E-01	145	-1.79E-02
-9.000E-01	144	-1.79E-02

-9.500E-01	143	-1.79E-02
-1.000E+00	142	-1.79E-02
-1.050E+00	141	-1.79E-02
-1.100E+00	140	-1.79E-02
-1.150E+00	139	-1.79E-02
-1.200E+00	138	-1.79E-02
-1.250E+00	137	-1.79E-02
-1.300E+00	136	-1.79E-02
-1.350E+00	135	-1.79E-02
-1.400E+00	134	-1.79E-02
-1.450E+00	133	-1.79E-02
-1.500E+00	132	-1.79E-02
-1.550E+00	131	-1.79E-02
-1.600E+00	130	-1.79E-02
-1.650E+00	129	-1.79E-02
-1.700E+00	128	-1.79E-02
-1.750E+00	127	-1.79E-02
-1.800E+00	126	-1.79E-02
-1.850E+00	125	-1.79E-02
-1.900E+00	124	-1.79E-02
-1.950E+00	123	-1.79E-02
-2.000E+00	122	-1.79E-02
-2.050E+00	121	-1.79E-02
-2.100E+00	120	-1.79E-02
-2.150E+00	119	-1.79E-02
-2.200E+00	118	-1.78E-02
-2.250E+00	117	-1.78E-02
-2.300E+00	116	-1.78E-02
-2.350E+00	115	-1.78E-02
-2.400E+00	114	-1.78E-02
-2.450E+00	113	-1.77E-02
-2.500E+00	112	-1.77E-02
-2.550E+00	111	-1.76E-02
-2.600E+00	110	-1.75E-02
-2.650E+00	109	-1.74E-02
-2.700E+00	108	-1.73E-02
-2.750E+00	107	-1.71E-02
-2.800E+00	106	-1.69E-02
-2.850E+00	105	-1.67E-02
-2.900E+00	104	-1.64E-02
-2.950E+00	103	-1.61E-02
-3.000E+00	102	-1.58E-02
-3.050E+00	101	-1.54E-02
-3.100E+00	100	-1.26E-03

I = 2
X = 5.00E-01

-- REALIZATION 2P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 --

Z =	K =	
2.500E-02	162	-5.10E-01
-2.500E-02	161	-5.60E-01
-7.500E-02	160	-6.10E-01
-1.250E-01	159	-6.60E-01
-1.750E-01	158	-7.10E-01
-2.250E-01	157	-7.60E-01
-2.750E-01	156	-8.10E-01
-3.250E-01	155	-8.60E-01
-3.750E-01	154	-9.10E-01
-4.250E-01	153	-9.60E-01
-4.750E-01	152	-1.01E+00
-5.250E-01	151	-1.06E+00
-5.750E-01	150	-1.11E+00
-6.250E-01	149	-1.16E+00
-6.750E-01	148	-1.21E+00
-7.250E-01	147	-1.26E+00
-7.750E-01	146	-1.31E+00
-8.250E-01	145	-1.36E+00
-8.750E-01	144	-1.41E+00
-9.250E-01	143	-1.46E+00
-9.750E-01	142	-1.51E+00
-1.025E+00	141	-1.56E+00
-1.075E+00	140	-1.61E+00
-1.125E+00	139	-1.66E+00

-1.175E+00	138	-1.71E+00
-1.225E+00	137	-1.76E+00
-1.275E+00	136	-1.81E+00
-1.325E+00	135	-1.86E+00
-1.375E+00	134	-1.91E+00
-1.425E+00	133	-1.96E+00
-1.475E+00	132	-2.01E+00
-1.525E+00	131	-2.06E+00
-1.575E+00	130	-2.11E+00
-1.625E+00	129	-2.16E+00
-1.675E+00	128	-2.21E+00
-1.725E+00	127	-2.26E+00
-1.775E+00	126	-2.31E+00
-1.825E+00	125	-2.36E+00
-1.875E+00	124	-2.41E+00
-1.925E+00	123	-2.46E+00
-1.975E+00	122	-2.51E+00
-2.025E+00	121	-2.56E+00
-2.075E+00	120	-2.61E+00
-2.125E+00	119	-2.66E+00
-2.175E+00	118	-2.71E+00
-2.225E+00	117	-2.77E+00
-2.275E+00	116	-2.82E+00
-2.325E+00	115	-2.87E+00
-2.375E+00	114	-2.92E+00
-2.425E+00	113	-2.97E+00
-2.475E+00	112	-3.03E+00
-2.525E+00	111	-3.08E+00
-2.575E+00	110	-3.14E+00
-2.625E+00	109	-3.20E+00
-2.675E+00	108	-3.26E+00
-2.725E+00	107	-3.32E+00
-2.775E+00	106	-3.39E+00
-2.825E+00	105	-3.47E+00
-2.875E+00	104	-3.56E+00
-2.925E+00	103	-3.67E+00
-2.975E+00	102	-3.82E+00
-3.025E+00	101	-4.07E+00
-3.075E+00	100	-4.95E+00

I = 2
X = 5.00E-01

- REALIZATION 2THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -*-*

Z =	K =	
2.500E-02	162	5.18E-01
-2.500E-02	161	5.18E-01
-7.500E-02	160	5.18E-01
-1.250E-01	159	5.18E-01
-1.750E-01	158	5.18E-01
-2.250E-01	157	5.18E-01
-2.750E-01	156	5.18E-01
-3.250E-01	155	5.18E-01
-3.750E-01	154	5.18E-01
-4.250E-01	153	5.18E-01
-4.750E-01	152	5.18E-01
-5.250E-01	151	5.18E-01
-5.750E-01	150	5.18E-01
-6.250E-01	149	5.18E-01
-6.750E-01	148	5.18E-01
-7.250E-01	147	5.18E-01
-7.750E-01	146	5.18E-01
-8.250E-01	145	5.18E-01
-8.750E-01	144	5.18E-01
-9.250E-01	143	5.18E-01
-9.750E-01	142	5.18E-01
-1.025E+00	141	5.18E-01
-1.075E+00	140	5.18E-01
-1.125E+00	139	5.18E-01
-1.175E+00	138	5.18E-01
-1.225E+00	137	5.18E-01
-1.275E+00	136	5.18E-01
-1.325E+00	135	5.18E-01
-1.375E+00	134	5.18E-01

-1.425E+00 133 5.18E-01
 -1.475E+00 132 5.18E-01
 -1.525E+00 131 5.18E-01
 -1.575E+00 130 5.18E-01
 -1.625E+00 129 5.18E-01
 -1.675E+00 128 5.18E-01
 -1.725E+00 127 5.18E-01
 -1.775E+00 126 5.18E-01
 -1.825E+00 125 5.18E-01
 -1.875E+00 124 5.18E-01
 -1.925E+00 123 5.18E-01
 -1.975E+00 122 5.18E-01
 -2.025E+00 121 5.18E-01
 -2.075E+00 120 5.17E-01
 -2.125E+00 119 5.17E-01
 -2.175E+00 118 5.17E-01
 -2.225E+00 117 5.16E-01
 -2.275E+00 116 5.16E-01
 -2.325E+00 115 5.15E-01
 -2.375E+00 114 5.14E-01
 -2.425E+00 113 5.13E-01
 -2.475E+00 112 5.11E-01
 -2.525E+00 111 5.09E-01
 -2.575E+00 110 5.06E-01
 -2.625E+00 109 5.03E-01
 -2.675E+00 108 4.99E-01
 -2.725E+00 107 4.93E-01
 -2.775E+00 106 4.85E-01
 -2.825E+00 105 4.76E-01
 -2.875E+00 104 4.62E-01
 -2.925E+00 103 4.44E-01
 -2.975E+00 102 4.18E-01
 -3.025E+00 101 3.76E-01
 -3.075E+00 100 2.79E-01

I = 2
 X = 5.00E-01

STEP NO.	TIME	U	V	W	P	T	C	TIMESTEP	REF. VAR.	INDEX
400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-8.942E-01	5.141E-01	0.000E+00	1.2528E-02	4.544E-05	0.454
[-REFERENCE VALUES AT NODE (2, 2,155) FOR REALI NO. 22--] [CONVERGENCE RATE / RESIDUALS]										
0	0.0000E+00	0.000E+00	0.000E+00	0.000E+00	-1.003E+02	1.000E+00	0.000E+00	2.8571E-04	4.544E-05	0.454
10	3.7734E-03	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	4.6540E-04	1.240E-05	0.124
20	9.9198E-03	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	7.5809E-04	2.927E-05	0.293
30	1.9932E-02	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	1.2348E-03	5.573E-05	0.557
40	3.6240E-02	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	2.0114E-03	8.832E-05	0.883
50	6.2804E-02	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	3.2764E-03	1.389E-05	0.139
60	1.0608E-01	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	5.3369E-03	1.799E-05	0.180
70	1.7656E-01	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	8.6933E-03	2.105E-05	0.211
80	2.9137E-01	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	1.4160E-02	2.227E-05	0.223
90	4.7838E-01	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	2.3066E-02	1.785E-05	0.179
100	7.8301E-01	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	3.7572E-02	8.539E-05	0.854
110	1.2792E+00	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	6.1200E-02	2.255E-06	0.226E-01
120	2.0875E+00	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	9.9689E-02	1.663E-05	0.166
130	3.0875E+00	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	1.0000E-01	4.103E-05	0.410
140	4.0875E+00	0.000E+00	0.000E+00	-2.231E-12	-1.003E+02	1.933E-02	0.000E+00	1.0000E-01	4.011E-05	0.401

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 0.1000 NEW TIMESTEP= 2.0000E-02

150	4.4785E+00	0.000E+00	0.000E+00	-2.233E-12	-1.003E+02	1.933E-02	0.000E+00	2.8142E-02	3.113E-05	0.311
160	4.8501E+00	0.000E+00	0.000E+00	-2.577E-12	-1.003E+02	1.933E-02	0.000E+00	4.5840E-02	2.713E-05	0.271
170	5.4555E+00	0.000E+00	0.000E+00	-2.385E-09	-7.128E+01	2.390E-02	0.000E+00	7.4669E-02	3.600E-05	0.360

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 0.1000 NEW TIMESTEP= 2.0000E-02

180	6.1518E+00	0.000E+00	0.000E+00	-3.789E-05	-9.019E-01	4.462E-01	0.000E+00	2.2050E-02	5.633E-05	0.563
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SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 3.4207E-02 NEW TIMESTEP= 6.8414E-03

190	6.3869E+00	0.000E+00	0.000E+00	-8.237E-04	-3.605E-01	9.711E-01	0.000E+00	7.1834E-03	1.623E-05	0.162
200	6.4818E+00	0.000E+00	0.000E+00	-2.002E-03	-3.040E-01	1.000E+00	0.000E+00	1.1701E-02	8.450E-05	0.845
210	6.6363E+00	0.000E+00	0.000E+00	-4.654E-03	-2.574E-01	1.000E+00	0.000E+00	1.9060E-02	2.785E-05	0.279

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220	6.8880E+00	0.000E+00	0.000E+00	-2.766E-02	-2.536E-01	1.000E+00	0.000E+00	3.1046E-02	2.062E-05	0.206
230	7.2981E+00	0.000E+00	0.000E+00	-8.977E-03	-3.439E-01	9.892E-01	0.000E+00	5.0571E-02	3.559E-05	0.356
240	7.9659E+00	0.000E+00	0.000E+00	-2.926E-02	-3.778E-01	9.475E-01	0.000E+00	8.2375E-02	9.921E-05	0.992

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 0.1000 NEW TIMESTEP= 2.0000E-02

250	8.7796E+00	0.000E+00	0.000E+00	-2.829E-02	-3.602E-01	9.715E-01	0.000E+00	2.1000E-02	1.970E-05	0.197
260	9.0570E+00	0.000E+00	0.000E+00	-1.969E-02	-3.948E-01	9.216E-01	0.000E+00	3.4207E-02	5.235E-05	0.524
270	9.5087E+00	0.000E+00	0.000E+00	-1.717E-02	-3.594E-01	9.724E-01	0.000E+00	5.5719E-02	5.195E-05	0.519
280	1.0245E+01	0.000E+00	0.000E+00	-1.616E-02	-3.884E-01	9.316E-01	0.000E+00	9.0761E-02	4.105E-05	0.410
290	1.1240E+01	0.000E+00	0.000E+00	-1.739E-02	-3.992E-01	9.146E-01	0.000E+00	1.0000E-01	4.907E-05	0.491
300	1.2240E+01	0.000E+00	0.000E+00	-1.777E-02	-4.033E-01	9.082E-01	0.000E+00	1.0000E-01	4.327E-05	0.433

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 0.1000 NEW TIMESTEP= 2.0000E-02

310	1.2631E+01	0.000E+00	0.000E+00	-1.810E-02	-4.031E-01	9.085E-01	0.000E+00	2.8142E-02	3.186E-05	0.319
320	1.3003E+01	0.000E+00	0.000E+00	-1.797E-02	-4.047E-01	9.059E-01	0.000E+00	4.5840E-02	8.649E-05	0.865

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 6.4502E-02 NEW TIMESTEP= 1.2900E-02

330	1.3386E+01	0.000E+00	0.000E+00	-1.789E-02	-4.041E-01	9.068E-01	0.000E+00	1.4934E-02	6.572E-05	0.657
340	1.3583E+01	0.000E+00	0.000E+00	-1.799E-02	-4.046E-01	9.061E-01	0.000E+00	2.4326E-02	4.031E-05	0.403
350	1.3904E+01	0.000E+00	0.000E+00	-1.793E-02	-4.051E-01	9.052E-01	0.000E+00	3.9624E-02	5.134E-05	0.513
360	1.4427E+01	0.000E+00	0.000E+00	-1.793E-02	-4.051E-01	9.052E-01	0.000E+00	6.4543E-02	7.285E-05	0.729

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 0.1000 NEW TIMESTEP= 2.0000E-02

370	1.5115E+01	0.000E+00	0.000E+00	-1.790E-02	-4.053E-01	9.049E-01	0.000E+00	2.1000E-02	3.823E-05	0.382
380	1.5393E+01	0.000E+00	0.000E+00	-1.791E-02	-4.054E-01	9.048E-01	0.000E+00	3.4207E-02	4.583E-06	0.458E-01
390	1.5845E+01	0.000E+00	0.000E+00	-1.790E-02	-4.055E-01	9.046E-01	0.000E+00	5.5719E-02	5.885E-05	0.588

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 7.4669E-02 NEW TIMESTEP= 1.4934E-02

400	1.6250E+01	0.000E+00	0.000E+00	-1.790E-02	-4.055E-01	9.046E-01	0.000E+00	1.8152E-02	3.808E-05	0.381
410	1.6490E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.045E-01	0.000E+00	2.9568E-02	1.576E-05	0.158
420	1.6881E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.045E-01	0.000E+00	4.8163E-02	9.419E-05	0.942
430	1.7517E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.045E-01	0.000E+00	7.8453E-02	9.749E-05	0.975
440	1.8472E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.045E-01	0.000E+00	1.0000E-01	8.635E-05	0.863
450	1.9472E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.045E-01	0.000E+00	1.0000E-01	9.493E-05	0.949
460	2.0472E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.045E-01	0.000E+00	1.0000E-01	4.774E-05	0.477

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 0.1000 NEW TIMESTEP= 2.0000E-02

470	2.0792E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	2.9549E-02	9.603E-05	0.960
480	2.1183E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	4.8132E-02	5.464E-05	0.546

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 6.4502E-02 NEW TIMESTEP= 1.2900E-02

490	2.1533E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	1.5681E-02	8.255E-05	0.825
500	2.1740E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	2.5542E-02	7.955E-05	0.796
510	2.2077E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	4.1605E-02	3.275E-05	0.328
520	2.2627E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	6.7770E-02	3.843E-05	0.384
530	2.3506E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	1.0000E-01	2.346E-05	0.235
540	2.4506E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	1.0000E-01	5.725E-05	0.573

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 0.1000 NEW TIMESTEP= 2.0000E-02

550	2.5193E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	2.3152E-02	4.873E-05	0.487
560	2.5498E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	3.7713E-02	3.613E-05	0.361
570	2.5996E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	6.1430E-02	5.152E-05	0.515

SOLUTION DID NOT CONVERGE. OLD TIMESTEP= 6.4502E-02 NEW TIMESTEP= 1.2900E-02

580	2.6159E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	2.0013E-02	2.689E-05	0.269
590	2.6423E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	3.2599E-02	1.745E-05	0.174
600	2.6853E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	5.3100E-02	5.356E-05	0.536
610	2.7555E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	8.6494E-02	7.091E-05	0.709
620	2.8541E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	1.0000E-01	5.133E-05	0.513
630	2.9541E+01	0.000E+00	0.000E+00	-1.790E-02	-4.056E-01	9.044E-01	0.000E+00	1.0000E-01	7.881E-05	0.788

????? EXECUTION STOPPED BECAUSE SOLUTION DOES NOT CONVERGE: CHECK TIME STEP SIZE AND MAT. PROPERTIES ??????

WHC-EP-0445

CONVERGENCE INDEX = 324.9

STEP NO.	TIME	[-REFERENCE VALUES AT NODE (2, 2,155) FOR REALI NO. 23--]					[CONVERGENCE RATE / RESIDUALS]			
		U	V	W	P	T	C	TIMESTEP	REF. VAR.	INDEX
0	0.0000E+00	0.000E+00	0.000E+00	0.000E+00	-1.003E+02	1.000E+00	0.000E+00	2.8571E-04	3.249E-02	325.
10	3.7734E-03	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	4.6540E-04	1.275E-05	0.127
20	9.9198E-03	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	7.5809E-04	2.537E-05	0.254
30	1.9932E-02	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	1.2348E-03	4.170E-05	0.417
40	3.6240E-02	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	2.0114E-03	5.890E-05	0.589
50	6.2804E-02	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	3.2764E-03	7.395E-05	0.740
60	1.0608E-01	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	5.3369E-03	7.923E-05	0.792
70	1.7656E-01	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	8.6933E-03	4.420E-05	0.442
80	2.9137E-01	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	1.4160E-02	9.332E-05	0.933
90	4.7838E-01	0.000E+00	0.000E+00	-3.955E-09	-1.003E+02	2.082E-02	0.000E+00	2.3066E-02	2.982E-05	0.298
100	7.8301E-01	0.000E+00	0.000E+00	-5.662E-08	-9.967E+01	2.093E-02	0.000E+00	3.7572E-02	2.706E-05	0.271
110	1.2792E+00	0.000E+00	0.000E+00	-9.186E-03	-5.632E+00	2.008E-01	0.000E+00	6.1200E-02	8.274E-05	0.827
120	2.0875E+00	0.000E+00	0.000E+00	-1.482E-02	-3.705E+00	2.811E-01	0.000E+00	9.9689E-02	9.698E-05	0.970
130	3.0875E+00	0.000E+00	0.000E+00	-1.611E-02	-3.066E+00	3.272E-01	0.000E+00	1.0000E-01	4.604E-05	0.460
140	4.0875E+00	0.000E+00	0.000E+00	-1.673E-02	-2.777E+00	3.542E-01	0.000E+00	1.0000E-01	4.987E-05	0.499
150	5.0875E+00	0.000E+00	0.000E+00	-1.709E-02	-2.611E+00	3.719E-01	0.000E+00	1.0000E-01	4.493E-05	0.449
160	6.0875E+00	0.000E+00	0.000E+00	-1.732E-02	-2.506E+00	3.842E-01	0.000E+00	1.0000E-01	9.038E-05	0.904
170	7.0875E+00	0.000E+00	0.000E+00	-1.748E-02	-2.435E+00	3.931E-01	0.000E+00	1.0000E-01	6.658E-05	0.666
180	8.0875E+00	0.000E+00	0.000E+00	-1.759E-02	-2.386E+00	3.995E-01	0.000E+00	1.0000E-01	5.558E-05	0.556
190	9.0875E+00	0.000E+00	0.000E+00	-1.767E-02	-2.350E+00	4.043E-01	0.000E+00	1.0000E-01	9.797E-05	0.980
200	1.0087E+01	0.000E+00	0.000E+00	-1.772E-02	-2.324E+00	4.078E-01	0.000E+00	1.0000E-01	9.588E-05	0.959
210	1.1087E+01	0.000E+00	0.000E+00	-1.777E-02	-2.305E+00	4.105E-01	0.000E+00	1.0000E-01	9.982E-05	0.998
220	1.2087E+01	0.000E+00	0.000E+00	-1.780E-02	-2.290E+00	4.125E-01	0.000E+00	1.0000E-01	7.715E-05	0.771
230	1.3087E+01	0.000E+00	0.000E+00	-1.782E-02	-2.280E+00	4.140E-01	0.000E+00	1.0000E-01	9.246E-05	0.925
240	1.4087E+01	0.000E+00	0.000E+00	-1.784E-02	-2.271E+00	4.152E-01	0.000E+00	1.0000E-01	7.029E-05	0.703
250	1.5087E+01	0.000E+00	0.000E+00	-1.786E-02	-2.265E+00	4.161E-01	0.000E+00	1.0000E-01	8.532E-05	0.853
260	1.6087E+01	0.000E+00	0.000E+00	-1.787E-02	-2.261E+00	4.168E-01	0.000E+00	1.0000E-01	6.819E-05	0.682
270	1.7087E+01	0.000E+00	0.000E+00	-1.787E-02	-2.257E+00	4.173E-01	0.000E+00	1.0000E-01	7.839E-05	0.784
280	1.8087E+01	0.000E+00	0.000E+00	-1.788E-02	-2.254E+00	4.177E-01	0.000E+00	1.0000E-01	7.013E-05	0.701
290	1.9087E+01	0.000E+00	0.000E+00	-1.788E-02	-2.252E+00	4.180E-01	0.000E+00	1.0000E-01	7.014E-05	0.701
300	2.0087E+01	0.000E+00	0.000E+00	-1.789E-02	-2.251E+00	4.182E-01	0.000E+00	1.0000E-01	7.681E-05	0.768
310	2.1087E+01	0.000E+00	0.000E+00	-1.789E-02	-2.250E+00	4.184E-01	0.000E+00	1.0000E-01	6.011E-05	0.601
320	2.2087E+01	0.000E+00	0.000E+00	-1.789E-02	-2.249E+00	4.185E-01	0.000E+00	1.0000E-01	8.939E-05	0.894
330	2.3087E+01	0.000E+00	0.000E+00	-1.789E-02	-2.248E+00	4.186E-01	0.000E+00	1.0000E-01	4.908E-05	0.491
340	2.4087E+01	0.000E+00	0.000E+00	-1.790E-02	-2.247E+00	4.187E-01	0.000E+00	1.0000E-01	8.944E-05	0.894
350	2.5087E+01	0.000E+00	0.000E+00	-1.790E-02	-2.247E+00	4.187E-01	0.000E+00	1.0000E-01	3.852E-05	0.385
360	2.6087E+01	0.000E+00	0.000E+00	-1.790E-02	-2.247E+00	4.188E-01	0.000E+00	1.0000E-01	4.502E-05	0.450
370	2.7087E+01	0.000E+00	0.000E+00	-1.790E-02	-2.246E+00	4.188E-01	0.000E+00	1.0000E-01	8.775E-05	0.878
380	2.8087E+01	0.000E+00	0.000E+00	-1.790E-02	-2.246E+00	4.188E-01	0.000E+00	1.0000E-01	5.518E-05	0.552
390	2.9087E+01	0.000E+00	0.000E+00	-1.790E-02	-2.246E+00	4.189E-01	0.000E+00	1.0000E-01	6.598E-05	0.660
400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-2.246E+00	4.189E-01	0.000E+00	1.2528E-02	2.135E-05	0.214

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

----> WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT

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

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

----> WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD

<---- DATA SET NUMBER: 2 WRITTEN TO ARCHIVES ---->

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

----> WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 3 WRITTEN TO ARCHIVES ---->

400 3.0000E+01 0.000E+00 0.000E+00 -1.790E-02 -2.246E+00 4.189E-01 0.000E+00 1.2528E-02 2.135E-05 0.214

-- REALIZATION 23W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 --
 Z = K =
 0.000E+00 162 -1.79E-02

-5.000E-02	161	-1.79E-02
-1.000E-01	160	-1.79E-02
-1.500E-01	159	-1.79E-02
-2.000E-01	158	-1.79E-02
-2.500E-01	157	-1.79E-02
-3.000E-01	156	-1.79E-02
-3.500E-01	155	-1.79E-02
-4.000E-01	154	-1.79E-02
-4.500E-01	153	-1.79E-02
-5.000E-01	152	-1.79E-02
-5.500E-01	151	-1.79E-02
-6.000E-01	150	-1.79E-02
-6.500E-01	149	-1.79E-02
-7.000E-01	148	-1.79E-02
-7.500E-01	147	-1.79E-02
-8.000E-01	146	-1.79E-02
-8.500E-01	145	-1.79E-02
-9.000E-01	144	-1.79E-02
-9.500E-01	143	-1.79E-02
-1.000E+00	142	-1.79E-02
-1.050E+00	141	-1.79E-02
-1.100E+00	140	-1.79E-02
-1.150E+00	139	-1.79E-02
-1.200E+00	138	-1.79E-02
-1.250E+00	137	-1.79E-02
-1.300E+00	136	-1.79E-02
-1.350E+00	135	-1.79E-02
-1.400E+00	134	-1.79E-02
-1.450E+00	133	-1.79E-02
-1.500E+00	132	-1.79E-02
-1.550E+00	131	-1.79E-02
-1.600E+00	130	-1.79E-02
-1.650E+00	129	-1.79E-02
-1.700E+00	128	-1.79E-02
-1.750E+00	127	-1.79E-02
-1.800E+00	126	-1.79E-02
-1.850E+00	125	-1.79E-02
-1.900E+00	124	-1.79E-02
-1.950E+00	123	-1.79E-02
-2.000E+00	122	-1.79E-02
-2.050E+00	121	-1.79E-02
-2.100E+00	120	-1.79E-02
-2.150E+00	119	-1.79E-02
-2.200E+00	118	-1.79E-02
-2.250E+00	117	-1.79E-02
-2.300E+00	116	-1.79E-02
-2.350E+00	115	-1.79E-02
-2.400E+00	114	-1.78E-02
-2.450E+00	113	-1.78E-02
-2.500E+00	112	-1.78E-02
-2.550E+00	111	-1.78E-02
-2.600E+00	110	-1.78E-02
-2.650E+00	109	-1.78E-02
-2.700E+00	108	-1.78E-02
-2.750E+00	107	-1.78E-02
-2.800E+00	106	-1.78E-02
-2.850E+00	105	-1.78E-02
-2.900E+00	104	-1.78E-02
-2.950E+00	103	-1.78E-02
-3.000E+00	102	-1.78E-02
-3.050E+00	101	-1.78E-02
-3.100E+00	100	-1.77E-02

I = 2
X = 5.00E-01

**-- REALIZATION 23P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 **--

Z =	K =	
2.500E-02	162	-1.90E+00
-2.500E-02	161	-1.95E+00
-7.500E-02	160	-2.00E+00
-1.250E-01	159	-2.05E+00
-1.750E-01	158	-2.10E+00
-2.250E-01	157	-2.15E+00

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-2.750E-01	156	-2.20E+00
-3.250E-01	155	-2.25E+00
-3.750E-01	154	-2.30E+00
-4.250E-01	153	-2.35E+00
-4.750E-01	152	-2.40E+00
-5.250E-01	151	-2.45E+00
-5.750E-01	150	-2.50E+00
-6.250E-01	149	-2.55E+00
-6.750E-01	148	-2.60E+00
-7.250E-01	147	-2.65E+00
-7.750E-01	146	-2.70E+00
-8.250E-01	145	-2.75E+00
-8.750E-01	144	-2.80E+00
-9.250E-01	143	-2.85E+00
-9.750E-01	142	-2.90E+00
-1.025E+00	141	-2.95E+00
-1.075E+00	140	-3.00E+00
-1.125E+00	139	-3.05E+00
-1.175E+00	138	-3.10E+00
-1.225E+00	137	-3.15E+00
-1.275E+00	136	-3.20E+00
-1.325E+00	135	-3.25E+00
-1.375E+00	134	-3.30E+00
-1.425E+00	133	-3.35E+00
-1.475E+00	132	-3.40E+00
-1.525E+00	131	-3.45E+00
-1.575E+00	130	-3.50E+00
-1.625E+00	129	-3.55E+00
-1.675E+00	128	-3.60E+00
-1.725E+00	127	-3.65E+00
-1.775E+00	126	-3.70E+00
-1.825E+00	125	-3.75E+00
-1.875E+00	124	-3.80E+00
-1.925E+00	123	-3.85E+00
-1.975E+00	122	-3.90E+00
-2.025E+00	121	-3.95E+00
-2.075E+00	120	-4.00E+00
-2.125E+00	119	-4.05E+00
-2.175E+00	118	-4.10E+00
-2.225E+00	117	-4.15E+00
-2.275E+00	116	-4.20E+00
-2.325E+00	115	-4.25E+00
-2.375E+00	114	-4.31E+00
-2.425E+00	113	-4.36E+00
-2.475E+00	112	-4.41E+00
-2.525E+00	111	-4.46E+00
-2.575E+00	110	-4.51E+00
-2.625E+00	109	-4.56E+00
-2.675E+00	108	-4.61E+00
-2.725E+00	107	-4.66E+00
-2.775E+00	106	-4.71E+00
-2.825E+00	105	-4.77E+00
-2.875E+00	104	-4.82E+00
-2.925E+00	103	-4.87E+00
-2.975E+00	102	-4.92E+00
-3.025E+00	101	-4.97E+00
-3.075E+00	100	-5.02E+00

I = 2
X = 5.00E-01

-- REALIZATION 23THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 --

Z =	K =	
2.500E-02	162	4.19E-01
-2.500E-02	161	4.19E-01
-7.500E-02	160	4.19E-01
-1.250E-01	159	4.19E-01
-1.750E-01	158	4.19E-01
-2.250E-01	157	4.19E-01
-2.750E-01	156	4.19E-01
-3.250E-01	155	4.19E-01
-3.750E-01	154	4.19E-01
-4.250E-01	153	4.19E-01
-4.750E-01	152	4.19E-01

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-5.250E-01 151 4.19E-01
 -5.750E-01 150 4.19E-01
 -6.250E-01 149 4.19E-01
 -6.750E-01 148 4.19E-01
 -7.250E-01 147 4.19E-01
 -7.750E-01 146 4.19E-01
 -8.250E-01 145 4.19E-01
 -8.750E-01 144 4.19E-01
 -9.250E-01 143 4.19E-01
 -9.750E-01 142 4.19E-01
 -1.025E+00 141 4.19E-01
 -1.075E+00 140 4.19E-01
 -1.125E+00 139 4.19E-01
 -1.175E+00 138 4.19E-01
 -1.225E+00 137 4.19E-01
 -1.275E+00 136 4.19E-01
 -1.325E+00 135 4.19E-01
 -1.375E+00 134 4.19E-01
 -1.425E+00 133 4.19E-01
 -1.475E+00 132 4.19E-01
 -1.525E+00 131 4.19E-01
 -1.575E+00 130 4.19E-01
 -1.625E+00 129 4.19E-01
 -1.675E+00 128 4.18E-01
 -1.725E+00 127 4.18E-01
 -1.775E+00 126 4.18E-01
 -1.825E+00 125 4.18E-01
 -1.875E+00 124 4.18E-01
 -1.925E+00 123 4.18E-01
 -1.975E+00 122 4.18E-01
 -2.025E+00 121 4.18E-01
 -2.075E+00 120 4.18E-01
 -2.125E+00 119 4.18E-01
 -2.175E+00 118 4.18E-01
 -2.225E+00 117 4.18E-01
 -2.275E+00 116 4.18E-01
 -2.325E+00 115 4.18E-01
 -2.375E+00 114 4.18E-01
 -2.425E+00 113 4.17E-01
 -2.475E+00 112 4.17E-01
 -2.525E+00 111 4.17E-01
 -2.575E+00 110 4.17E-01
 -2.625E+00 109 4.17E-01
 -2.675E+00 108 4.17E-01
 -2.725E+00 107 4.17E-01
 -2.775E+00 106 4.16E-01
 -2.825E+00 105 4.16E-01
 -2.875E+00 104 4.16E-01
 -2.925E+00 103 4.16E-01
 -2.975E+00 102 4.15E-01
 -3.025E+00 101 4.15E-01
 -3.075E+00 100 4.15E-01

I = 2
 X = 5.00E-01

STEP NO.	TIME	U	V	W	P	T	C	TIMESTEP	REF. VAR.	RESIDUALS INDEX
400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-6.888E-01	6.290E-01	0.000E+00	1.2528E-02	3.351E-05	0.335
[-REFERENCE VALUES AT NODE (2, 2,155) FOR REALI NO. 49--] [CONVERGENCE RATE / RESIDUALS]										
10	3.7734E-03	0.000E+00	0.000E+00	0.000E+00	-1.003E+02	1.000E+00	0.000E+00	2.8571E-04	3.351E-05	0.335
20	9.9198E-03	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	4.6540E-04	8.083E-05	0.808
30	1.9932E-02	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	7.5809E-04	1.319E-05	0.132
40	3.6240E-02	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	1.2348E-03	3.536E-05	0.354
50	6.2804E-02	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	2.0114E-03	7.568E-05	0.757
60	1.0608E-01	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	3.2764E-03	1.523E-05	0.152
70	1.7656E-01	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	5.3369E-03	2.479E-05	0.248
80	2.9137E-01	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	8.6933E-03	3.426E-05	0.343
90	4.7838E-01	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	1.4160E-02	3.979E-05	0.398
100	7.8301E-01	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	2.3066E-02	2.208E-05	0.221
110	1.2792E+00	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	3.7572E-02	2.259E-05	0.226
120	2.0875E+00	0.000E+00	0.000E+00	-1.026E-10	-1.003E+02	3.373E-02	0.000E+00	6.1200E-02	8.510E-05	0.851
130	3.0875E+00	0.000E+00	0.000E+00	-2.254E-08	-9.101E+01	3.544E-02	0.000E+00	9.9689E-02	2.698E-05	0.270
								1.0000E-01	9.307E-05	0.931

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140	4.0875E+00	0.000E+00	0.000E+00	-4.931E-03	-6.716E-01	5.491E-01	0.000E+00	1.0000E-01	8.480E-05	0.848
150	5.0875E+00	0.000E+00	0.000E+00	-1.871E-02	-6.268E-01	5.814E-01	0.000E+00	1.0000E-01	4.750E-05	0.475
160	6.0875E+00	0.000E+00	0.000E+00	-1.717E-02	-6.061E-01	5.981E-01	0.000E+00	1.0000E-01	1.417E-05	0.142
170	7.0875E+00	0.000E+00	0.000E+00	-1.775E-02	-5.939E-01	6.086E-01	0.000E+00	1.0000E-01	5.685E-05	0.569
180	8.0875E+00	0.000E+00	0.000E+00	-1.781E-02	-5.901E-01	6.120E-01	0.000E+00	1.0000E-01	2.185E-05	0.219
190	9.0875E+00	0.000E+00	0.000E+00	-1.785E-02	-5.876E-01	6.142E-01	0.000E+00	1.0000E-01	6.270E-05	0.627
200	1.0087E+01	0.000E+00	0.000E+00	-1.788E-02	-5.867E-01	6.151E-01	0.000E+00	1.0000E-01	4.037E-05	0.404
210	1.1087E+01	0.000E+00	0.000E+00	-1.789E-02	-5.861E-01	6.155E-01	0.000E+00	1.0000E-01	8.265E-05	0.827
220	1.2087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.859E-01	6.157E-01	0.000E+00	1.0000E-01	2.292E-05	0.229
230	1.3087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.858E-01	6.159E-01	0.000E+00	1.0000E-01	2.980E-05	0.298
240	1.4087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	5.101E-05	0.510
250	1.5087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	3.972E-05	0.397
260	1.6087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	6.256E-05	0.626
270	1.7087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	1.696E-05	0.170
280	1.8087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	8.680E-05	0.868
290	1.9087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	9.533E-05	0.953
300	2.0087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	9.798E-05	0.980
310	2.1087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.159E-01	0.000E+00	1.0000E-01	7.427E-05	0.743
320	2.2087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	8.154E-05	0.815
330	2.3087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	6.867E-05	0.687
340	2.4087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	6.723E-05	0.672
350	2.5087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	8.134E-05	0.813
360	2.6087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	6.071E-05	0.607
370	2.7087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	8.727E-06	0.873E-01
380	2.8087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	8.822E-05	0.882
390	2.9087E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.0000E-01	2.025E-05	0.203
400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.2528E-02	4.837E-05	0.484

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

----> WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT

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

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

----> WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD

<---- DATA SET NUMBER: 2 WRITTEN TO ARCHIVES ---->

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

----> WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 3 WRITTEN TO ARCHIVES ---->

400 3.0000E+01 0.000E+00 0.000E+00 -1.790E-02 -5.857E-01 6.160E-01 0.000E+00 1.2528E-02 4.837E-05 0.484

- REALIZATION 49W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -**

Z =	K =	
0.000E+00	162	-1.79E-02
-5.000E-02	161	-1.79E-02
-1.000E-01	160	-1.79E-02
-1.500E-01	159	-1.79E-02
-2.000E-01	158	-1.79E-02
-2.500E-01	157	-1.79E-02
-3.000E-01	156	-1.79E-02
-3.500E-01	155	-1.79E-02
-4.000E-01	154	-1.79E-02
-4.500E-01	153	-1.79E-02
-5.000E-01	152	-1.79E-02
-5.500E-01	151	-1.79E-02
-6.000E-01	150	-1.79E-02
-6.500E-01	149	-1.79E-02
-7.000E-01	148	-1.79E-02
-7.500E-01	147	-1.79E-02
-8.000E-01	146	-1.79E-02
-8.500E-01	145	-1.79E-02
-9.000E-01	144	-1.79E-02

-9.500E-01	143	-1.79E-02
-1.000E+00	142	-1.79E-02
-1.050E+00	141	-1.79E-02
-1.100E+00	140	-1.79E-02
-1.150E+00	139	-1.79E-02
-1.200E+00	138	-1.79E-02
-1.250E+00	137	-1.79E-02
-1.300E+00	136	-1.79E-02
-1.350E+00	135	-1.79E-02
-1.400E+00	134	-1.79E-02
-1.450E+00	133	-1.79E-02
-1.500E+00	132	-1.79E-02
-1.550E+00	131	-1.79E-02
-1.600E+00	130	-1.79E-02
-1.650E+00	129	-1.79E-02
-1.700E+00	128	-1.79E-02
-1.750E+00	127	-1.79E-02
-1.800E+00	126	-1.79E-02
-1.850E+00	125	-1.79E-02
-1.900E+00	124	-1.79E-02
-1.950E+00	123	-1.78E-02
-2.000E+00	122	-1.78E-02
-2.050E+00	121	-1.77E-02
-2.100E+00	120	-1.77E-02
-2.150E+00	119	-1.77E-02
-2.200E+00	118	-1.78E-02
-2.250E+00	117	-1.87E-02
-2.300E+00	116	-2.15E-02
-2.350E+00	115	-2.81E-04
-2.400E+00	114	-3.42E-08
-2.450E+00	113	-1.07E-10
-2.500E+00	112	-1.03E-10
-2.550E+00	111	-1.03E-10
-2.600E+00	110	-1.03E-10
-2.650E+00	109	-1.03E-10
-2.700E+00	108	-1.03E-10
-2.750E+00	107	-1.03E-10
-2.800E+00	106	-1.03E-10
-2.850E+00	105	-1.03E-10
-2.900E+00	104	-1.03E-10
-2.950E+00	103	-1.03E-10
-3.000E+00	102	-1.03E-10
-3.050E+00	101	-1.03E-10
-3.100E+00	100	-1.03E-10

I = 2
X = 5.00E-01

-- REALIZATION 49P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -*-*

Z =	K =	
2.500E-02	162	-2.36E-01
-2.500E-02	161	-2.86E-01
-7.500E-02	160	-3.36E-01
-1.250E-01	159	-3.86E-01
-1.750E-01	158	-4.36E-01
-2.250E-01	157	-4.86E-01
-2.750E-01	156	-5.36E-01
-3.250E-01	155	-5.86E-01
-3.750E-01	154	-6.36E-01
-4.250E-01	153	-6.86E-01
-4.750E-01	152	-7.36E-01
-5.250E-01	151	-7.86E-01
-5.750E-01	150	-8.36E-01
-6.250E-01	149	-8.86E-01
-6.750E-01	148	-9.36E-01
-7.250E-01	147	-9.86E-01
-7.750E-01	146	-1.04E+00
-8.250E-01	145	-1.09E+00
-8.750E-01	144	-1.14E+00
-9.250E-01	143	-1.19E+00
-9.750E-01	142	-1.24E+00
-1.025E+00	141	-1.29E+00
-1.075E+00	140	-1.34E+00
-1.125E+00	139	-1.39E+00

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-1.175E+00	138	-1.44E+00
-1.225E+00	137	-1.49E+00
-1.275E+00	136	-1.54E+00
-1.325E+00	135	-1.59E+00
-1.375E+00	134	-1.64E+00
-1.425E+00	133	-1.69E+00
-1.475E+00	132	-1.74E+00
-1.525E+00	131	-1.79E+00
-1.575E+00	130	-1.84E+00
-1.625E+00	129	-1.89E+00
-1.675E+00	128	-1.94E+00
-1.725E+00	127	-1.99E+00
-1.775E+00	126	-2.04E+00
-1.825E+00	125	-2.09E+00
-1.875E+00	124	-2.14E+00
-1.925E+00	123	-2.19E+00
-1.975E+00	122	-2.24E+00
-2.025E+00	121	-2.29E+00
-2.075E+00	120	-2.34E+00
-2.125E+00	119	-2.40E+00
-2.175E+00	118	-2.46E+00
-2.225E+00	117	-2.53E+00
-2.275E+00	116	-2.62E+00
-2.325E+00	115	-3.55E+00
-2.375E+00	114	-8.92E+01
-2.425E+00	113	-1.02E+02
-2.475E+00	112	-1.02E+02
-2.525E+00	111	-1.03E+02
-2.575E+00	110	-1.03E+02
-2.625E+00	109	-1.03E+02
-2.675E+00	108	-1.03E+02
-2.725E+00	107	-1.03E+02
-2.775E+00	106	-1.03E+02
-2.825E+00	105	-1.03E+02
-2.875E+00	104	-1.03E+02
-2.925E+00	103	-1.03E+02
-2.975E+00	102	-1.03E+02
-3.025E+00	101	-1.03E+02
-3.075E+00	100	-1.03E+02

I = 2
X = 5.00E-01

-- REALIZATION 49THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 --

Z =	K =	
2.500E-02	162	6.16E-01
-2.500E-02	161	6.16E-01
-7.500E-02	160	6.16E-01
-1.250E-01	159	6.16E-01
-1.750E-01	158	6.16E-01
-2.250E-01	157	6.16E-01
-2.750E-01	156	6.16E-01
-3.250E-01	155	6.16E-01
-3.750E-01	154	6.16E-01
-4.250E-01	153	6.16E-01
-4.750E-01	152	6.16E-01
-5.250E-01	151	6.16E-01
-5.750E-01	150	6.16E-01
-6.250E-01	149	6.16E-01
-6.750E-01	148	6.16E-01
-7.250E-01	147	6.16E-01
-7.750E-01	146	6.16E-01
-8.250E-01	145	6.16E-01
-8.750E-01	144	6.16E-01
-9.250E-01	143	6.16E-01
-9.750E-01	142	6.16E-01
-1.025E+00	141	6.16E-01
-1.075E+00	140	6.16E-01
-1.125E+00	139	6.16E-01
-1.175E+00	138	6.16E-01
-1.225E+00	137	6.16E-01
-1.275E+00	136	6.16E-01
-1.325E+00	135	6.16E-01
-1.375E+00	134	6.16E-01

-1.425E+00 133 6.16E-01
 -1.475E+00 132 6.16E-01
 -1.525E+00 131 6.16E-01
 -1.575E+00 130 6.16E-01
 -1.625E+00 129 6.16E-01
 -1.675E+00 128 6.16E-01
 -1.725E+00 127 6.16E-01
 -1.775E+00 126 6.15E-01
 -1.825E+00 125 6.15E-01
 -1.875E+00 124 6.15E-01
 -1.925E+00 123 6.14E-01
 -1.975E+00 122 6.13E-01
 -2.025E+00 121 6.11E-01
 -2.075E+00 120 6.09E-01
 -2.125E+00 119 6.04E-01
 -2.175E+00 118 5.96E-01
 -2.225E+00 117 5.81E-01
 -2.275E+00 116 5.49E-01
 -2.325E+00 115 3.06E-01
 -2.375E+00 114 3.62E-02
 -2.425E+00 113 3.37E-02
 -2.475E+00 112 3.37E-02
 -2.525E+00 111 3.37E-02
 -2.575E+00 110 3.37E-02
 -2.625E+00 109 3.37E-02
 -2.675E+00 108 3.37E-02
 -2.725E+00 107 3.37E-02
 -2.775E+00 106 3.37E-02
 -2.825E+00 105 3.37E-02
 -2.875E+00 104 3.37E-02
 -2.925E+00 103 3.37E-02
 -2.975E+00 102 3.37E-02
 -3.025E+00 101 3.37E-02
 -3.075E+00 100 3.37E-02

I = 2
 X = 5.00E-01

STEP NO.	TIME	U	V	W	P	T	C	TIMESTEP	CONVERGENCE RATE	RESIDUALS INDEX
400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-5.857E-01	6.160E-01	0.000E+00	1.2528E-02	4.837E-05	0.484
10	3.7734E-03	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	4.6540E-04	1.788E-05	0.179
20	9.9198E-03	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	7.5809E-04	4.045E-05	0.404
30	1.9932E-02	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	1.2348E-03	7.416E-05	0.742
40	3.6240E-02	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	2.0114E-03	1.281E-05	0.128
50	6.2804E-02	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	3.2764E-03	1.845E-05	0.184
60	1.0608E-01	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	5.3369E-03	2.339E-05	0.234
70	1.7656E-01	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	8.6933E-03	2.668E-05	0.267
80	2.9137E-01	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	1.4160E-02	2.376E-05	0.238
90	4.7838E-01	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	2.3066E-02	2.793E-05	0.279
100	7.8301E-01	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	3.7572E-02	1.800E-05	0.180
110	1.2792E+00	0.000E+00	0.000E+00	-6.122E-11	-1.003E+02	2.508E-02	0.000E+00	6.1200E-02	9.604E-05	0.960
120	2.0875E+00	0.000E+00	0.000E+00	-7.234E-11	-1.003E+02	2.508E-02	0.000E+00	9.9689E-02	6.481E-05	0.648
130	3.0875E+00	0.000E+00	0.000E+00	-1.726E-04	-1.878E+00	2.801E-01	0.000E+00	1.0000E-01	6.809E-05	0.681
140	4.0875E+00	0.000E+00	0.000E+00	-1.523E-02	-6.710E-01	6.082E-01	0.000E+00	1.0000E-01	5.526E-05	0.553
150	5.0875E+00	0.000E+00	0.000E+00	-1.694E-02	-6.554E-01	6.203E-01	0.000E+00	1.0000E-01	3.302E-05	0.330
160	6.0875E+00	0.000E+00	0.000E+00	-1.783E-02	-6.399E-01	6.329E-01	0.000E+00	1.0000E-01	4.413E-05	0.441
170	7.0875E+00	0.000E+00	0.000E+00	-1.779E-02	-6.317E-01	6.398E-01	0.000E+00	1.0000E-01	8.502E-05	0.850
180	8.0875E+00	0.000E+00	0.000E+00	-1.783E-02	-6.286E-01	6.424E-01	0.000E+00	1.0000E-01	6.193E-05	0.619
190	9.0875E+00	0.000E+00	0.000E+00	-1.788E-02	-6.271E-01	6.437E-01	0.000E+00	1.0000E-01	5.733E-05	0.573
200	1.0087E+01	0.000E+00	0.000E+00	-1.789E-02	-6.263E-01	6.444E-01	0.000E+00	1.0000E-01	6.098E-05	0.610
210	1.1087E+01	0.000E+00	0.000E+00	-1.789E-02	-6.260E-01	6.447E-01	0.000E+00	1.0000E-01	4.844E-05	0.484
220	1.2087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.258E-01	6.449E-01	0.000E+00	1.0000E-01	4.731E-05	0.473
230	1.3087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.257E-01	6.449E-01	0.000E+00	1.0000E-01	6.235E-05	0.623
240	1.4087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.257E-01	6.450E-01	0.000E+00	1.0000E-01	2.994E-05	0.299
250	1.5087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.257E-01	6.450E-01	0.000E+00	1.0000E-01	1.845E-05	0.185
260	1.6087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.257E-01	6.450E-01	0.000E+00	1.0000E-01	7.786E-05	0.779
270	1.7087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.257E-01	6.450E-01	0.000E+00	1.0000E-01	9.414E-05	0.941
280	1.8087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.257E-01	6.450E-01	0.000E+00	1.0000E-01	7.882E-05	0.788
290	1.9087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	5.332E-05	0.533
300	2.0087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	7.572E-05	0.757
310	2.1087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	6.700E-05	0.670

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320	2.2087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	8.328E-05	0.833
330	2.3087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	3.458E-05	0.346
340	2.4087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	1.012E-05	0.101
350	2.5087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	4.862E-05	0.486
360	2.6087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	8.340E-05	0.834
370	2.7087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	5.053E-05	0.505
380	2.8087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	4.931E-05	0.493
390	2.9087E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.0000E-01	3.873E-05	0.387
400	3.0000E+01	0.000E+00	0.000E+00	-1.790E-02	-6.256E-01	6.450E-01	0.000E+00	1.2528E-02	5.444E-05	0.544

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

----> WRITING VARIABLE: W - Z-DIR. VELOCITY COMPONENT

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

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

----> WRITING VARIABLE: P - PRESSURE OR PRESSURE HEAD

<---- DATA SET NUMBER: 2 WRITTEN TO ARCHIVES ---->

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

----> WRITING VARIABLE: THET- RELATIVE SATURATION LEVEL

<---- DATA SET NUMBER: 3 WRITTEN TO ARCHIVES ---->

400 3.0000E+01 0.000E+00 0.000E+00 -1.790E-02 -6.256E-01 6.450E-01 0.000E+00
 1.2528E-02 5.444E-05 0.544

- REALIZATION 50W - Z-DIR. VELOCITY COMPONENT FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -**

Z =	K =	
0.000E+00	162	-1.79E-02
-5.000E-02	161	-1.79E-02
-1.000E-01	160	-1.79E-02
-1.500E-01	159	-1.79E-02
-2.000E-01	158	-1.79E-02
-2.500E-01	157	-1.79E-02
-3.000E-01	156	-1.79E-02
-3.500E-01	155	-1.79E-02
-4.000E-01	154	-1.79E-02
-4.500E-01	153	-1.79E-02
-5.000E-01	152	-1.79E-02
-5.500E-01	151	-1.79E-02
-6.000E-01	150	-1.79E-02
-6.500E-01	149	-1.79E-02
-7.000E-01	148	-1.79E-02
-7.500E-01	147	-1.79E-02
-8.000E-01	146	-1.79E-02
-8.500E-01	145	-1.79E-02
-9.000E-01	144	-1.79E-02
-9.500E-01	143	-1.79E-02
-1.000E+00	142	-1.79E-02
-1.050E+00	141	-1.79E-02
-1.100E+00	140	-1.79E-02
-1.150E+00	139	-1.79E-02
-1.200E+00	138	-1.79E-02
-1.250E+00	137	-1.79E-02
-1.300E+00	136	-1.79E-02
-1.350E+00	135	-1.79E-02
-1.400E+00	134	-1.79E-02
-1.450E+00	133	-1.79E-02
-1.500E+00	132	-1.79E-02
-1.550E+00	131	-1.79E-02
-1.600E+00	130	-1.79E-02
-1.650E+00	129	-1.79E-02
-1.700E+00	128	-1.79E-02
-1.750E+00	127	-1.79E-02

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-1.800E+00	126	-1.79E-02
-1.850E+00	125	-1.79E-02
-1.900E+00	124	-1.79E-02
-1.950E+00	123	-1.79E-02
-2.000E+00	122	-1.79E-02
-2.050E+00	121	-1.79E-02
-2.100E+00	120	-1.79E-02
-2.150E+00	119	-1.79E-02
-2.200E+00	118	-1.79E-02
-2.250E+00	117	-1.79E-02
-2.300E+00	116	-1.78E-02
-2.350E+00	115	-1.78E-02
-2.400E+00	114	-1.77E-02
-2.450E+00	113	-1.76E-02
-2.500E+00	112	-1.74E-02
-2.550E+00	111	-1.73E-02
-2.600E+00	110	-1.72E-02
-2.650E+00	109	-1.76E-02
-2.700E+00	108	-2.02E-02
-2.750E+00	107	-1.01E-04
-2.800E+00	106	-9.14E-09
-2.850E+00	105	-6.21E-11
-2.900E+00	104	-6.12E-11
-2.950E+00	103	-6.12E-11
-3.000E+00	102	-6.12E-11
-3.050E+00	101	-6.12E-11
-3.100E+00	100	-6.12E-11

I = 2
X = 5.00E-01

-- REALIZATION 50P - PRESSURE OR PRESSURE HEAD FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -**

Z =	K =	
2.500E-02	162	-2.76E-01
-2.500E-02	161	-3.26E-01
-7.500E-02	160	-3.76E-01
-1.250E-01	159	-4.26E-01
-1.750E-01	158	-4.76E-01
-2.250E-01	157	-5.26E-01
-2.750E-01	156	-5.76E-01
-3.250E-01	155	-6.26E-01
-3.750E-01	154	-6.76E-01
-4.250E-01	153	-7.26E-01
-4.750E-01	152	-7.76E-01
-5.250E-01	151	-8.26E-01
-5.750E-01	150	-8.76E-01
-6.250E-01	149	-9.26E-01
-6.750E-01	148	-9.76E-01
-7.250E-01	147	-1.03E+00
-7.750E-01	146	-1.08E+00
-8.250E-01	145	-1.13E+00
-8.750E-01	144	-1.18E+00
-9.250E-01	143	-1.23E+00
-9.750E-01	142	-1.28E+00
-1.025E+00	141	-1.33E+00
-1.075E+00	140	-1.38E+00
-1.125E+00	139	-1.43E+00
-1.175E+00	138	-1.48E+00
-1.225E+00	137	-1.53E+00
-1.275E+00	136	-1.58E+00
-1.325E+00	135	-1.63E+00
-1.375E+00	134	-1.68E+00
-1.425E+00	133	-1.73E+00
-1.475E+00	132	-1.78E+00
-1.525E+00	131	-1.83E+00
-1.575E+00	130	-1.88E+00
-1.625E+00	129	-1.93E+00
-1.675E+00	128	-1.98E+00
-1.725E+00	127	-2.03E+00
-1.775E+00	126	-2.08E+00
-1.825E+00	125	-2.13E+00
-1.875E+00	124	-2.18E+00
-1.925E+00	123	-2.23E+00
-1.975E+00	122	-2.28E+00

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-2.025E+00	121	-2.33E+00
-2.075E+00	120	-2.38E+00
-2.125E+00	119	-2.43E+00
-2.175E+00	118	-2.48E+00
-2.225E+00	117	-2.53E+00
-2.275E+00	116	-2.58E+00
-2.325E+00	115	-2.63E+00
-2.375E+00	114	-2.68E+00
-2.425E+00	113	-2.74E+00
-2.475E+00	112	-2.79E+00
-2.525E+00	111	-2.85E+00
-2.575E+00	110	-2.91E+00
-2.625E+00	109	-2.98E+00
-2.675E+00	108	-3.06E+00
-2.725E+00	107	-4.79E+00
-2.775E+00	106	-9.62E+01
-2.825E+00	105	-1.03E+02
-2.875E+00	104	-1.03E+02
-2.925E+00	103	-1.03E+02
-2.975E+00	102	-1.03E+02
-3.025E+00	101	-1.03E+02
-3.075E+00	100	-1.03E+02

I = 2
X = 5.00E-01

-- REALIZATION 50THET- RELATIVE SATURATION LEVEL FOR PLANE J = 2 AT STEP 400, TIME= 3.0000E+01 -**

Z =	K =	
2.500E-02	162	6.45E-01
-2.500E-02	161	6.45E-01
-7.500E-02	160	6.45E-01
-1.250E-01	159	6.45E-01
-1.750E-01	158	6.45E-01
-2.250E-01	157	6.45E-01
-2.750E-01	156	6.45E-01
-3.250E-01	155	6.45E-01
-3.750E-01	154	6.45E-01
-4.250E-01	153	6.45E-01
-4.750E-01	152	6.45E-01
-5.250E-01	151	6.45E-01
-5.750E-01	150	6.45E-01
-6.250E-01	149	6.45E-01
-6.750E-01	148	6.45E-01
-7.250E-01	147	6.45E-01
-7.750E-01	146	6.45E-01
-8.250E-01	145	6.45E-01
-8.750E-01	144	6.45E-01
-9.250E-01	143	6.45E-01
-9.750E-01	142	6.45E-01
-1.025E+00	141	6.45E-01
-1.075E+00	140	6.45E-01
-1.125E+00	139	6.45E-01
-1.175E+00	138	6.45E-01
-1.225E+00	137	6.45E-01
-1.275E+00	136	6.45E-01
-1.325E+00	135	6.45E-01
-1.375E+00	134	6.45E-01
-1.425E+00	133	6.45E-01
-1.475E+00	132	6.45E-01
-1.525E+00	131	6.45E-01
-1.575E+00	130	6.45E-01
-1.625E+00	129	6.45E-01
-1.675E+00	128	6.45E-01
-1.725E+00	127	6.45E-01
-1.775E+00	126	6.45E-01
-1.825E+00	125	6.45E-01
-1.875E+00	124	6.45E-01
-1.925E+00	123	6.45E-01
-1.975E+00	122	6.45E-01
-2.025E+00	121	6.45E-01
-2.075E+00	120	6.45E-01
-2.125E+00	119	6.44E-01
-2.175E+00	118	6.44E-01
-2.225E+00	117	6.43E-01

-2.275E+00	116	6.42E-01
-2.325E+00	115	6.41E-01
-2.375E+00	114	6.39E-01
-2.425E+00	113	6.37E-01
-2.475E+00	112	6.33E-01
-2.525E+00	111	6.27E-01
-2.575E+00	110	6.18E-01
-2.625E+00	109	6.04E-01
-2.675E+00	108	5.77E-01
-2.725E+00	107	2.38E-01
-2.775E+00	106	2.61E-02
-2.825E+00	105	2.51E-02
-2.875E+00	104	2.51E-02
-2.925E+00	103	2.51E-02
-2.975E+00	102	2.51E-02
-3.025E+00	101	2.51E-02
-3.075E+00	100	2.51E-02

I = 2
X = 5.00E-01

400 3.0000E+01 0.000E+00 0.000E+00-1.790E-02-6.256E-01 6.450E-01 0.000E+00 1.2528E-02 5.444E-05 0.544

THIS OUTPUT IS PRODUCED BY THE COMPUTATIONAL MODEL

----- P O R M C -----

FOR TRANSIENT OR STEADY STATE STOCHASTIC 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

VERSION 1.0: DATED: 22 OCT 1989

DATE OF RUN: 3/21/1991 - TIME OF RUN: 08:48:20

ELAPSED TIME FOR THIS CASE : 813.52 MINUTES
TIME PER GRID NODE PER STEP: 813.52 MILLISECONDS
TIME PER NODE-STEP-EQUATION: 813.52 MILLISECONDS
1 EQUATIONS SOLVED AT 1458 NODES FOR 0 STEPS.

RECORD OF INPUT DATA STREAM

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

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APPENDIX C

ERROR MESSAGES OF PORMC

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APPENDIX C

ERROR MESSAGES OF PORMC

PORMC 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 PORMC. (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.
251	The time step specified for simulations of the SOLVE command is smaller than 1 E-20 or larger than 1 E+20.

Table C-1. Error Messages of PORMC. (sheet 2 of 3)

Error number	Error description
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.
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.

Table C-1. Error Messages of PORMC. (sheet 3 of 3)

Error number	Error description
651	The reference air-entry pressure, h^* , of Equations 6.42-1 and 6.42-6 that is specified by the CHAR acteristic 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 CHAR acteristic command is less than zero.
710	The dependent variable character string specified by the SOUR ce command is not one of C, P, or T, as required.
711	The total number of active source zones specified by the SOUR ce commands exceeds the LSZ parameter.
712	The zone number specified by the SOUR ce command was not previously defined by a ZONE command.

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