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**PORFLOW: A MULTIFLUID MULTIPHASE MODEL FOR
SIMULATING FLOW, HEAT TRANSFER, AND
MASS TRANSPORT IN FRACTURED POROUS MEDIA
USER'S MANUAL — VERSION 2.40**

Prepared for

**Nuclear Regulatory Commission
Contract NRC-02-88-005**

Prepared by

**Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas**

February 1992



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Prepared by

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February 1992

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This report is based on existing documents related to older versions of PORFLOW. The old documents were reviewed by various people at the time. In addition, the authors have benefitted greatly from discussions with numerous code users. This particular report was reviewed by Drs. Wes Patrick and Ross Bagtzoglou at the Center. We are thankful to all the reviewers and code users for their helpful suggestions.

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PREFACE

PORFLOW computer code, its pre- and post-processors FREEFORM and ACRPLOT respectively are copyrighted software of the Analytic and Computational Research Incorporated (ACRi), Los Angeles, California. The FREEFORM pre-processor for inputting data to PORFLOW is an integral part of PORFLOW, so that PORFLOW cannot be used without also using FREEFORM. However post-processors other than ACRPLOT can be used to process the output.

While assigning copyright on PORFLOW to ACRi, the U.S. Government retained limited right for its use. This right is limited in as much as this code cannot be used for commercial purposes. Executable copy of this code is available to the public from the National Energy Software Center (NESC) at Oak Ridge.

Dr. A.K. Runchal of ACRi, working as a consultant to the Center for Nuclear Waste Regulatory Analyses (Center), has recently added some desirable features to create PORFLOW, Version 2.40. This report is a documentation of PORFLOW, Version 2.40 developed jointly by Dr. Runchal (ACRi) and Dr. Sagar (CNWRA) for use by the staffs of the Center and the NRC. The Center and the NRC have access to the source code of Version 2.40 with the stipulation that it not be transferred to any party for commercial use. Other versions of the code, along with their documentation may be obtained from ACRi.

A version of the PORFLOW code used at the Hanford Site is also known as PORFLO-3 Version 1.0 (Runchal and Sagar, 1989^{*}; Sagar and Runchal, 1990^{*}). This older version of PORFLOW has been used at the Center in the Performance Assessment Research Project. For consistency and to honor the copyright, this code will be referred to as PORFLOW Version 1.0 from now on.

The Center has not acquired the post-processor, ACRPLOT. Instead, post-processors have been locally developed to interface with commercial plotting packages such as TECPLOT and IVM that currently function on a variety of hardware at the Center.

^{*}See list of references in the document for full citation.

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EXECUTIVE SUMMARY

The U.S. Nuclear Regulatory Commission (NRC), Office of Research (RES) is investigating techniques that would be used in assessing the performance of High-Level Nuclear Waste Repositories. The work reported in this document was performed at the Center for Nuclear Waste Analyses (Center) as part of the Performance Assessment Research Project sponsored by the NRC Office of Nuclear Regulatory Research, Division of Regulatory Applications.

This document describes the PORFLOW, Version 2.40 software package which has been developed by updating an older version for use in Center work. The PORFLOW computer code is designed to simulate flow, heat transfer, and mass transport in three-dimensional heterogeneous porous and fractured media. Two new features were added to produce Version 2.40. These are:

- A capability for phase changes between solid, liquid, and gas. With this feature, flow of water in the presence of phase changes into ice or steam and vice versa can be simulated. It is assumed that liquid water and its vapor pressure may not be in thermodynamic equilibrium.
- A capability to deal with a mixture of gases, e.g., air, vapor, and CO₂. This feature was specifically added because transport of radioactive gases is a distinct possibility in repositories located in the unsaturated zone. Currently, no module for kinetic generation of radioactive gases however, is available in PORFLOW.

In general, PORFLOW, Version 2.40 provides capabilities to solve transport problems in multiphase, multicomponent systems. Decay chains of up to four members can be employed to deal with radionuclide transport.

The primary objective of this document is to provide only a brief overview of the theory of PORFLOW but give detailed descriptions of the commands that a user must know to execute the code. Since PORFLOW implements rather complex numerical algorithms, it is recommended that the user have some background in nonisothermal flow and transport through porous media.

It may be noted that PORFLOW is a general purpose commercial software. That is, it is designed to solve a variety of problems of various dimensionality (from 1D to 3D), steady or transient nature, confined or unconfined systems, and porous and fractured media. Obviously, by a suitable combination of appropriate features and options, many seemingly dissimilar problems may be solved. Currently PORFLOW is limited to using rectangular parallelepiped computational elements although their sizes can freely vary within the grid.

NOTATION

Symbol	MEANING	UNITS		
		GENERIC	SI	FPS
B	Buoyancy parameter	---	---	---
c	Specific heat	$L^2 t^2 T^{-1}$	J/(kg K)	BTU/(lbm °F)
C	Species concentration in fluid	$M L^{-3}$	kg/m ³	lbm/ft ³
D	Dispersion coefficient	$L^2 t^{-1}$	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
F	General transport variable	various	various	various
g	Gravitational acceleration	$L t^{-2}$	m/s ²	ft/s ²
h	pressure head at reference density	L	m	ft
J	Diffusional flux of species	$M L^{-2} t^{-1}$	kg/(m ² s)	lbm/(ft ² s)
k	Intrinsic permeability	L^2	m ²	ft ²
k	Thermal conductivity of fluid	$ML t^{-3}T^{-1}$	W/(m K)	BTU/(ft s °F)
k _d	Partition coefficient	$M^{-1} L^3$	m ³ /kg	ft ³ /lbm
k _r	Relative hydraulic conductivity	---	---	---
K	Hydraulic conductivity	$L t^{-1}$	m/s	ft/s
m	Rate of injection of fluid	$M L^{-3} t^{-1}$	kg/(m ³ s)	lbm/(ft ³ s)
m	Mass fraction of a species	---	---	---
m _v	Volumetric mass injection rate	t^{-1}	m ³ /(m ³ s)	ft ³ /(ft ³ s)
M	Molecular weight	$M mol^{-1}$	kg/mol	lbm/mol
N	Coordinate normal to a boundary	L	m	ft
p	Thermodynamic pressure	$M L^{-1} t^{-2}$	N/m ²	lbf/ft ²
P	Total hydraulic head	L	m	ft
q	Flux of thermal energy	$M t^{-3}$	W/(m ²)	BTU/(ft ² s)
r	Radius of curvature	L	m	ft
R	Density ratio	---	---	---
R _d	Retardation factor	---	---	---
R _u	Universal gas constant	$L^2 t^2 T^{-1}$	J/(kg molK)	BTU/(lbm-mol R)
S	Saturation fraction of fluid	---	---	---
S	Source for a dependent variable	various	various	various
S _c	Source for a species	$M L^{-3} t^{-1}$	kg/(m ³ s)	lbm/ft ³ s)
S _e	Effective storativity	L^{-1}	1/m	1/ft
S _r	Residual liquid phase fraction for the soil	---	---	---

NOTATION - Continued

Symbol	MEANING	UNITS		
		GENERIC	SI	FPS
S_T	Heat source	$M L^{-1} t^{-3}$	W/(m ³)	BTU/(ft ³ s)
t	Time	t	s	s
T	Thermodynamic Temperature	T	K	R
T_s	Base to convert temp. to absolute units	T	K	R
T_c	Critical temperature	T	K	R
U	Darcy velocity in x-direction	$L t^{-1}$	m/s	ft/s
v	Pore or fluid particle velocity	$L t^{-1}$	m/s	ft/s
V	Darcy velocity in y-direction	$L t^{-1}$	m/s	ft/s
V_i	Velocity in i th direction	$L t^{-1}$	m/s	ft/s
\underline{V}	Total velocity vector	$L t^{-1}$	m/s	ft/s
W	Darcy velocity in z-direction	$L t^{-1}$	m/s	ft/s
x	x-coordinate	L	m	ft
y	y-coordinate	L	m	ft
z	z-coordinate	L	m	ft

GREEK SYMBOLS

Symbol	MEANING	UNITS		
		GENERIC	SI	FPS
α_f	Fluid compressibility	$M^{-1} L t^2$	m ² /N	ft ² /lbf
α_L	Longitudinal dispersivity	L	m	ft
α_s	Compressibility of solid matrix	$M^{-1} L t^2$	m ² /N	ft ² /lbf
α_s	Pressure coefficient of phase saturation	$M^{-1} L t^2$	m ² /N	ft ² /lbf
α_T	Transverse dispersivity	L	m	ft
β_f	Expansion coefficient for fluid	T^{-1}	1/K	1/°F
β_s	Temperature coefficient of phase saturation	T^{-1}	1/K	1/°F
Γ	Diffusion coefficient	$M L^{-1} t^{-1}$	kg/(m s)	lbm/(ft s)
ϵ	A small quantity	—	—	—
Θ	Angular coordinate	radian	radian	radian
Θ	Porosity of the matrix	—	—	—
λ	Reaction rate for species	t^{-1}	1/s	1/s

NOTATION - Continued

GREEK SYMBOLS - Continued

Symbol	MEANING	UNITS		
		GENERIC	SI	FPS
μ	Fluid viscosity	$M L^{-1} t^{-1}$	kg/(m s)	lbm/(ft s)
ρ	Fluid density	$M L^{-3}$	kg/m ³	lbm/ft ³
σ	Generation fraction for species	---	---	---
τ	Tortuosity factor	---	---	---
ϕ	Volume fraction filled with a given fluid	---	---	---

SUBSCRIPTS

SYMBOL	PERTAINING TO
D	Diffusional component of porosity or fluid filled volume fraction
E	Effective component of porosity or fluid filled volume fraction
e	Equivalent of effective value for the fluid-solid matrix
f	The fluid phase
i	The i th coordinate direction
j	The j th coordinate direction
j	The j th chemical species
s	The solid phase
t	The time coordinate
T	Total porosity or fluid filled volume fraction
x	The x direction
y	The y or r direction
z	The z or Θ direction
1	The primary fluid
2	The secondary fluid
3	The third fluid

NOTATION - Continued

SUPERSCRIPTS

SYMBOL	PERTAINING TO
n	The n th fluid or the n th chemical species
k	The k th time step
1	The primary fluid
2	The second fluid
3	The third fluid
*	A reference state of the system
~	A representative or average value
^	A non-dimensional value

1 OVERVIEW AND INTRODUCTION

PORFLOW[®] is a software package for solution of multiphase fluid flow, heat transfer, and mass transport problems in variably saturated porous or fractured media. It is a highly flexible, modular and user-oriented computer code. Due to its modular nature, the user may readily customize the code for specific applications. It employs the FREEFORM[®] command language pre-processor to provide a flexible, simple to use, and format-free user interface. The code also interfaces with the ACRPLOT[®] post-processor to display the computed results in a variety of graphical images. The software is written in FORTRAN 77 language and is essentially independent of any specific computer hardware.

This document describes Version 2.40 which is operational on a range of micro, mini, mainframe and super computers. An outline of the theory and a complete description of the input and output options are given in the following chapters. The theory on which the PORFLOW software is based is more completely described in a number of publications which are available in the published literature. The code is currently being applied to realistic test problems. The results of such tests will be reported in another document. This chapter provides an introduction to the various capabilities of PORFLOW.

1.1 OVERVIEW

The PORFLOW software package is a comprehensive mathematical model for simulation of multiphase fluid flow, heat transfer, and mass transport processes in heterogeneous porous and fractured media. A sophisticated pre-processor allows the user to communicate with PORFLOW through conversational, English-like FREEFORM command language developed by Analytic and Computational Research, Inc., (ACRi) of Los Angeles, California (Appendix A). FREEFORM is designed to allow control of data input and output through simple, format-free, English-like commands. Only a few input commands need to be frequently used and, in the absence of specification by the user, built-in default values are assumed; this enables a newcomer to use PORFLOW easily without much delay or costly training.

The PORFLOW software may be used to simulate transient or steady-state problems in cartesian or cylindrical geometry. The geologic medium may be anisotropic and heterogeneous, and it may contain distinct embedded elements, such as discrete fractures or boreholes, within a porous matrix. PORFLOW is based on a unified theoretical treatment of a number of concepts relevant to transport processes in fluids. The physical processes incorporated into PORFLOW are shown in Figure 1-1. As can be seen from this figure, various levels of interaction and coupling exist between the different components of the flow system. In the PORFLOW computer code, these components may be employed either in a coupled or uncoupled mode. Some of the important features of PORFLOW are:

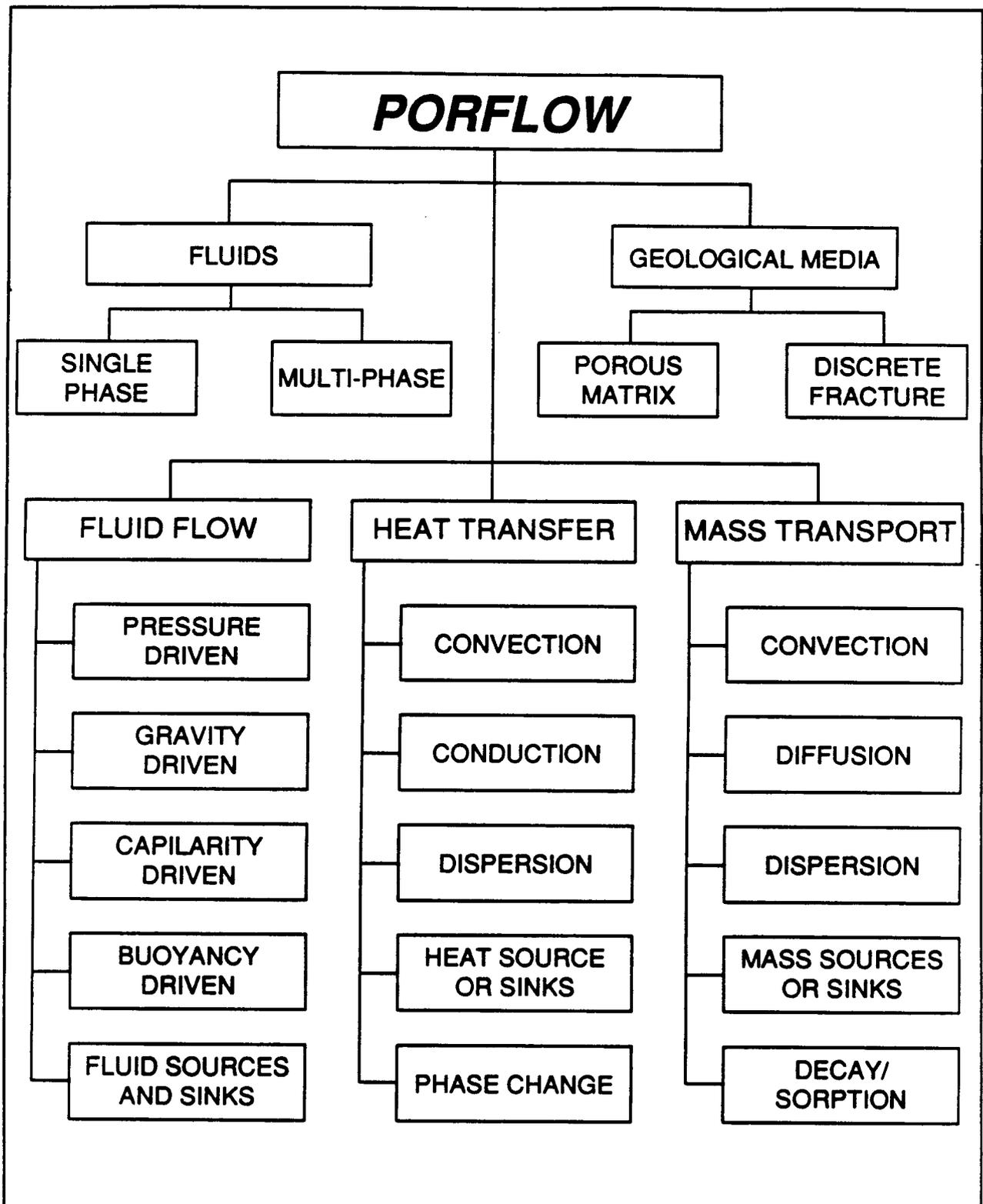


Figure 1-1. Processes incorporated into PORFLOW

- Cartesian or cylindrical geometry,
- Transient or steady-state simulation,
- Horizontal or vertical cross-sections or fully three-dimensional domains,
- Multi-fluid, multiphase and variably saturated matrix,
- Dynamically active liquid-solid and liquid-vapor phase change,
- Inhomogeneous, anisotropic and time-dependent properties,
- Inherently mass-conservative numerical method,
- Buoyancy effects due to density variations,
- Alternate constitutive equations for porous medium properties,
- Arbitrarily non-uniform grid,
- Time-dependent physical input,
- Format-free, conversational input with built-in default values,
- Flexible operational and output control,
- Choice of basis functions for integration of equations,
- Alternate methods for solving systems of linear equations,
- Option to solve any or all of the governing equations, and
- Dynamic coupling between flow, heat and mass transport.

1.2 USER'S MANUAL ORGANIZATION

Chapter 1:	Overview and introduction
Chapter 2:	Mathematical basis
Chapter 3:	Numerical basis
Chapter 4:	Specification of problem geometry and grid
Chapter 5:	Introduction to input and output options
Chapter 6:	Description of PORFLOW [®] keyword commands
Appendix A:	ACRi FREEFORM command language
Appendix B:	Error messages of PORFLOW

1.3 VALIDATION AND PREVIOUS APPLICATIONS

PORFLOW benefits from over twenty years of experience gained from the computer codes written for use by the industry, and academic and research organizations. The important elements of PORFLOW, such as the discretization schemes and the solution methods have all been independently verified over a number of years. The primary contribution of PORFLOW is in welding these disparate elements into a software package which is general, flexible, economical, and easy to use. PORFLOW has been extensively verified against a number of analytic solutions, experimental and field data, and other numerical models. Over 40 publications and technical reports on the applications of PORFLOW are currently available. These include Runchal (1980), Runchal and Hocking (1981), Runchal (1981), Runchal et al. (1982), Fujioka and Runchal (1983), Kline et al. (1983), Eyler and Budden (1984), Runchal et al. (1985), Runchal (1987a), Aimo (1987), Walton and Sagar (1987), Loiseau (1988), Walton and Sagar (1988), Baca et al. (1988), Walton and Sagar (1989), Smoot and Sagar (1990),

Rockhold et al. (1990), and Magnuson et al. (1990). The specific applications of the PORFLOW models have included:

- Analysis of high and low level nuclear waste repositories,
- Chemical pollution of ground water aquifers,
- Organic contamination of ground water,
- Ground water resource and pumping studies,
- Flow, heat transfer and chemical reaction in porous beds,
- Storage and withdrawal of hot water in deep aquifers,
- Salinity intrusion in coastal aquifers,
- Thawing/freezing of ground due to buried oil and gas pipes,
- Propagation of freezing front in soils,
- Analysis of oil pipelines buried under sea,
- Interaction of ground water systems with atmosphere,
- Corrosion in waste canisters and liners,
- Hydrologic analysis due to reverse circulation drilling,
- Performance enhancement of oil wells by liner perforation,
- Dewatering of mines,
- Consolidation of soils, and
- Geological evolution of sedimentary formations.

1.4 STRUCTURE OF PORFLOW

The structure of PORFLOW is designed to achieve four major objectives:

1. User-friendliness,
2. Generality,
3. Flexibility, and
4. Economy of computation.

To meet the first of these objectives, PORFLOW employs a very friendly user interface which allows the specification of the input and output requirements through conversational, English-like, FREEFORM command language developed by ACRi. The output from the model may be displayed in convenient tabular or graphical form.

To achieve the second of these objectives, a simple and convenient method is employed to define the geometry and the physics of the system. The domain of interest is considered to be composed of several distinct zones. The zones may differ from each other by virtue of a physical property such as hydraulic conductivity or a special feature such as a fracture. A zone may consist of a single element of the grid; it may be a layer of elements or it may encompass whole of the domain of interest. Furthermore, a zone may consist of contiguous elements or it may be spread over scattered elements of the grid.

The last two objectives are achieved by employing a highly modular structure for PORFLOW which, for current versions, consists of over 100 individual modules. In general, each of these modules is dedicated to a single function and can be replaced by an alternate module without any significant change to the rest of the modules or the structure of PORFLOW. The code provides options for alternate discretization schemes, solution methods, and calculation of fluid and medium properties. Any option, not required for a given problem, is easily bypassed by simple index specifications; this allows efficient and economical solution of a wide range of problems of varying complexity. One example of the economy and efficiency of the PORFLOW code is that it is *fully operational on IBM-PC and compatible microcomputers*.

1.5 SCOPE AND LIMITATIONS OF PORFLOW

1.5.1 System of Equations

PORFLOW provides for the numerical solution of a variable set of general transport equations: those for multiphase fluids, thermal energy, and one or more chemical species. The governing equations are supplemented by constitutive equations, phase change relations, equations of state and initial and boundary conditions. The equations are coupled through convection, buoyancy, temperature, phase change, and fluid density and viscosity effects. These equations may be solved individually or simultaneously in a coupled or uncoupled manner, depending on the nature of a specific problem and options selected by the user.

The current version of PORFLOW provides for up to three phase (or fluid) flow systems. Examples of such systems are water-oil-vapor-air, water-steam-air, water-steam, water-ice, or water-air.

1.5.2 Spatial Dimensionality

The code is primarily designed to solve two-dimensional (2D) or three-dimensional (3D) problems. It can accept user input in either a 2D or 3D mode. Full details of these input modes are given in Chapters 5 and 6. One dimensional problems can be solved 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- two or three-dimensional problem.

1.5.3 Problem Geometry

The problem geometry can be defined in terms of either cartesian (x,y,z) or cylindrical (x,r,θ) coordinates. In the 2D mode, only the (x,y) or (x,r) planes are allowed. Two or one dimensional problems, of course, can be simulated in the 3D mode in any combination of coordinates by allowing for a minimum of three nodes in each direction.

Orientation of the axes with respect to the gravitational acceleration vector is arbitrary. The gravitational vector may be aligned with any of the directions or it may be at any arbitrary angle to the coordinate directions. It influences both the buoyancy effects due to density gradients and the definition of the hydraulic head [see Eqn. (2.1.8)].

1.5.4 Temporal Dependence

Either transient or steady-state problems can be solved. Except for the geometry and 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 can be designed to change the data values at specified time intervals.

1.5.5 Spatial Dependence

The values of most parameters are allowed to vary over the spatial grid. The model domain can be divided into zones, each differing from the others in some distinct way such as a material property. The material properties can also be anisotropic.

1.5.6 Boundary Conditions

Varied types of boundary conditions can be specified in PORFLOW. Dirichlet (specified values of hydraulic head, temperature, or concentration), Neumann (specified fluxes of fluid, heat, or mass), gradient (gradient of hydraulic head, temperature, and concentration), 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 1.5.4, this feature can be used to solve a large variety of problems with space- and time-dependent boundary conditions.

1.5.7 Methods for Solving Governing Equations

The method of Nodal Point Integration (NPI) is employed for integration of the governing differential equations by temporal and spatial discretization over each of the control volumes of the physical domain. The numerical method leads to solutions that automatically conserve fluid, heat, and mass locally within every grid element, as well as for the entire model domain. The resulting system of linear algebraic equations is then solved by one or more of a variety of matrix inversion algorithms. The accumulation term in the equations may be approximated by the Picard or a modified-Picard method and the flux terms may be approximated by the governing variable or its change from a current state (delta formulation). In the current versions, the control volumes (elements) used to define the problem geometry can vary in size across the coordinate system, but their geometry is restricted to that of a rectangular parallelepiped or segment of a solid cylinder. Three distinct discretization schemes are

available: the hybrid (Runchal, 1972), the exponential (Spalding, 1972) and the CONDIF (Runchal, 1987b) schemes. The nature of these schemes is described in Chapter 3.

The resulting matrix of algebraic equations may be solved by a suitable matrix inversion method. The available options include the explicit method of Point Successive Over-Relaxation, the semi-implicit method of the Alternating Direction Implicit (ADI), and the implicit methods of Conjugate Gradient, the Cholesky Decomposition and the Gaussian Elimination. In addition, PORFLOW provides the flexibility to use any other matrix inversion technique through coupling with an external matrix-inversion algorithm.

1.5.8 Multiple Phases and Variable Saturation

Though the framework of PORFLOW is general enough to allow for any number of phases (or fluids), the current versions allow for a one (say, water), two (say, water and air), or three (say, water, oil and air) phase fluid flow. Different phases of a fluid (such as liquid and gas) are treated as different fluids. A one fluid or a single phase system is also called a "fully" saturated flow whereas a multiphase system is referred to as a "variably" saturated flow.

In case of a multiphase system, the current versions assume that the phases are immiscible and that each phase has a distinct pressure which is, of course, a function of space and time. The pressure of each phase differs from that of the adjoining phase by a capillary pressure.

Problems with variable saturation can be solved with PORFLOW. In the partially saturated zone, liquids (water, oil etc.) and gas (air, vapor etc.) are assumed to coexist. Degree of saturation of each phase is determined at each grid node as part of the solution.

1.5.9 Free Surface and Unconfined Flow

In its default mode, PORFLOW assumes that the flow domain is confined. The multiphase provision may be invoked to solve for an unconfined flow domain. However, the multiphase approach is generally considerably more expensive than the saturated flow option. If the vadose zone is not of interest, then PORFLOW provides for an alternative method to solve for the unconfined flow. In this mode, only the saturated region of the flow, below the water table, is solved.

1.5.10 Phase Change

The PORFLOW provides for liquid-vapor (such as water-steam) and liquid-solid (such as water-ice) phase change in a dynamic manner. The phase change algorithm is reversible and general, and provides for nonequilibrium thermodynamics. The phase change parameters and fluid property relations may be arbitrarily changed by the user.

1.5.11 Special Geologic Features

In addition to the capability to consider heterogeneity and anisotropy of the porous media, an option is included in PORFLOW that permits the user to consider planar geologic features such as fractures, faults, and clastic dikes, and linear features such as boreholes. These features are distinguished from the parent media (soil and/or rock) by their distinctively different length scales and properties. For example, if one of the three dimensions of a fracture is small relative to the other two, then it behaves essentially as a two-dimensional (planar) element that is embedded in the three-dimensional domain. Similarly, boreholes or other small man-made excavations are essentially one-dimensional features.

It is possible to treat all of these features as distinct three-dimensional zones. However, due to the different length scales involved, this treatment may make excessive demands on computer resources. An alternate option, to consider such features as two- or one-dimensional elements that are embedded within three-dimensional media, is available. The choice of this option greatly reduces the required grid sizes and computational time.

1.5.12 Pore Structure

PORFLOW assumes a pore structure which is classified in terms of three types of porosities. The largest of these is the total porosity which is the volume fraction of the total pore space to the total volume of the host matrix. Not all of these pores, however, actively participate in movement of fluid. Some pores are completely isolated from the interconnected pathways for flow and others form dead ends at the extremes of isolated pathways, much in the manner of a maze. The effective porosity is thus defined as the volume fraction of the pore space through which fluid flow occurs compared to the total matrix volume. A third porosity of interest is the diffusional porosity which is defined as the ratio of the volume of the pores that participate in diffusion to the total matrix volume. It includes the pores through which fluid movement occurs plus the dead-end pores that are assumed to not contribute to fluid flow, but that are assumed to facilitate the diffusion of heat and mass. By definition, its numerical value is intermediate between the total and effective values.

1.5.13 Sources and Sinks

Several options are provided in PORFLOW for incorporating sources and sinks of fluid, heat, and mass. Fluid injection or withdrawal, and sources (or sinks) of heat or chemical species may occur anywhere in the interior of the domain of interest. Spatially variable sources and sinks can be specified. The strength of the source or sink either can be constant or can vary with time. For mass species, the sources can be limited by their inventory, solubility, or both.

1.5.14 Operational and Output Control

Through design of the input, the user can exert extensive control over the operation of the code. For example, the execution of the code can be stopped to change boundary conditions 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 in a tabular form or written in a file for post-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.

2 MATHEMATICAL BASIS

PORFLOW solves a set of coupled transport equations for fluid velocities, pressure, temperature, and concentration of chemical species in multiphase or multifluid, variably saturated, fractured or porous media flow. The number of phases (or fluids) and that of species equations to be solved can be easily varied to accommodate specific user requirements. The equations may be solved in their two- or three-dimensional, transient or steady state form.

These equations are based on the conservation principles of continuum mechanics, except that the Darcy's equations are used in place of the Navier-Stokes equations. A brief summary of the governing equations is provided in this chapter. The principal processes incorporated in these equations were summarized earlier in Figure 1-1.

2.1 GOVERNING EQUATIONS FOR FLUID FLOW

2.1.1 Continuity or Mass Balance Equations

The equation of continuity for the conservation of a compressible fluid mass in nondeforming media in cartesian tensor notation is written as:

$$\partial_t(\rho^n S^n \Theta_E) + \sum_{i=1}^d \partial_i(\rho^n V_i^n) = m^n + q^n \quad , \quad (2.1.1)$$

where:

- ∂_t denotes the partial derivative with respect to the time coordinate, t ,
 t is the time coordinate,
- ρ^n is the mass density of the n^{th} phase,
- S^n is the saturation of the n^{th} phase,
- Θ_E is the effective porosity of the matrix defined as the component of the pore space, expressed as a fraction of the total matrix volume, through which flow occurs (see Section 1.5.12),
- ∂_i denotes the partial derivative with respect to the coordinate in the i^{th} direction,
 V_i^n is the specific discharge or Darcy velocity component of the n^{th} phase in the i^{th} direction,
- m^n is the rate of mass injection (>0) or withdrawal (<0) of the n^{th} phase per unit volume,
- q^n is the rate of formation (>0) or disappearance (<0) of the n^{th} phase as a result of phase change, and
- d is the number of space dimensions.

From considerations of continuity, the sum of saturation of all phases is equal to unity; that is:

$$\sum_n S^n = 1 \quad . \quad (2.1.2)$$

Therefore, for a total of N phases, only N-1 partial differential equations of the form of Eqn. (2.1.1) need to be solved; saturation for the Nth phase can be obtained from Eqn. (2.1.2) as:

$$S^N = 1 - \sum_{n=1}^{N-1} S^n \quad . \quad (2.1.3)$$

2.1.2 Momentum Balance Equations

The momentum balance for the nth phase in a porous media is assumed to be adequately expressed by Darcy's Law which, for variable density conditions, may be written as (Bear, 1972):

$$V_i^n = \sum_{j=1}^d -K_{ij}^n (\partial_j P^n - B_j^n) \quad . \quad (2.1.4)$$

In this equation:

$$K_{ij}^n = k_{ij} k_r^n \rho^{n*} g / \mu^n \quad . \quad (2.1.5)$$

In PORFLOW, $k_{ij} = 0$ if $i \neq j$; and:

$$P^n = h^n + \sum_j (x_j^* - x_j) g_j / g \quad , \quad (2.1.6)$$

$$B_j^n = (R^n - 1) g_j / g \quad , \quad (2.1.7)$$

$$h^n = p^n / (\rho^{n*} g) \quad , \quad (2.1.8)$$

$$R^n = \rho^n / \rho^{n*} \quad , \quad (2.1.9)$$

$$g = \sqrt{\sum_j g_j^2} \quad , \quad (2.1.10)$$

where the superscript n denotes the nth phase and:

- K_{ij} is the hydraulic conductivity tensor,
- P is the hydraulic head at a reference density,
- B_j is the buoyancy vector,
- k_{ij} is the intrinsic permeability tensor,
- $*$ denotes a reference value of the corresponding quantity,
- g is the constant of gravitational acceleration,
- μ is the dynamic viscosity of the fluid,
- h is the pressure head at a reference fluid density,
- x_j is the coordinate distance along the jth direction,
- x_j^* is the jth coordinate value for the datum,
- g_j is component of gravity in the jth direction,
- p is the thermodynamic pressure from a reference datum, and
- R is the ratio of local fluid density to its reference value.

In general, the pressure head, h^n , and hence the hydraulic head, P^n , can be defined from any arbitrarily level since it is only the gradients of pressure which appear in the momentum equation [Eqn. (2.1.4)]. For multiphase or partially saturated flow, the pressure head, h^n , is often defined with atmospheric pressure as the datum. In that case, h^n is positive if fluid pressure is above atmospheric pressure and negative if below.

2.1.3 Pressure Equations

The governing equation for fluid pressure of the nth phase is obtained by substituting Eqn. (2.1.4) into (2.1.1). After some algebraic manipulation, this equation may be written as:

$$\partial_i (R^n S^n \Theta_E) - \sum_{i=1}^d \partial_i \left[R^n \sum_{j=1}^d K_{ij}^n (\partial_j P^n - B_j^n) \right] + m_v^n \quad , \quad (2.1.11)$$

where, m_v^n , the rate of addition or loss of fluid per unit volume, is given by:

$$m_v^n = (m^n + q^n) / p^n \quad . \quad (2.1.12)$$

PORFLOW provides for three alternate formulations of the pressure equation which may be selected by the user. The first of these is the classical "storage coefficient" formulation. If we assume that:

$$\Theta_E = \Theta_E(P^n) \quad , \quad (2.1.13)$$

$$\rho^n = \rho^n(P^n, T) \quad , \quad (2.1.14)$$

$$S^n = S^n(P^k, T) ; \quad k=1, \dots, n+1 \quad , \quad (2.1.15)$$

then Eqn. (2.1.11) transforms into:

$$\begin{aligned} S_o^n \partial_t P^n &= \sum_{i=1}^d \partial_i \left[R^n \sum_{j=1}^d K_{ij}^n (\partial_j P^n - B_j^n) \right] \\ &+ R^n \Theta_E (S^n \beta_f^n + \beta_s^n) \partial_t T + m_v^n \quad , \end{aligned} \quad (2.1.16)$$

with:

$$S_o^n = R^n S^n \alpha_s^n + R^n \Theta_E (S^n \alpha_f^n + \alpha_s^n) \quad , \quad (2.1.17)$$

$$\alpha_s^n = \partial \Theta_E / \partial P^n \quad , \quad (2.1.18)$$

$$\alpha_f^n = (\rho^n)^{-1} (\partial \rho^n / \partial P^n) |_T \quad , \quad (2.1.19)$$

$$\alpha_s^n = \sum_m (\partial S^n / \partial P^m) (\partial P^m / \partial P^n) \quad , \quad (2.1.20)$$

$$\beta_f^n = -(\rho^n)^{-1} (\partial \rho^n / \partial T) |_P \quad , \quad (2.1.21)$$

$$\beta_s^n = (\partial S^n / \partial T) |_P \quad . \quad (2.1.22)$$

In these equations, for the n^{th} phase, denoted by the superscript n :

- S_o is the effective storativity,
- α_s is the compressibility of the host solid matrix divided by specific weight of the fluid,
- α_f is the fluid compressibility divided by specific weight of the fluid,
- α_s is the pressure coefficient of phase saturation,

- β_f is the fluid thermal expansion coefficient,
- β_s is the temperature coefficient of phase saturation,
- T is the fluid temperature, and
- m_v is the volumetric rate of mass addition (>0) or loss (<0) of phase per unit volume.

This storage coefficient formulation is primarily of use when the accumulation term in Eqn. (2.1.11) is small compared to the pressure and source terms. This is often the case for incompressible or slightly-compressible flow and for single-phase flow when the speed of pressure propagation is much larger than the flow speed. The other two formulations rely upon the use of a pressure difference in the derivation of the governing equation. With Φ as the existing hydraulic head for the n^{th} phase and P^n as the hydraulic head at the new state of the system, the difference between the two is given by:

$$\Delta = P^n - \Phi \tag{2.1.23}$$

For computational purposes, Eqn. (2.1.11) may be replaced by a "modified storage coefficient" formulation which is expressed as:

$$S_o^n \partial_t \Delta = \sum_{i=1}^d \partial_i [R^n K_{ij}^n (\partial_j P^n - B_j^n)] + m_v^n - \partial_t (R^n S^n \Theta_E) \tag{2.1.24}$$

From a comparison of Eqns. (2.1.11) and (2.1.24), it is clear that the two are equivalent as $\Phi \rightarrow P^n$ (and $\Delta \rightarrow 0$). The coefficient S_o^n now plays the role of the classical relaxation factor or pseudo-transient storativity. However, it should be noted that the choice of this coefficient does not affect the final solution so long as $\Phi \rightarrow P^n$. The role played by the storage coefficient in the conventional formulation of the pressure equation is now included implicitly in the accumulation term which is the last term on the right hand side of Eqn. (2.1.24). An appropriate choice of S_o^n is nonetheless important since it will affect the convergence of Φ to P^n . It may be conjectured that the optimum choice for this quantity is that given by Eqn. (2.1.17).

The third and final formulation of the pressure equation, called the "delta" formulation, is obtained by expressing the right hand side of Eqn. (2.1.24) also in terms of Δ ; so that:

$$S_o^n \partial_t \Delta = \sum_{i=1}^d \partial_i [R^n K_{ij}^n (\partial_j \Delta - B_j^n)] \tag{2.1.25}$$

$$+ \partial_j (R^n K_{ij}^n \partial_j \Phi) + m_v^n - \partial_t (R^n S^n \Theta_E) .$$

For multiphase or partially-saturated flow, phase saturations are often strong nonlinear functions of the phase pressures. The accumulation term can therefore be large in these circumstances. Equations (2.1.24) and (2.1.25) ensure that mass is conserved unconditionally for such systems irrespective of the nature of the relationship between the storage coefficient and the fluid pressure. Equation (2.1.16), on the other hand, assures mass conservation only if the changes in the effective storativity are small compared to the changes in the flow due to pressure differences. Hence, for multiphase or highly compressible flows, these latter forms of the equations are preferable to Eqn. (2.1.16).

2.2 GOVERNING EQUATIONS FOR HEAT TRANSFER

The governing equation for heat transfer in PORFLOW is based on the assumption that thermal equilibrium exists between all the fluid phases and the solid constituents of the porous matrix. Thus, at any given location, the solid and fluid constituents are all at the same temperature. The equation for the conservation of thermal energy is then written as:

$$\partial_t (H_e) + \sum_{i=1}^d \partial_i (V_i^e H) = \sum_{i=1}^d \partial_i (\Gamma_{ij}^T \partial_j T) + S_T \quad , \tag{2.2.1}$$

where:

- H_e is the effective enthalpy per unit volume of the porous media,
- V_i^e is the effective specific discharge component for all the fluid phases in the i^{th} direction,
- H is the total enthalpy of all the fluid phases per unit volume,
- Γ_{ij}^T is the effective diffusion (and dispersion) coefficient for heat, and
- S_T is the rate of heat generated (>0) or dissipated (<0) per unit volume.

In PORFLOW, $\Gamma_{ij}^T = 0$ if $i \neq j$.

The effective internal energy of the fluid and that of the geologic media is then given by:

$$H = \sum_n \rho^n S^n h^n \quad , \quad (2.2.2)$$

$$H_e = (1 - \Theta_T) \rho_s c_s T + \Theta_T H \quad , \quad (2.2.3)$$

where:

- h^n is the enthalpy of the n^{th} phase per unit mass,
- Θ_T is the total porosity of the matrix which is defined as the ratio of the total pore space to the total volume of the matrix (see Section 1.5.12),
- c_s is the specific heat of the solid in dry condition,
- ρ_s is the density of porous media in dry condition, and
- T is the temperature.

The effective enthalpy of the fluid and that of the porous matrix may be expressed as:

$$H_e = \alpha_h T \quad , \quad (2.2.4)$$

$$H = \beta_h T \quad , \quad (2.2.5)$$

so that:

$$\alpha_h = (1 - \Theta_T) \rho_s c_s + \Theta_T \beta_h \quad , \quad (2.2.6)$$

$$\beta_h = \sum_n \rho^n S^n h^n / T \quad . \quad (2.2.7)$$

The diffusional heat flux is composed of three components: thermal conduction in the solid, thermal conduction in the fluid, and hydrodynamic dispersion. The effective coefficient for the total diffusional flux is given by:

$$\Gamma_{ij}^T = (1 - \Theta_T) k_s + \Theta_T \tau_{ij} \sum_n S^n k_f^n + \Theta_E D_{ij} \sum_n S^n \rho^n c_f^n \quad , \quad (2.2.8)$$

where:

- k_s is the thermal conductivity of the solid,
- τ_{ij} is a constrictivity or tortuosity factor tensor,

k_T^n is the thermal conductivity of the n^{th} phase,
 D_{ij} is the hydrodynamic dispersion tensor (discussed further in Section 2.5.9), and
 c_T^n is the specific heat of the n^{th} phase.

Combination of Eqns. (2.2.1) through (2.2.8) leads to the governing equation for temperature:

$$\partial_t(\alpha_h T) + \sum_{i=1}^d \partial_i(\beta_h V_i T) = \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij}^T \partial_j T \right) + S_T \quad (2.2.9)$$

Much in the manner of the three different formulations employed for the pressure equation, the temperature equation may also be expressed in terms of a storage coefficient, modified storage coefficient or the delta formulation as:

$$\alpha_h^T \partial_t T + \sum_{i=1}^d \partial_i(\beta_h V_i T) = \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij}^T \partial_j T \right) + S_T \quad (2.2.10)$$

$$\alpha_h^T \partial_t \Delta + \sum_{i=1}^d \partial_i(\beta_h V_i T) = \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij}^T \partial_j T \right) - \partial_t(\alpha_h T) + S_T \quad (2.2.11)$$

$$\begin{aligned} \alpha_h^T \partial_t \Delta + \sum_{i=1}^d \partial_i(\beta_h V_i \Delta) &= \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij}^T \partial_j \Delta \right) \\ &+ \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij}^T \partial_j \Phi \right) - \sum_{i=1}^d \partial_i(\beta_h V_i \Phi) - \partial_t(\alpha_h T) + S_T \quad (2.2.12) \end{aligned}$$

where Φ is the existing temperature, T is the temperature at the new state of the system, and:

$$\Delta = T - \Phi \quad (2.2.13)$$

$$\alpha_h^T = \alpha_h + T \partial \alpha_h / \partial T \quad (2.2.14)$$

From a comparison of Eqns. (2.2.9) and (2.1.11), it is clear that numerical implementation of Eqn. (2.2.10) is likely to conserve energy only if α_h is constant or if it varies slowly so that any changes are negligible compared to the changes in other terms. The other two forms of the equations provide a more rigorous framework for an energy-conservative formulation.

2.3 GOVERNING EQUATIONS FOR MASS TRANSPORT

The equation for conservation of mass species, can be written as:

$$\partial_t C_e^n + \sum_{i=1}^d \partial_i (v_i C^n) = \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij}^C C^n \right) + S_C^n - \lambda^n C_e^n + \sum_m \sigma^{nm} \lambda^m C_e^m \quad , \quad (2.3.1)$$

where:

- C_e^n is the mass concentration of the n^{th} species per unit volume of the porous matrix,
- C^n is the mass concentration of the n^{th} species in fluid,
- Γ_{ij}^C is the effective diffusion (and dispersion) coefficient for mass,
- S_C^n is the source of the n^{th} species,
- λ^n is the decay rate for the n^{th} species, and
- σ^{nm} is the fraction of decay of the m^{th} species which generates the n^{th} species.

To derive the governing mass transport equation, it is assumed that the species transport is limited within only one phase, say the k^{th} phase, of the fluid system. Then:

$$C_e^n = \phi_D C^n + (1 - \Theta_T) C_s^n \quad , \quad (2.3.2)$$

$$\phi_D = S^k \Theta_D \quad , \quad (2.3.3)$$

where:

- ϕ_D is the diffusional porosity of the host matrix saturated with the k^{th} phase,
- C_s^n is the concentration of the species in the solid phase,
- S^k is the saturation of the k^{th} phase, and
- Θ_D is the diffusional porosity of the host matrix (see Section 1.5.12).

We now assume that a chemical equilibrium exists between the fluid and the solid constituents of the porous matrix and that the concentrations in the fluid and the solid are related through a linear Freundlich isotherm (Freeze and Cherry, 1979). With k_d^n as the sorption or partition coefficient for the n^{th} phase, the concentrations in the solid and the fluid are related by:

$$C_s^n = \rho_s k_d^n C^n \quad . \quad (2.3.4)$$

Equations (2.3.2) and (2.3.4) combine to yield:

$$C_e^n = \phi_D R_D^n C^n \quad , \quad (2.3.5)$$

where, R_D^n , the retardation coefficient, is given by:

$$R_D^n = 1 + (1 - \Theta_T) \rho_s k_d^n / \phi_D \quad . \quad (2.3.6)$$

Two options are provided to compute the effective diffusion coefficient for mass. The first option is based on the assumption that Γ_{ij}^C is composed of two components: that due to molecular diffusion and that due to hydrodynamic dispersion, so that:

$$\Gamma_{ij}^C = \phi_D \tau_{ij} D_M + \phi_E D_{ij} \quad , \quad (2.3.7)$$

$$\phi_E = S^k \Theta_E \quad , \quad (2.3.8)$$

where D_M is the molecular diffusion coefficient, τ_{ij} is the tortuosity factor, and ϕ_E is the effective saturated porosity for the k^{th} phase. The second option, following Kemper and van Schaik (1966), provides for an exponential dependence of Γ_{ij}^C on ϕ_D in the form:

$$\Gamma_{ij}^C = D_M \cdot \alpha_1 \exp(\alpha_2 \cdot \phi_D) \quad . \quad (2.3.9)$$

The governing equation for mass species is now obtained as:

$$\begin{aligned} \partial_t(\phi_D R_D^n C^n) + \sum_{i=1}^d \partial_i(V_i C^n) &= \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij}^C \partial_j C^n \right) \\ + S_C^n - \phi_D R_D^n \lambda^n C^n + \sum_m \phi_D R_D^m \sigma^{mm} \lambda^m C^m \quad . \end{aligned} \quad (2.3.10)$$

In a manner analogous to that for the temperature equation, this equation may also be expressed in terms of the three different formulations employed for the temperature equation. The resulting equations are identical to the corresponding formulations for the temperature equation except that the coefficients and source terms are derived from Eqn. (2.3.10) rather than Eqn. (2.2.9).

2.4 THE GENERAL TRANSPORT EQUATION

The transport equations for ground water flow, thermal energy and mass transport, Eqns. (2.1.11), (2.2.9), and (2.3.10), respectively, all have similar mathematical form and therefore can all be represented by a general transport equation of the form:

$$\partial_t(\alpha F) + \sum_{i=1}^d \partial_i(\beta V_i F) = \sum_{i=1}^d \partial_i \left(\sum_{j=1}^d \Gamma_{ij} \partial_j F \right) + S_F - s_F F \quad , \quad (2.4.1)$$

where F is the transported property, α , β , and Γ are the fluid or host media property coefficients, S_F is the source term of F and s_F is the rate constant for reaction or removal of property F. The coefficients α , β and Γ of this equation are summarized in Table 2-1.

TABLE 2-1. COEFFICIENTS AND SOURCE TERMS OF THE GENERAL TRANSPORT EQUATION

F	α	β	Γ_{ij}	S_F	s_F
P^a	$R^a S^a \Theta_E$	0	$R^a K_{ij}^a$	$m_v^a - \partial_i (R^a K_{ij}^a B_j^a)$	0.
T	α_h	β_h	Γ_{ij}^T	S_T	0.
C^a	$\Theta_D R_d$	1	Γ_{ij}^C	$S_C^a + \phi_D \sum_m R_D^m \sigma^{am} \lambda^m C^m$	$\phi_D R_D^a \lambda^a$

Though the derivation of Eqn. (2.4.1) has included the full diffusion coefficient tensor, the current version of PORFLOW assumes that the coordinate directions coincide with the principal axes of the diffusion tensor; therefore all the off-diagonal terms of the tensor are zero.

In the more familiar cartesian and cylindrical polar coordinate notation, this equation is written as:

$$\begin{aligned} \partial_t(\alpha F) + \partial_x(\beta UF) + r^{-1} \partial_y(r \beta VF) + r^{-1} \partial_z(\beta WF) = \partial_x(\Gamma_x \partial_x F) \\ + r^{-1} \partial_y(r \Gamma_y \partial_y F) + r^{-1} \partial_z(\Gamma_z r^{-1} \partial_z F) + S_F - s_F F \quad . \end{aligned} \quad (2.4.2)$$

For the cartesian coordinate system, x, y and z are the cartesian coordinates and r is set to unity. For cylindrical polar coordinate system, x, y and z represent, respectively, the axial coordinate (x), the radius (r), and the angular coordinate (Θ).

The Darcy velocity components for the n^{th} phase are given from Eqn. (2.1.4) as:

$$\begin{aligned}
 U^n &= -K_x^n (\partial_x P^n - B_x^n) \quad , \\
 V^n &= -K_y^n (\partial_y P^n - B_y^n) \quad , \\
 W^n &= -K_z^n (\partial_z P^n - B_z^n) \quad ,
 \end{aligned}
 \tag{2.4.3}$$

where K_x^n , K_y^n and K_z^n are the principal components of the hydraulic conductivity tensor, K_{ij}^n , for the n^{th} phase along the x, y and z directions, respectively.

2.5 THE AUXILIARY EQUATIONS

2.5.1 Introduction

A number of auxiliary relations are required to solve the governing transport equations. These include the specification of fluid and host matrix properties, constitutive relations for properties of the media and specification of source terms, and initial and boundary conditions. The mathematical framework of PORFLOW is general enough to accommodate virtually any relation for these quantities, and many options are continually being added. Some of the commonly employed expressions which are provided as built-in options are summarized below.

2.5.2 Fluid Density

The changes in the fluid density have significant effect on the flow and pressure equations through the introduction of the buoyancy term in the velocity and pressure equations. Some secondary effects of density variation include changes in the storativity, thermal capacity and thermal diffusivity of the fluid. These latter effects are, generally, much smaller than the former. PORFLOW provides for calculation of fluid density by any one of the following alternative equations:

$$\rho = \rho^* [(T_c - T) / (T_c - T^*)]^{n_1} \quad , \tag{2.5.1}$$

$$\rho = \rho^* [1 + a_1(T^* - T) + a_2(T^* - T)^2 + a_3(T^* - T)^3] \quad , \tag{2.5.2}$$

$$\rho = \rho^* [1 + a_1(T^* - T) + a_2(C^* - C)] \quad , \tag{2.5.3}$$

$$\rho = (p + p^*) / [R_u(T + T_s) \sum_j (m_j / M_j)] \quad , \tag{2.5.4}$$

where:

- ρ^* is the fluid reference density,
- T_c is the critical temperature for the fluid,
- T^* is the reference temperature,
- a_1 to a_3 are empirically determined constants,
- C^* is the reference mass concentration,
- p^* is the reference datum for thermodynamic pressure,
- R_u is the universal gas constant,
- T_a is a constant to convert temperature to absolute units,
- m_j is mass fraction of the j^{th} chemical species in the gas, and
- M_j is the molecular weight of the j^{th} species.

The first three of these equations are primarily used for liquids. The last is the equation of state for a perfect gas. For water, Eqn. (2.5.1) gives a good fit to the experimental data with $\rho^* = 996.59 \text{ kg/m}^3$, $T_c = 647.3 \text{ K}$, $T^* = 300 \text{ K}$ and $a_1 = 0.20$. With these values the water density computed from Eqn. (2.5.1) differs from the reference values by less than 1 percent in the temperature range between 4 and 200°C and by less than 2.5 percent between 0 and 350°C (Perry and Chilton, 1973, pp. 3-230).

2.5.3 Fluid Viscosity

The changes in fluid viscosity affect the hydraulic conductivity of the porous matrix. In general, the viscosity of a fluid is a much stronger function of temperature than that of pressure. The effect of pressure is therefore ignored in PORFLOW which provides for two different options for calculation of viscosity:

$$\mu = \mu_0 \exp\left[\frac{a_1}{T + T_a}\right] \quad , \quad (2.5.5)$$

$$\mu = \mu^* \left[1 + a_1(T^* - T) + a_2(T^* - T)^2 + a_3(T^* - T)^3\right] \quad , \quad (2.5.6)$$

where μ^* is the fluid viscosity at reference temperature, T^* , and a_1 through a_3 are empirically determined constants. For water, Eqn. (2.5.5) is recommended by Perry and Chilton (1973, pp. 3-246). With μ_0 and a_1 equal to $6.4 \times 10^{-6} \text{ kg/(m}\cdot\text{s)}$ and 1436 K, respectively, the calculated values differ from the reference values by less than 8 percent between 25 and 250°C, by less than 15 percent between 20 and 350°C, and by 31 percent at 0°C.

In PORFLOW, it is the viscosity ratio rather than the viscosity which is required to account for the influence of viscosity variation on hydraulic conductivity [see Eqn. (2.5.27) below]. The error in this ratio can be considerably decreased from the above values by a

selection of the reference temperature, T^* , to lie towards the middle of the expected temperature range. Equation (2.5.5) can be written in terms of μ^* as:

$$\mu - \mu^* \exp\left[\frac{a_1}{(T + T_a)} - \frac{a_1}{(T^* + T_a)}\right] \quad (2.5.7)$$

2.5.4 Characteristic Saturation Relations

PORFLOW allows for multiple phase flow systems. For example, the flow stream may consist of one (say, water or gas), two (say, water-air, water-gas, water-ice) or three (say, water-oil-gas) phases. The phase change relationships in PORFLOW, which determine S^n , are based on the Clapeyron relation:

$$S^n - S^n(\psi) \quad , \quad (2.5.8)$$

$$\psi - AP + BT \quad , \quad (2.5.9)$$

where ψ may be interpreted as a mean curvature of the phase interface, P and T are the characteristic pressure and temperature of the system, and A and B are empirical constants. However, the Clapeyron phase change relations are applicable in a more general sense and the coefficients need not be interpreted on the basis of surface curvature.

The characteristic saturation relationship, often called soil characteristic, is a basic soil (or rock) property for multiphase (variably saturated) flow and is usually based on empirical measurements. Further, these relations are generally expressed in terms of a cumulative relative saturation, \hat{S}^n , rather than the absolute value of the saturation, S^n . For a three phase system:

$$\hat{S}^1 - (S^1 - S_r)/(1 - S_r) \quad , \quad (2.5.10)$$

$$\hat{S}^2 - (S^1 + S^2 - S_r)/(1 - S_r) \quad , \quad (2.5.11)$$

$$\hat{S}^3 - \frac{(S^1 + S^2 + S^3 - S_r)}{1 - S_r} \quad (2.5.12)$$

where \hat{S}^n is the cumulative relative saturation of the n^{th} phase and S_r is the "residual" or "irreducible" saturation of the primary fluid. From Eqn. (2.1.2), for a three phase system, absolute saturations of the first and second fluids are then given by:

$$S^1 = S_r + (1 - S_r) \hat{S}^1 \quad , \quad (2.5.13)$$

$$S^2 = S_r + (1 - S_r) \hat{S}^2 - S^1 \quad , \quad (2.5.14)$$

$$S^3 = 1 - S^1 - S^2 \quad . \quad (2.5.15)$$

For a two-phase system, S^1 is determined from Eqn. (2.5.13), S^3 is zero and:

$$S^2 = 1 - S^1 \quad . \quad (2.5.16)$$

PORFLOW provides for a number of methods for computation of phase saturations. Many practical applications, especially in ground water hydrology and environmental pollution applications, involve isothermal or near-isothermal fluid systems. In such cases, empirical evidence suggests that the phase saturation is primarily determined by the capillary pressure difference between adjoining phases and the effect of temperature is negligible. In such cases, S^n is specified by empirical functional relations between S^n and δh^n , where δh^n is the capillary pressure between the n^{th} phase and the adjoining $(n+1)^{\text{th}}$ phase; that is:

$$\delta h^n = h^{n+1} - h^n \quad . \quad (2.5.17)$$

The quantity δh^n , which represents the magnitude of capillary pressure is always defined in such a way that "n" refers to the fluid with higher "wettability" (say, water) compared to the fluid denoted by "n+1" (say, air). Therefore, if the capillary pressure, δh^n , is positive, then both fluids are simultaneously present in that pore space (at a macroscopic level); otherwise the pore space is assumed to be saturated with the "wetter" fluid.

For the $(S^n - \delta h^n)$ relations, two options are provided in PORFLOW. The first option is for the characteristic relation to be provided in a tabular form. The second option is to use the general class of saturation characteristic given by:

$$\begin{aligned} \hat{S}^k &= [C + (\delta h^k / H^k)^n]^m ; & \delta h^k > H^k(1 - C) \quad , \\ &- 1 ; & \delta h^k \leq H^k(1 - C) \quad , \end{aligned} \quad (2.5.18)$$

where C , H^k , n , and m are empirical constants. The empirical constant H^k in this equation is the so-called air-entry pressure head. When C is unity and H^k is equal to $1/\alpha^k$, Eqn. (2.5.18) leads to the van Genuchten relation (1978):

$$\begin{aligned} \hat{S}^k &= [1 + (\alpha^k \delta h^k)^n]^{-m} ; & \delta h^k > 0 , \\ &= 1 ; & \delta h^k \leq 0 , \end{aligned} \tag{2.5.19}$$

When C is equal to zero, Eqn. (2.5.18) leads to the Brooks and Corey (1966) formulation:

$$\begin{aligned} \hat{S}^k &= (\delta h^k / H^k)^{-\lambda} ; & \delta h^k > H^k , \\ &= 1 ; & \delta h^k \leq H^k , \end{aligned} \tag{2.5.20}$$

where λ , an empirical constant, is related to m and n by:

$$\lambda = m \cdot n . \tag{2.5.21}$$

From Eqn. (2.5.18), it is easy to conclude that the van Genuchten and Brooks and Corey formulations become identical as the capillary pressure, δh , becomes much larger than the air-entry pressure, H^k .

In contrast to the capillary pressure driven systems, for the water-ice systems, the phase saturation is primarily governed by temperature rather than pressure. The built-in characteristic for phase saturation in PORFLOW employs the constitutive relation given by Wheeler (1973) which is suitable for medium-to-coarse grained soils. In this characteristic relation:

$$\begin{aligned} S_1 &= S_r + \alpha_1 \left\{ 1 + \frac{T_F - T}{T_D} \right\}^{-n} ; & T \leq T_F , \\ &= 0 ; & T > T_F , \end{aligned} \tag{2.5.22}$$

$$S_2 = 1 - S_1 , \tag{2.5.23}$$

where:

- S_1 is the saturation of the liquid phase,
- S_2 is the saturation of the solid phase,
- S_r is the residual "unfreezable" liquid phase fraction for the soil,
- α_1 is a characteristic constant for the soil,
- T_F is the freezing temperature,
- T_D is a characteristic delay temperature for freezing, and
- n is an empirical power law exponent.

2.5.5 Effective Storativity

The effective storativity, S_e of Eqn. (2.1.17) is given by:

$$S_e^n = R^n S^n \alpha_s^n + R^n \Theta_E (S^n \alpha_f^n + \alpha_s^n) \quad (2.5.24)$$

For a porous matrix, α_s^n , the compressibility of the matrix, is assumed to be a constant which is specified from experimental data. R^n and α_f^n are obtained from the fluid density relations. For a liquid, compressibility, α_f^n , is generally quite small and is assumed to be specified by the user as input. For a gas, it can be calculated from the perfect gas law [Eqn. (2.5.4)] as:

$$\alpha_f^n = 1/h^n \quad (2.5.25)$$

For a one phase system, saturation is unity for that phase and zero for all other phases. In such a system α_s^n is zero for confined flow and unity for unconfined flow. For a multiphase system, α_s^n is determined from the saturation characteristic. For tabular input of saturation characteristics, this coefficient is computed numerically. For the saturation characteristics of Eqn. (2.5.18), for the adjoining k^{th} and $k+1^{\text{th}}$ phases, α_s^k is given by:

$$\begin{aligned} \alpha_s^k &= m \cdot n \{1 - C(\hat{S}^k)^{1/m}\} \hat{S}^k / \delta h^k ; & \delta h^k > H^k(1 - C) \quad , \\ &= 0 ; & \delta h^k \leq H^k(1 - C) \quad , \end{aligned} \quad (2.5.26)$$

2.5.6 Hydraulic Conductivity

The hydraulic conductivity tensor, K_{ij} of Eqn. (2.1.5) may be written as:

$$K_{ij}^n = K_{ij}^* k_r^n \rho^n \mu^* / (\rho^* \mu^n) \quad , \quad (2.5.27)$$

$$K_{ij}^* = k_{ij} \rho^* g / \mu^* \quad , \quad (2.5.28)$$

where k_r^n , $0 \leq k_r^n \leq 1$, is the relative permeability for the n^{th} phase, and K_{ij}^* are the reference values of the hydraulic conductivity tensor for a reference fluid (usually water) of density ρ^* and viscosity μ^* . The K_{ij}^* are assumed to be specified from field data for a given soil or rock formation or are calculated from the intrinsic permeability of the porous matrix according to Eqn. (2.5.28). The density and viscosity ratios are calculated from one of the relations given above.

For a single phase system, k_r is equal to unity. For a multiphase system, the k_r may be specified either from empirical data or it may be obtained from the saturation characteristic relations by one or other of the available predictive models. The general form of the resulting expression for the Mualem (1976) or Burdine (1953) predictive models is given by:

$$k_r^n = [\hat{S}^n - \hat{S}^{n-1}]^A \left[\{1 - (\hat{S}^{n-1})^{1/m}\}^m - \{1 - (\hat{S}^n)^{1/m}\} \right]^B, \quad (2.5.29)$$

for the van Genuchten relations, and:

$$k_r^n = [\hat{S}^n - \hat{S}^{n-1}]^A \left[(\hat{S}^{n-1})^{B+2/\lambda} - (\hat{S}^n)^{B+2/\lambda} \right], \quad (2.5.30)$$

for the Brooks and Corey (1966) relations. In these equations, exponents A and B are, respectively, 1/2 and 2 for the Mualem (1976), and 2 and 1 for the Burdine (1953) model. The superscript n takes the values of 1, 2, and 3, with the additional relation that:

$$\hat{S}^0 = 0. \quad (2.5.31)$$

2.5.7 Fluid Enthalpy and Specific Heat

The enthalpy of the n^{th} fluid phase, with h_o^n as its enthalpy of formation and c_p^n as its specific heat, is written as:

$$h^n = h_o^n + \int_T c_p^n dT. \quad (2.5.32)$$

In the current implementations of PORFLOW, it is assumed that the heat of formation for all fluid phases, except for the component which changes phase, is zero. It is further assumed that for all components in solid or liquid form, the specific heat is constant. Thus the enthalpy for these components is given by:

$$h^n = c_p^n T. \quad (2.5.33)$$

For the component which changes phase, the heat of formation and the specific heat are assumed to be defined by:

$$h_v = c_0 + c_1 T + c_2 T^2 + c_3 T^3, \quad (2.5.34)$$

where c_0 through c_3 are empirical constants.

The default set of values in PORFLOW, which are suitable for evaporation of water, are: $c_0 = 3.9202E6$, $c_1 = 3681.00$, $c_2 = -11.76$, and $c_3 = 0.01772$. In this case, T is

in degrees K and h_v in J/kg. Bixler et al. (1985) have proposed a simpler set of values with $c_0 = 3.92017E6$, $c_1 = -2441.00$ and $c_2 = c_3 = 0$.

2.5.8 Vapor Formation Equation

The vapor formation equation in PORFLOW is based on the mass transfer equilibrium principal similar to that implemented by Bixler et al. (1985). The net transfer rate is given by:

$$q_v = C_m \Theta_E (S_l - S_r) (p_s - p_v) / p_g \quad , \quad (2.5.35)$$

where:

- q_v is the rate of evaporation or condensation,
- C_m is an empirical constant,
- S_l is the saturation fraction of liquid,
- S_r is the residual liquid saturation,
- p_s is the saturation pressure of the vapor at equilibrium,
- p_v is the actual thermodynamic pressure of the vapor, and
- p_g is the thermodynamic pressure of the gas phase.

2.5.9 Equilibrium Vapor Pressure

The built-in equilibrium vapor pressure formula in PORFLOW is:

$$p_s = a_0 \exp \left\{ a_1 - \frac{a_2}{T - a_3} \right\} \quad , \quad (2.5.36)$$

where a_0 through a_3 are empirical constants. With $a_0 = 131.57894$, $a_1 = 18.3443$, $a_2 = 3841.1954$, and $a_3 = 45$, and T in degrees Kelvin, the values of saturation pressure for water are in good agreement with the experimental data in the 0°C to 350°C range as shown in Table 2-2.

2.5.10 Hydrodynamic Dispersion

The general form of the hydrodynamic dispersion tensor as given by Scheidegger (1961) is:

$$D_{ij} = \alpha_T \delta_{ij} \underline{y} + (\alpha_L - \alpha_T) |v_i v_j| / \underline{y} \quad , \quad (2.5.37)$$

where α_L and α_T are, respectively, the longitudinal and transverse dispersivities for the porous matrix, δ_{ij} is the Kronecker delta function, and \underline{y} is the magnitude of the local pore or fluid

TABLE 2-2. VAPOR PRESSURE FOR WATER

TEMPERATURE		p, (pascals x 10 ⁵)	
deg C	K	Equation (2.5.36)	Steam Tables
0	273.15	0.00594	0.00611
20	293.15	0.02309	0.02337
50	323.15	0.12260	0.12335
100	393.15	1.00539	1.0133
150	425.15	4.72619	4.7597
170	443.15	7.87248	7.9203
200	473.15	15.47723	15.5506
250	523.15	39.54853	39.776
300	573.15	84.61033	85.92
350	623.15	158.7037	165.37

particle velocity vector, v_i . The particle velocity vector, in turn, is related to the Darcy velocity vector, V_i , and the soil moisture by:

$$y = \left[\sum_i (v_i^2) \right]^{1/2} \quad , \quad (2.5.38)$$

$$v_i = V_i / \phi_E \quad . \quad (2.5.39)$$

The current versions of PORFLOW assume that the principal axes of the dispersion tensor are aligned with the coordinate directions. Consequently, all off-diagonal components are zero and the diagonal components, in (x,y,z) notation, are given by:

$$\begin{aligned}
 D_x &= [\alpha_L U^2 + \alpha_T (V^2 + W^2)] / (\phi_E Y) \quad , \\
 D_y &= [\alpha_L V^2 + \alpha_T (W^2 + U^2)] / (\phi_E Y) \quad , \\
 D_z &= [\alpha_L W^2 + \alpha_T (U^2 + V^2)] / (\phi_E Y) \quad ,
 \end{aligned}
 \tag{2.5.40}$$

and

$$Y = (U^2 + V^2 + W^2)^{1/2} \quad .
 \tag{2.5.41}$$

2.5.11 Fluid, Heat, and Mass Sources

Source terms can be specified for inclusion in the fluid, heat and mass transport equations. These terms may be positive or negative in value. Thus, for example, if fluid is being injected into a zone, the source term for that zone will be positive. On the other hand, if fluid is being withdrawn (or pumped) from a zone, then the source term will be negative; in such a case it should, strictly, be referred to as the sink term. PORFLOW allows for both constant and time-varying sources. In the latter case, these may be either tabulated or analytic functions of time. The tabulated values may vary arbitrarily with time. The analytic options provide for two formulations: an exponential decay with time and a solubility-limited option.

The built-in exponential decay formulation, for a source comprised of N components, is of the form:

$$S_F = \sum_{n=1}^N s_n \exp(-f_n t) \quad ,
 \tag{2.5.42}$$

where S_F is any of m_v , S_T or S_C^a , s_n is the strength of the n^{th} component of source, f_n is the characteristic frequency (or time) constant for the n^{th} component, and t is the time.

The solubility-limited source term option is available for mass species only; that is, the S_C^a term. In this option, it is assumed that a finite inventory of the source material, such as a chemical or radionuclide species, is initially present. This material is then dissolved by the fluid such that the maximum concentration in the fluid phase does not exceed the solubility of the species. Specifically, the rate of dissolution is given by:

$$S_C^a = f_s (C_s^a - C^a) \quad ,
 \tag{2.5.43}$$

where S_C^a is the rate of species dissolution, f_s is a dissolution frequency, and C_s^a is the saturation limit of the species in the fluid. In implementation of Eqn. (2.5.43), the amount of inventory

dissolved is computed at every time step and the frequency term is set to a large number as long as the source inventory has not been exhausted, otherwise it is set to zero.

PORFLOW also accommodates decay of a species due to radioactivity or first-order Arrhenius chemical reaction. With $t_{1/2}^n$ as the half life of the species, the decay rate is:

$$\lambda^n = \ln(1/2)/t_{1/2}^n \quad (2.5.44)$$

A fraction of the decay of the n^{th} species may generate the next species in the chain; this fraction is denoted by σ^{nm} and, along with $t_{1/2}^n$, is specified as part of the input by the user.

2.5.12 Boundary Conditions

The general form of boundary condition for the transport equation is:

$$-\Gamma \partial F / \partial N - h_F (F - F_o) + q_F = 0 \quad (2.5.45)$$

where F represents P^n , T , or C^n , N is the direction coordinate normal to the boundary, and Γ , h_F , F_o , and q_F are specified quantities. Appropriate selection of these quantities, results in three types of boundary conditions, called the Dirichlet, the Neumann and the mixed (also called radiation, Robbins or third kind) boundary conditions. All three boundary conditions are available in PORFLOW; these are discussed below.

Dirichlet condition: With $\Gamma = q_F = 0$, and F_o as the specified value at the boundary, Eqn. (2.5.45) reduces to:

$$F = F_o \quad (2.5.46)$$

Neumann condition: When $h_F = 0$, the resulting expression is:

$$-\Gamma \partial F / \partial N = q_F \quad (2.5.47)$$

Here Γ is either unity if the gradient of the variable is specified or it represents the appropriate component of the hydraulic conductivity (K_{ij}), thermal conductivity (Γ_{ij}^T), or the dispersion coefficient (Γ_{ij}^C) tensor for the corresponding equation if the flux of the variable is specified. It is internally computed from other input data and separate specification is not required. The quantity q_F is the specified boundary gradient or flux of fluid, heat, or chemical species.

Mixed condition: With $q_F = 0$, Eqn. (2.5.45) simplifies to:

$$-\Gamma \partial F / \partial N - h_F (F - F_0) \quad . \quad (2.5.48)$$

In this equation, Γ has the same meaning as for the Neumann condition, h_F is the fluid, heat, or mass transfer coefficient, and F_0 is the equilibrium value of F .

2.5.13 Initial Conditions

The governing equations require the specification of a well posed set of initial conditions. The initial conditions for pressure, P , the temperature, T , and the species C^a may be specified explicitly or they are taken to be zero by default. In addition, the Darcy velocity components, U , V , and W , may be initialized to values other than zero. The variable values may be initialized arbitrarily or according to the relation:

$$F = F_0 + a_1 x + a_2 y + a_3 z \quad , \quad (2.5.49)$$

where F_0 , a_1 , a_2 , and a_3 are constants, and x , y , and z are the coordinates of a point either in the interior of the domain or on the boundary.

3 NUMERICAL BASIS

The governing partial differential equations of PORFLOW are solved by the Nodal Point Integration method. A choice of integration profiles or basis functions is provided for spatial discretization of the equations. These lead to the hybrid, the exponential and the CONDIF numerical schemes. The system of algebraic equations resulting from the discretization process is solved by one of five matrix solution methods. Numerical solution of the governing equations described in Chapter 2 requires three steps: (1) A grid arrangement to divide the domain of interest into discrete intervals, (2) discretization and derivation of the algebraic analogues of the equations by a "numerical scheme", and (3) solution of the resulting algebraic equations by a matrix "solution method". Like all numerical methods, the numerical stability and accuracy of the algorithms employed in PORFLOW are functions of the discretization process. These issues are discussed in this Chapter.

3.1 THE GRID ARRANGEMENT

The first step towards obtaining a numerical solution is spatial discretization of the domain of interest. In PORFLOW, the field of interest is divided into a number of contiguous elements each of which is an individual control volume. A nodal point, which represents the intersection of the three coordinate lines, is associated with each of the elements. Examples of such a grid in cartesian and cylindrical coordinate systems are shown in Figures 3-1 and 3-2, respectively. In these figures, the cell boundaries are drawn midway between the grid lines, and each cell encloses one grid node. If the grid spacing is nonuniform, then the node is not at the centroid of the cell. As indicated in Figures 3-1 and 3-2, each node is denoted by an ordered alphanumeric triplet (I,J,K), in the respective grid directions (x,y,z) or (x,r,θ).

PORFLOW employs a staggered grid approach. All the state variables, except the velocity components, are defined at the grid nodes. The velocity components, U, V and W, and the fluxes of heat, and mass are defined at cell boundaries (solid lines). The U, V and W velocity locations fall midway between the grid nodes in the x, y (or r) and z (or θ) directions, respectively. Details of this arrangement of variables and the integration cell are shown in Figures 3-3 through 3-5. This use of a 'staggered' grid leads to a more natural description of the physical system where the fluxes are defined at the element boundaries and the intrinsic properties at the node points.

3.2 DISCRETIZATION SCHEME

The discretized form of the governing equation [Eqn. (2.4.1)] is obtained by integrating it over each cell such as the one shown in Figure 3-5. The integration method used is called the Nodal Point Integration (NPI). The NPI method is a variation of the finite-volume or the integrated finite-difference method and bears some resemblance to the finite-element method.

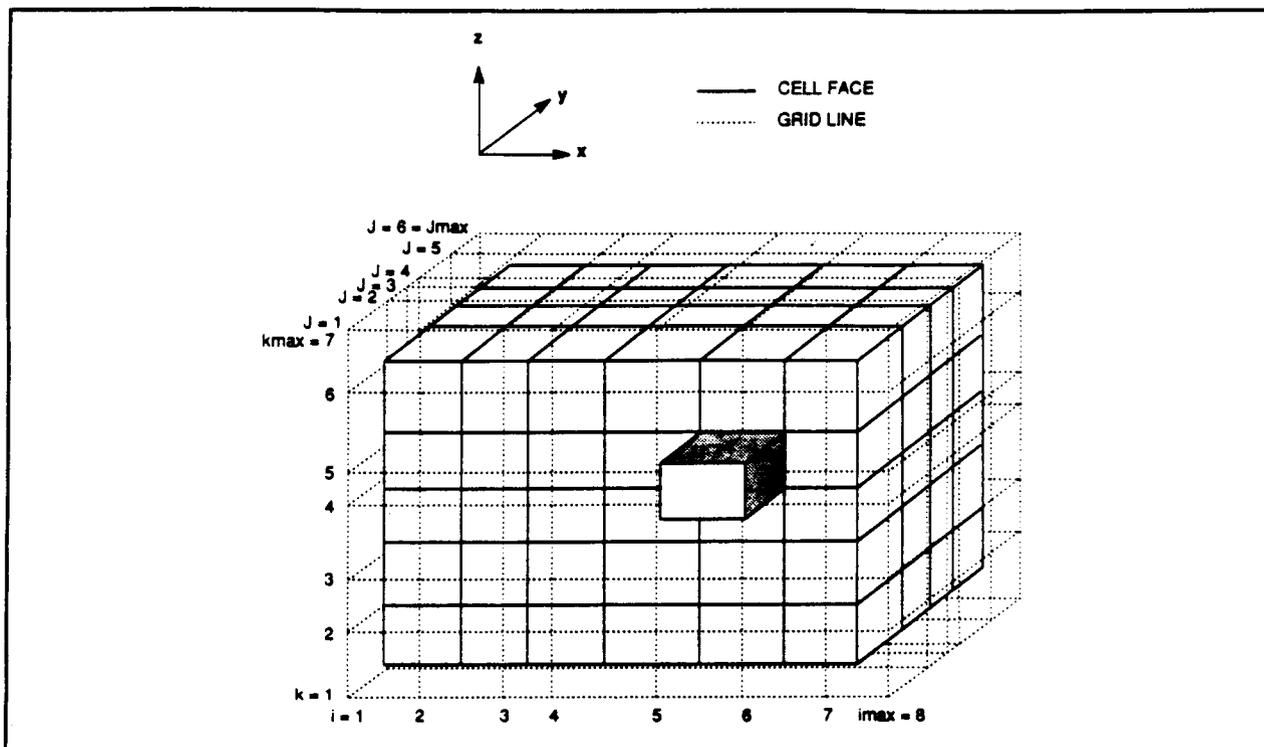


Figure 3-1. Cartesian grid arrangement

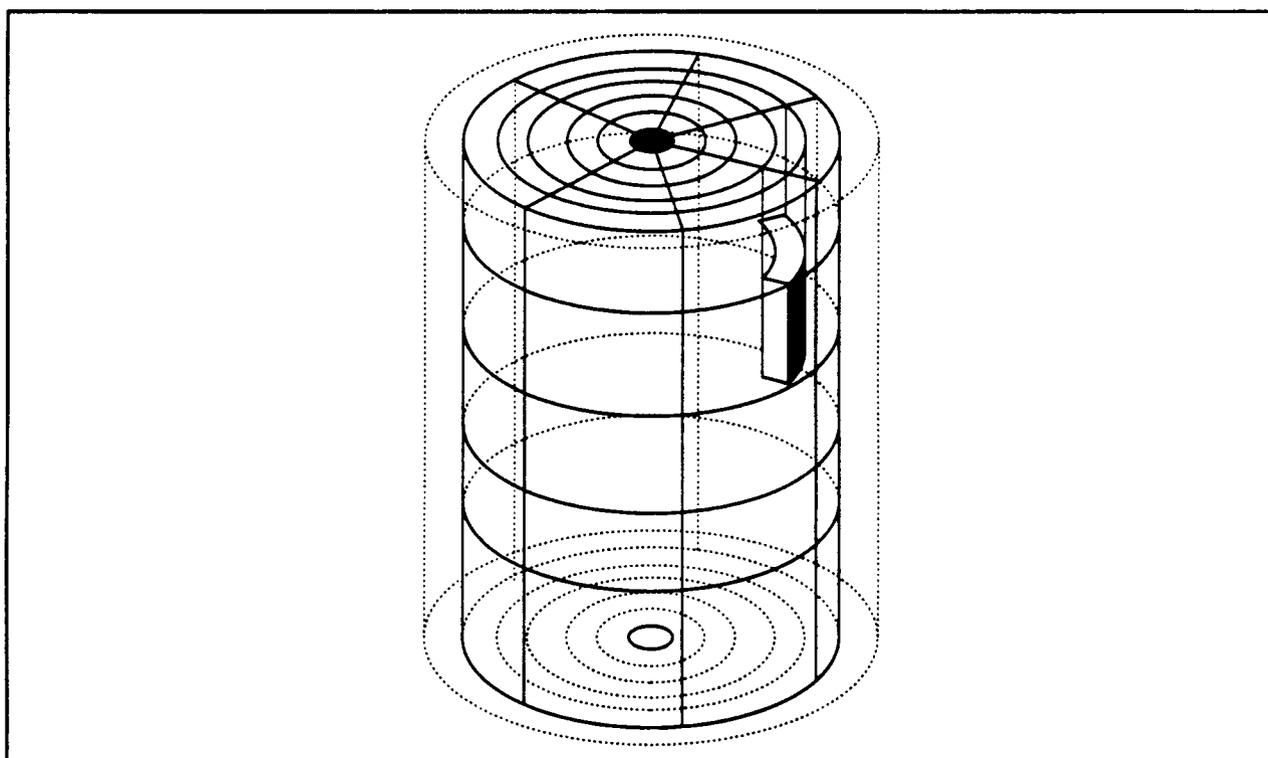


Figure 3-2. Cylindrical grid arrangement

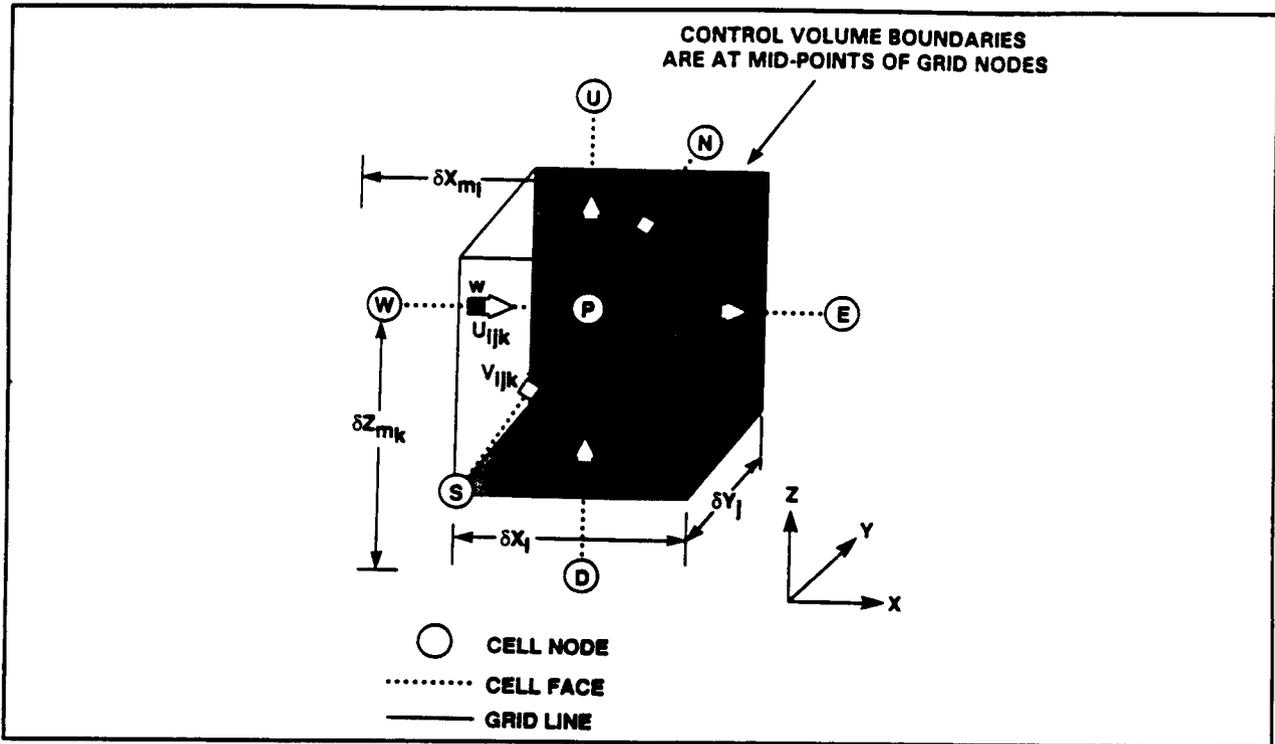


Figure 3-3. Typical grid cell in cartesian coordinates

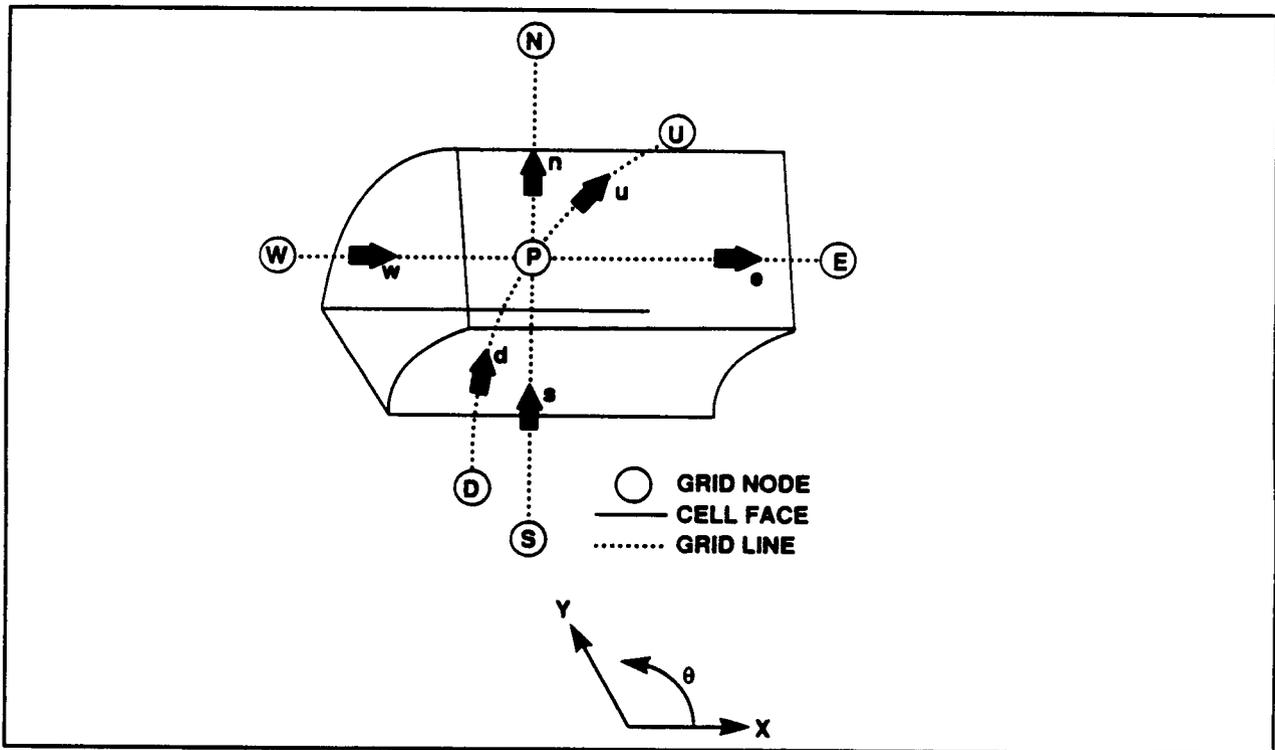


Figure 3-4. Typical grid cell in cylindrical coordinates

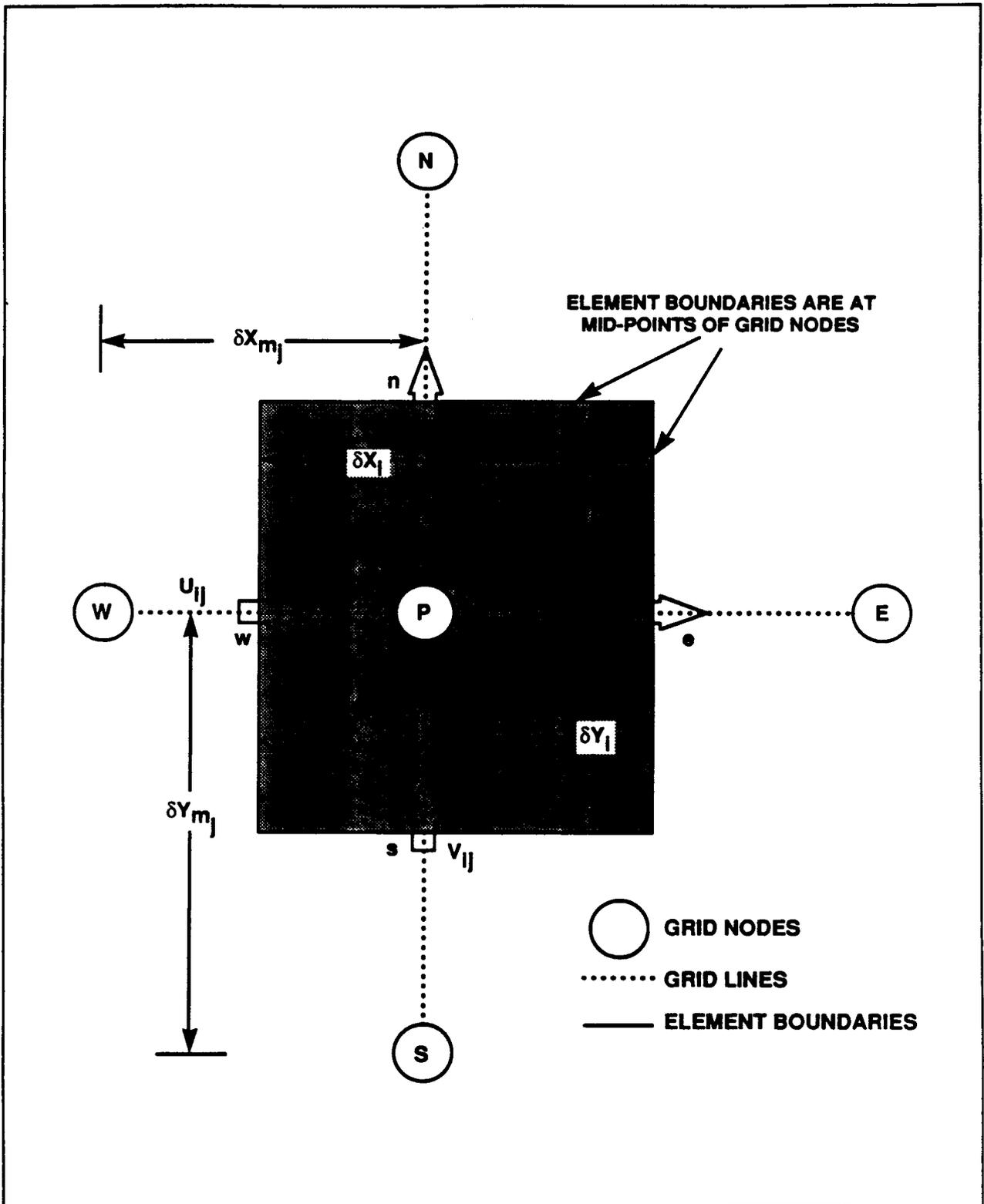


Figure 3-5. Typical grid cell arrangement in x-y plane

However, it is simpler and more economical than the finite-element methods. A major advantage of the NPI method, over the finite-difference and finite-element methods, is that it intrinsically preserves the mass, material and thermal fluxes both at local and global scales. It is thus inherently mass-conservative and leads to more accurate and stable numerical formulations. The details of the NPI method are available, for example, in Runchal (1987a).

PORFLOW employs a numerical approach for spatial integration which leads to unconditional (linear) stability. The spatial variation of state variables is approximated by appropriate profiles to ensure accuracy and stability. The governing transport equation consists of three types of terms: the convective terms, the diffusive terms and the source terms. The NPI method treats the convective and diffusive terms in a unified manner; the other terms are treated individually (Runchal, 1987a).

The numerical integration starts with the assumption of an integration profile for the state variable. The current version of PORFLOW employs three different kinds of profiles. These are the first order polynomial, the second order polynomial and, the exponential profile. These result, respectively, in the upwind, the central difference and the exponential scheme. The first two are used in PORFLOW in a special combination, called the hybrid scheme. The central difference scheme, which provides second-order accuracy, is the preferred scheme in PORFLOW. It is well known, however, that the central difference scheme may lead to numerical instabilities if the magnitude of the local grid Peclet number exceeds 2. With U , δL and Γ , respectively, as the velocity component, grid interval and diffusivity in a given direction, the grid Peclet number, Pe , is defined as:

$$Pe = U\delta L/\Gamma \quad (3.2.1)$$

The value of local Peclet number at each grid node, in each direction, is constantly monitored and if $Pe > 2$, then an automatic shift to the 'upwind' formulation is made. This method of enhancing stability is known as the hybrid scheme (Runchal, 1972). The hybrid scheme is second-order accurate if the $Pe < 2$; otherwise it is only first-order accurate. It is known that "upwinding" leads to an increasing amount of numerical diffusion as the angle between the velocity vector and the grid lines increases. PORFLOW therefore provides for the exponential numerical scheme (Spalding, 1972) which represents the exact solution of the one-dimensional form of transport equations without sources. The exponential scheme cannot be accurately classified; however, in practice, it is known to decrease numerical diffusion if the flow is primarily unidirectional and source terms are small, otherwise its accuracy has been found to be comparable to that of the hybrid scheme. An alternate method to obtain stability with second-order accuracy is that of the CONDIF scheme (Runchal, 1987b) which is a member of the TVD family of numerical schemes (Harten, 1984). CONDIF leads to an unconditionally stable formulation in the form of a modified central difference scheme.

The method of evaluation of the integrals, which is equivalent to the selection of a basis function in the finite-element technique, is under user control in PORFLOW. For most

problems it proves sufficient to employ the hybrid scheme. If the grid is very coarse, then the CONDIF, or in some cases, exponential scheme should be employed.

The discretization with respect to time may be either explicit or implicit. In the explicit scheme, all terms of Eqn. (2.4.1), except the storage term $\partial_t(\alpha F)$, are evaluated from known values at the previous time step. The values at the current time step can then be calculated by a straightforward backward discretization of the storage term. In an implicit scheme, by comparison, some or all of the convection, diffusion, and source terms appearing in Eqn. (2.4.1) are taken at the new time step. Each algebraic equation in this case has more than one unknown, and matrix methods are required to solve the set of equations. The storage term in the general transport equation may be treated in one of the three ways: these are the storage coefficient, the modified storage coefficient, and the delta formulations described in Section 2. These are also referred to as the Picard, the modified Picard and the Delta formulations later in this document.

An algebraic analogue of the general transport equation, Eqn. (2.4.1), can be written in terms of appropriate expressions for the storage, convection, diffusion and source terms. This analogue relates the value of a dependent variable at the central node to those at the neighboring nodes by the equation:

$$A_P(F_P^{k+1} - F_P^k) + \sum_K A_N[\Theta(F_P^{k+1} - F_K^{k+1}) + (1 - \Theta)(F_P^k - F_K^k)] - \delta V S_{FP} - s_{FP}[\Theta F_P^{k+1} + (1 - \Theta)F_P^k] \quad (3.2.2)$$

In Eqn. (3.2.2), the subscript P denotes the node point at location (I,J,K), δV is the volume of the cell at P and summation is carried over all the neighboring nodes shown in Figure 3-3. That is: the subscript K denotes the grid node values at E, W, N, S, U and D, respectively. The coefficients, A's, are functions of grid size, fluid velocity, and properties of the fluid and the porous media. Their exact forms depend on the spatial and temporal discretization scheme adopted. The superscripts k and k+1 denote the value of the variable F at two successive time steps. The parameter Θ determines whether the numerical scheme is explicit ($\Theta = 0$), implicit ($\Theta = 1$), or semi-implicit ($0 < \Theta < 1$). The choice of Θ in PORFLOW is made internally and is based upon the method of solution selected by the user.

3.3 SOLUTION METHOD

One algebraic equation, similar to Eqn. (3.2.2), is obtained for each grid node. To solve this set of algebraic equations, five options are currently available and new options are continually being evaluated for inclusion.

The first option is for use with explicit schemes. In this case, there is only one unknown (F_p^{k+1}) per equation; all other F's are known from the previous time step, previous iterate, or initial conditions. Equation (3.2.2) can then be solved for the new value at each node. For steady state solution, the process is repeated until the calculated values do not change by more than a specified tolerance limit. This procedure is termed the method of Successive Over-Relaxation (SOR).

The second method, the Alternating Direction Implicit (ADI) method, solves the set of algebraic equations in three sweeps, one each along the x-, y-, and z- coordinate directions. It is semi-implicit in nature. For each sweep, Eqn. (3.2.2) is written only with the values at the grid nodes in that direction at the advanced time step. All other values are taken at the previous time step. In this manner, each equation has only three unknowns (e.g., F_p^{k+1} , F_E^{k+1} , and F_W^{k+1} in the x-direction sweep) which gives rise to a tri-diagonal system of equations that are solved by the Thomas Algorithm (Varga, 1962).

The remaining three methods, Cholesky Decomposition, Gaussian Elimination and Conjugate Gradient, are implicit in nature. The first two of these are direct matrix solvers; the third is an iterative solver. The Cholesky Decomposition is applicable only to a symmetrical matrix. In PORFLOW, the pressure equation always generates a symmetrical matrix; the thermal and species equations generate a symmetrical matrix only if the convection terms are zero. Therefore the application of this method is rather limited. However, it is one of the most efficient direct solvers for large matrices. In this method, the symmetric coefficient matrix of the algebraic equations is decomposed into a special form that consists of a diagonal matrix, and lower and upper triangular matrices. Once the decomposition is done, the solution is obtained by back substitution. Gauss Elimination without any preconditioning is the fourth method of solving implicit equations. This method is applicable to both symmetric and nonsymmetric matrices and, therefore, to all three governing equations of PORFLOW. Direct solution methods suffer from two drawbacks: the computer time and storage requirements increase as N^3 and N^5 , respectively, where N is the number of grid nodes.

The fifth solution method available in PORFLOW is the method of Conjugate gradients. It is applicable to both symmetric and nonsymmetric matrices. Unlike the Cholesky and Gauss methods, it is an iterative method. The computer storage requirements of this method are proportional to N; the computer time increases as N^m where m is generally between 1 and 2.

3.4 NUMERICAL STABILITY AND ACCURACY

3.4.1 General Considerations

The numerical schemes and solution methods employed in PORFLOW represent the best options currently available for solving a wide variety of porous media flow and transport problems. In general these provide accurate, economical, and numerically stable solutions. However, as in all numerical solution methods, an instability may arise in the numerical solution

when the physical process being simulated exhibits nonlinearity or when strong coupling between various components of the model exists. A numerical instability may exhibit itself either as "weak instability" or "exponential growth." Weak instability usually can be identified in terms of a step-to-step oscillation about a mean value. In PORFLOW this trend becomes obvious by examination of the diagnostic output. Exponential growth can be identified in terms of an uncontrolled growth in the values of the state variables.

The hybrid, exponential and CONDIF numerical schemes used in PORFLOW are unconditionally stable for any spatial discretization in the linear sense (von Neumann analysis). The stability of the temporal discretization depends upon the solution method adopted. The direct matrix solvers always provide a solution (except for round-off) to the matrix of algebraic equations, provided one exists. The ADI and Conjugate gradient methods are stable in the linear sense. The SOR is conditionally stable provided certain criteria are met. It should be noted that no methods currently exist to establish the stability of the complete, coupled, nonlinear system of PORFLOW equations. It is known that instabilities in such systems may arise due to the coupling and nonlinear terms. The numerical accuracy of the schemes employed in PORFLOW varies from first order to second order with respect to spatial discretization. With respect to temporal discretization, the accuracy is second order for the ADI and first order for all other solution methods.

The accuracy of the numerical solution improves with a decrease in grid size and time step. The stability of a scheme, on the other hand, generally improves with a decrease in the time step but is adversely affected by a decrease in the grid size. The numerical efficiency, or economy, is often adversely affected by a decrease in both the grid size and the time steps. Thus, considerations of numerical stability, accuracy and economy often impose conflicting requirements on the discretization process. The physical processes and numerical approximations inherent in the PORFLOW code imply the existence of several characteristic temporal and spatial scales. For efficient, accurate and stable numerical solution, these scales must be duly considered in the selection of the grid distribution and time step. The influence of the time step is, of course, limited to transient solution process; it plays no role in the steady state simulations. These issues are discussed further below.

3.4.2 Time Scale of Pressure Propagation

The characteristic time scale for propagation of transient pressure effects is given by:

$$\delta t_{\text{press}} = S_e \delta L^2 / (2K) \quad , \quad (3.4.1)$$

where S_e , δL , and K are, respectively, the representative values of effective storativity, grid size, and hydraulic conductivity.

This characteristic time scale is of importance for transient fluid flow problems. All pressure disturbances propagate across a grid interval of length δL in this time. For explicit schemes (e.g. SOR), the time step employed must not exceed the value given by Eqn. (3.4.1). For the other methods, although no numerical stability conditions apply, it is recommended that, for accurate representation of transient effects, the time step employed should be within an order of magnitude of the value calculated from Eqn. (3.4.1).

For iterative schemes, sometimes numerical instability may be encountered due to nonlinear and coupling effects if the time step employed is much larger than this time scale. In such cases either the time step must be decreased or a direct solution method must be adopted.

Many problems of practical interest are characterized by very small values of effective storativity (or zero for steady-state problems). The pressure propagation time is then very small or zero. In such cases it may be better to use PORFLOW in its quasi- or fully steady-state mode where the pressure equation is solved by the modified ADI or direct method. The alternative is to use an artificially large value for specific storativity which then allows the use of large time steps. In such a case, the storativity essentially acts as a relaxation parameter in the solution procedure (see, for example, Varga, 1962). In this instance the transient solution obtained will not be accurate.

3.4.3 Time Scale of Diffusion

An important time scale for physical phenomena that are significantly influenced by diffusion is given as:

$$\delta t_{\text{diff}} = \alpha_e \delta L^2 / (2\Gamma_e) \quad , \quad (3.4.2)$$

where α_e is a representative value of the accumulation coefficient, α , and Γ_e is a representative value of the effective diffusivity, Γ_{ij} in Eqn. (2.4.1).

This time scale is similar to that for pressure propagation, except that α_e and Γ_e play the roles of the S_e and K , respectively. Both temperature and species equations contain diffusion terms. The general implications of this time scale are similar to those for the pressure propagation scale. The time step employed should be kept within an order of magnitude of the value given by Eqn. (3.4.2). For the explicit solution method, the time step employed must not, for reasons of stability, exceed the value given by this equation.

3.4.4 Time Scale of Convection

With U and δL as the characteristic velocity component and grid interval, the convection time scale, δt_{conv} , is defined as:

$$\delta t_{\text{conv}} = \delta L/U \quad (3.4.3)$$

The constraint based on this time scale is often stated in terms of the Courant number, Co , which is defined as:

$$Co = \delta t / \delta t_{\text{conv}} = U \delta t / \delta L \quad , \quad (3.4.4)$$

where δt is a representative time step for the numerical solution.

The explicit solution method requires that the Courant number must not exceed unity; the other methods are not subject to any Courant-number-based constraint, as indicated by linear stability analysis. Nonetheless, for useful simulation of a physical process that is significantly influenced by convection, the time step employed should be within an order of magnitude of the convection time scale for the physical process, δt_{conv} .

3.4.5 Other Pertinent Time Scales

For any specific problem, it is likely that other pertinent time scales may need to be considered. These time scales may arise, for example, from the presence of uniform or time-varying pumping or injection rates, propagation of saturation front, buoyancy, heat or mass sources, chemical reaction, radioactive decay, and time-dependent boundary conditions. Each of these imposes certain physical and numerical time-scale constraints on the solution process. These constraints can be determined by recourse to the corresponding governing differential equation.

3.4.6 Grid Peclet Number

The grid Peclet number, as defined by Eqn. (3.2.1) above, plays an important role in the numerical stability and accuracy of a numerical scheme, if both the convective and diffusive terms are nonzero¹ (β and Γ of Table 2-1). The hybrid and the exponential schemes used in PORFLOW, are unconditionally stable for arbitrary values of the grid Peclet number. However, the numerical accuracy, especially that of the steady-state component of the solution, is strongly governed by the grid Peclet number (Roache, 1972; Runchal, 1977). In particular, it can be shown that, depending on the assumptions made for spatial variation of the state variables, significant numerical errors may occur if the local grid Peclet number is greater than 2.

¹Since the pressure equation does not contain any convective terms, the Peclet number is important only for temperature and concentration equations.

In PORFLOW, the spatial profile employed for integration of the governing equations is chosen on the basis of the local value of the grid Peclet number. If the grid Peclet number is less than 2, then a second-order polynomial (equivalent to a central difference scheme) profile is employed. If, however, this number exceeds a value of 2, then PORFLOW provides for three alternative options. These options are the hybrid, the exponential and the CONDIF methods as discussed in Section 3.2. The actual choice must be based on a balance between accuracy and economy.

In practice, the second-order approximation with automatic shift to upwind differences is often adequate for solution of the temperature equation. The characteristic velocity for this equation is the Darcy velocity, which is typically small and allows large time steps according to the criterion above. For the concentration equation on the other hand, the characteristic velocity is the pore velocity. Therefore, for this equation, it may be advisable to employ one of the other options.

3.5 CONVERGENCE

PORFLOW contains both iterative and direct methods for solution of the matrix of algebraic equations which result from the discretization process (see Section 3.2). These equations can be expressed in the matrix form:

$$A_{ij} \phi_i - b_j \quad , \quad (3.5.1)$$

where A_{ij} is the matrix of coefficients, ϕ_i is the unknown solution vector and b_j is the forcing function. For direct solution methods, the matrix inversion process leads to an exact solution of the above set of equations (within the round-off error limits of the computer).

For iterative solution methods, however, Eqn. (3.5.1) is rearranged as a successive approximation equation:

$$\phi_i^k - T_{ij} \phi_j^{k-1} + c_i \quad , \quad (3.5.2)$$

where ϕ^k is the k^{th} approximation to ϕ_i , T_{ij} is a modified coefficients matrix and c_i is a modified forcing function. This process starts with an initial condition, or initial estimate to the solution vector, ϕ_i , and the process is repeated until the successive iterates converge to a pre-specified tolerance. In PORFLOW, two criteria are used to test for convergence. The first criterion relies upon a test of the residuals such that:

$$R_1 = \frac{1}{N} \sum_{i=1}^N |A_{ij} \phi_i - b_j| \leq \epsilon \quad , \quad (3.5.3)$$

where ϵ is a small quantity (typically on the order of the computer accuracy) and N is the number of grid nodes.

The second criterion is based upon the successive departure of the iterates and can be expressed as:

$$R_2 - \max(1 - \phi_i^k / \phi_i^{k-1}) \leq e, \quad i = 1, 2, 3, \dots, N, \quad (3.5.4)$$

where ϕ_i are the successive iterates at the i^{th} node.

4 SPECIFICATION OF PROBLEM GEOMETRY AND GRID

The first step in solving a given problem is to specify the problem geometry and a corresponding grid for spatial discretization. Details of this input are given in Chapters 5 and 6. This chapter provides some hints which may prove useful in selecting and specifying a suitable geometry and grid for a problem. The geometry of the problem is specified in terms of basic geometric elements of PORFLOW called "zones" or "sub-domains." For complex problems, much of the input specification is made by sub-dividing the domain of interest into a number of zones or sub-domains that differ from the others in some respect. This chapter outlines the manner in which zones or sub-domains are defined and later employed, to accommodate disparate geometric components of a physical problem.

4.1 SPECIFICATION OF PROBLEM GEOMETRY

The problem geometry in PORFLOW is defined by a set of cartesian (x,y,z) or cylindrical (x,r,θ) coordinates. The domain of interest is specified in terms of basic geometric elements called zones or sub-domains. Any sub-region of the domain of interest that has distinct physical properties or other characteristics which distinguish it from other sub-regions is defined as a distinct zone. Distinguishing features include, for example, different rock or soil types or layers, fractures, or boreholes.

Once the physical domain of the problem has been identified in terms of the zones, the next step is to impose a discrete spatial grid over the domain of interest (see Figures 3-1 and 3-2). Some criteria and hints for the selection of this grid are discussed below in Section 4.2. Intersections of these grid lines are called the grid nodes. Each of these nodes is associated with an element or control volume which is formed by the mid-points of the grid lines (Figure 3-3). Location of each grid node is identified by its physical coordinates (x,y,z) or (x,r,θ) and by a unique set of grid indices (I,J,K) where I , J and K refer, respectively, to the x , y (or r) and z (or θ) direction. All the state variables, except velocity components, are defined at the grid nodes. The U , V and W velocity components, as shown in Figure 3-3, are defined at locations which are, respectively, midway between the grid nodes in the x , y (or r) and z (or θ) directions. The index notation employed is such that the velocity components at the west, south and bottom face of the control volume are denoted by the same I , J and K indices as the F values at the grid node. The use of this staggered grid approach results in a more natural description of the physical system whereby the fluxes are defined at the element boundaries and the intrinsic properties at the element node.

The grid must be selected in such a manner that the physical boundaries of each zone are coincident with the boundaries of the control volumes. An exception to this is allowed for the outermost zones lying at the boundaries of the domain of interest. The boundaries for these may coincide with either the control volume boundaries or the grid node locations. This arrangement

allows the fluxes across the zone boundaries to be correctly incorporated into the PORFLOW algorithm. The fluxes at the boundaries of the outermost zones are computed from the specified boundary conditions. As mentioned in Section 2.7, the Dirichlet boundary conditions for these may be specified at the grid nodes or cell interfaces; all other types of boundary conditions are always specified at the cell interface. If the outer boundary of an outermost zone coincides with the cell interface, then the outermost node lies outside the domain of interest and acts as a fictitious node for implementation of boundary conditions.

At times, a physical boundary of the domain of interest may be inclined to the principal directions. Such boundaries may be specified by the arrangement shown in Figure 4-1. The inclined boundary consists of the diagonals of the nearest elements that straddle the inclined boundary. The specification of the boundary is then made in terms of the stair-stepped zone shown in Figure 4-1. With reference to Figure 4-1, all elements below the stair-stepped boundary can be defined as nodes belonging to a zone that is distinct from the zone of the nodes above the stair-stepped boundary. For example, all elements below and to the right of the stair-stepped boundary may be defined as aquitard nodes if the inclined boundary represents a barrier to ground water movement.

4.2 SPECIFICATION OF SPATIAL AND TEMPORAL GRID

4.2.1 Basic Considerations

Several considerations influence the design of the computational grid for a given problem. These include:

1. Computer resources,
2. Desired numerical accuracy,
3. Special geometric and physical features of the problem,
4. Stability of the numerical solution process,
5. Nature and type of boundary conditions, and
6. Special output requirements.

Some of these considerations lead to conflicting requirements. For example, the accuracy of the numerical process generally increases with the number of grid nodes, but so does the cost. Also, it may not be possible to resolve all the special features of geometry or boundary conditions within the constraints of the available computer resources. Similar compromises may be necessary to accommodate other features of a given problem.

4.2.2 Computer Resources

The first step in selection of grid size and time step is a consideration of the available computer resources of memory size and computation time. This provides an upper limit on the number of nodes and time steps which can be employed for numerical simulation.

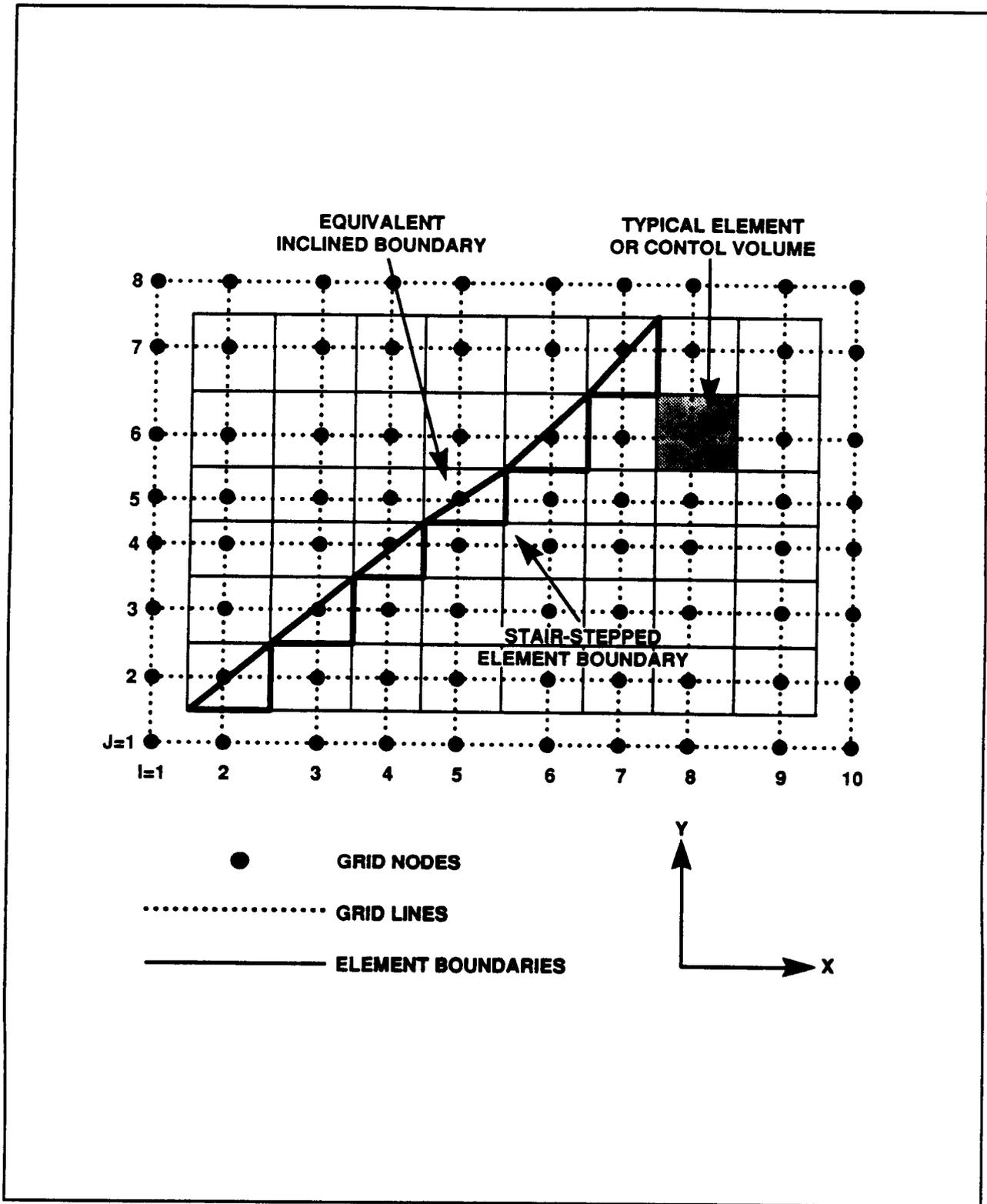


Figure 4-1. Incorporation of inclined physical boundaries

This leads to average spatial (δx , δy and δz , or δx , δr , and $\delta \theta$) and temporal (δt) scales of resolution.

4.2.3 Numerical Stability and Accuracy

The criteria of stability and accuracy outlined in Section 3.4 should be applied to determine the approximate upper and lower limits of the grid size and time step. This determination should be based on the known or expected values of the other pertinent parameters (such as velocity, diffusivity, etc.) of the problem. Any adjustments to grid size or number of nodes imposed by these criteria should then be made accordingly.

4.2.4 Scale of Heterogeneity

Variations in hydraulic, thermal, and mass transport properties should be adequately represented by the grid. These properties are specified at grid nodes and are assumed to remain constant within a cell. If they change in a discontinuous manner, as commonly would occur in layered media, the grid should be designed such that a cell face coincides with the discontinuity. For regions with continuously varying properties, the grid should be finer where the variation in properties is relatively rapid, and coarser 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.

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

4.2.5 Scale of Physical Resolution

For a variety of reasons, in specific parts of the domain, solutions may be needed at a finer scale than in other parts. For example, interest may be focused on those areas where temperatures or chemical concentrations are high. In such areas, smaller cells should be used. On the other hand, it may prove necessary to resolve certain features at a larger scale than that of the feature itself. For example, for a problem involving simulation of field pumping tests, the size of an individual pumping well may be too small (e.g., a few centimeters) in comparison to the spatial scale of the problem (e.g., on the order of hundreds to thousands of meters). In such a case, the pumping is typically distributed over an entire grid element that may have a length dimension on the order of a few meters. The resulting solution will not be accurate for prediction of local effects close to pumping; however, it will provide acceptable approximation of the effects of pumping on the rest of the flow field.

4.2.6 Planar and Linear Features

Geologic or man-made features such as fractures and clastic dikes, and bore holes, wells, and tunnels, are distinguishable from the geologic continuum by distinctive contrasts in their physical properties and scales. They may be represented as distinct zones if the geometric dimensions are such that they can be adequately resolved by the grid elements of PORFLOW. However, the fracture width or the borehole diameter is often too small to be economically resolved by grid 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.

In these cases, PORFLOW permits geometric features and properties of the planar and linear features to be identified independent of the remaining input. A restriction is placed on the geometry of these discrete structures; they must begin and end at the nodes of the grid. These planar and linear features are then automatically embedded in the porous media by the PORFLOW code. Although these features are embedded within the porous media and communicate with it by means of the applicable governing mathematical formulations, PORFLOW tracks the flow and transport in them separate from that of the porous media.

4.2.7 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. If this proves prohibitive, then it may be necessary to distribute the source (or sink) over a larger area with the knowledge that the solution in the immediate vicinity of the source may be limited in its accuracy.

4.2.8 Boundary Conditions

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

In PORFLOW, the physical (external) boundaries of the problem geometry must either coincide with the grid lines or with the cell (element) boundaries. As shown in Figure 3-3, the latter boundaries are exactly in the middle of the grid lines. The location of the external

boundary in relation to the grid, is best defined with reference to the boundary conditions (see also Section 2.5.8). For boundary conditions of the Dirichlet type, the boundary may be located at either a grid line or a control volume boundary. For boundary conditions of the Neumann and mixed type, the boundary must coincide with the control volume boundary. Because PORFLOW provides for solution of more than one dependent variable, often the boundary conditions for all variables are not of the same kind. In such a case, the preferable course of action is to locate the physical boundary at the control volume boundary. However, if the physical boundary is located at the grid line, PORFLOW will automatically impose the Neumann and mixed type of boundary conditions at the nearest mid-point and the Dirichlet boundary conditions at the grid line.

4.2.9 Input and Output Requirements

At times it may be necessary to make adjustment to grid size and time step to accommodate certain input or output requirements. For example, output may be required during a simulation at a regular frequency. The time step may then be adjusted such that it is an integral fraction of frequency of output. Similarly, data for hydraulic or thermal properties may be available only at certain locations or the boundary conditions may change at certain space or time intervals. These and similar factors must be accounted for in a judicious selection of grid size and time step.

5 INTRODUCTION TO INPUT AND OUTPUT OPTIONS

PORFLOW is a flexible and user-oriented software package. The computer program is modular in nature so that selected parts can be updated without significant changes to the overall structure of the program. It employs the FREEFORM command language to provide a flexible, simple to use and format-free user interface. The structure and syntax of the command language are fully described in Appendix A. The FREEFORM command language is a "keyword" oriented language. A complete discussion of the input and output options, and the keyword commands are described in Chapter 6. The input and much of the operation of the program is user controlled, hence, it can be modified during the progress of the calculations by convenient user-specified options. The output is largely controlled by the user, both in terms of its extent and its frequency. This chapter provides an introduction to the important input and output features of PORFLOW.

5.1 OVERVIEW OF KEYWORD COMMAND LANGUAGE

The PORFLOW input is divided into several groups. Each group is identified by a "keyword" command and may consist of one or more input records, each no more than 80 characters in length. Each record group, in addition to the keyword, may contain "numeric data", "modifiers" and "comments". The keyword, the numeric data and the modifiers must be separated from each other by separator, terminator or comment fields. Comments may be embedded within input records to enhance the clarity and readability of the input. A detailed description of the FREEFORM command language is given in Appendix A.

The PORFLOW, Version 2.40, I/O interface consists of 51 keyword commands which are listed in Table 5-1. A complete description of the commands, and of the modifiers and numeric data associated with them, is given in Chapter 6 in alphabetical order. Illustrations of the PORFLOW input are included as Appendix B. Some commands may be changed during the course of simulations (see Section 5.11). These commands are marked by a "C" in Table 5-1 under the subheading "Type"; other commands which provide 'fixed' input are marked with an "F".

5.2 ORDER OF INPUT COMMANDS

In general, the input records may be specified in any convenient order. However, some constraints are imposed by common sense. For example, the command that initiates the solution of the equations must follow complete specification of the geometry and physics of the problem. Similarly, the command that signifies the end of calculations must be the last input record for a given problem. Table 5-2 lists the relationship of these keyword commands to various functional aspects of problem specification; it may be convenient, though not necessary, to

TABLE 5-1. KEYWORDS OF PORFLOW AND THEIR FUNCTIONS

NO.	KEYWORD	INPUT FUNCTION	TYPE
1	BANNer	Print user & program identification to output file	C
2	BOUNDary	Override built-in boundary conditions	C
3	CONVergence	Specify convergence criterion	C
4	COORDinate	Specify grid coordinates	F
5	DATUm	Specify reference datum level for hydraulic head	F
6	DEBUg	Specify debug options	C
7	DECAy	Specify species decay constants	C
8	DEFIne	Specify value of a symbolic variable	C
9	DENSity	Select fluid mass density options	C
10	DIAGnostic	Diagnostic output options	C
11	DISAbLe	Disable certain built-in default options	F
12	END	End of a problem	F
13	FIXEd	Fixed pressure, temperature or concentration nodes	F
14	FLUX	Compute flux of species crossing a sub-domain	C
15	FLUId	Specify thermal and transport properties of the fluid	C
16	FOR	Specify zone designation for property input	C
17	GRAVity	Specify constants of gravitational acceleration	C
18	GRID	Number of grid nodes in the x, y and z directions	F
19	HISTory	Provide time history output at selected nodes	F
20	HYDRauiC	Hydraulic properties of porous matrix	C
21	INITial	Initial conditions for state variables	F
22	INTEgration	Index for selection of integration profile	C
23	LOCAtE	Specify location of internal or open boundary	F
24	MATRIx	Specify options for solution of matrix of equations	C
25	METHod	Select solution method for the governing differential equations	C
26	MULTIphase	Specify multi-phase or multi-fluid hydraulic characteristics	C
27	OUTPut	Frequency and extent of tabular output	C
28	PAUSE	Cause a temporary pause in processing	C
29	PERIodic	Specify periodic boundary conditions	F
30	PROBLEM	Specify general nature and type of problem	F

TABLE 5-1. KEYWORDS OF PORFLOW AND THEIR FUNCTIONS (Continued)

NO.	KEYWORD	INPUT FUNCTION	TYPE
31	PROPerty	Option for mode of property specification	F
32	READ	Read initial conditions from archive file	F
33	REFErence	Reference values for key variables	C
34	RELAX	Relaxation factors for governing variables	C
35	RENAme	Allows renaming of output variables listed in Table 5-5	C
36	ROCK	Material properties of solid component of matrix	C
37	SAVE	Frequency of output to archive file	C
38	SCALE	Internal scaling of specified input	C
39	SCREen	Echo some of the diagnostic output to screen	C
40	SOIL	Material properties of solid component of matrix	C
41	SOLVE	Start of solution of equations	C
42	SOURce	Specify source, injection or withdrawal terms	C
43	THERmal	Thermal properties of solid or porous matrix	C
44	TIME	Set initial time for simulations	C
45	TITLe	Problem title specification	F
46	TRACK	Compute particle tracks and corresponding elapsed time in flow field	C
47	TRANsport	Transport properties of porous matrix	C
48	USER	User identification for input and output files	F
49	VISCosity	Select fluid viscosity options	C
50	WINDow	Set sub-domain for output purposes	C
51	ZONE	Specify host media zones	C

**TABLE 5-2. FUNCTIONAL UNITS OF PORFLOW COMMANDS
AND SUGGESTED ORDER OF INPUT**

ORDER	FUNCTION	RELATED KEYWORD COMMAND
1	Identification	BANNer, TITLe, USER
2	Grid specification	COORDinate, GRID, SCALe
3	Problem definition	GRAVity, LOCAtE, PROBlEm, ZONE
4	Initial and boundary conditions	BOUNDary, DATUm, FIXEd, INITial, PERIodic, READ, TIME
5	Fluid properties	DENSity, FLUId, REFERENCE, VISCOsity
6	Soil/rock matrix properties	FOR, HYDRauiC, MULTIpHase, PROPErty, SOIL, ROCK, THERmal, TRANSport
7	Source and sink specifications	DECAy, SOURce
8	Solution options	DISABle, INTEGration, MATRIx, METHod, RELAx
9	Output control	DEBUg, DIAGNostic, FLUX, HISTory, OUTPut, RENAmE, SAVE, SCREEn, TRACK, WINDow
10	Operational control	CONVergence, DEFInE, END, PAUSE, SOLVe

follow this functional order. The **SOLVE**² command initiates the solution of the governing equations and must, therefore, follow complete specification of the problem. The **END** command terminates the execution of a problem and must, therefore, be the last command of an input sequence for a problem.

Although PORFLOW allows an order-free format for input, certain constraints may be inherent in problem specification itself. For example, any input in terms of grid coordinates (say, the **BOUNDary** or **INITial** commands), must, obviously, follow the coordinate specifications (**COORDinate** command). Similarly, the zone designation (**ZONE** command) for a subregion must precede any other reference to the zone number, such as for property specification.

5.3 SPECIFICATION OF GRID AND PROBLEM DIMENSIONALITY

The computations may be in three-dimensional (3D) or two-dimensional (2D) mode. One or the other mode is selected by the **GRID** command. In the 3D mode, the cartesian geometry

²The keywords are denoted by bold uppercase letters.

is specified in terms of the (x,y,z) and the cylindrical geometry in terms of (x,r,Θ) coordinates. In the 2D mode, the respective geometries are specified in terms of (x,y) and (x,r) coordinates. Irrespective of the physical coordinates, the grid indices always vary from $(1,1,1)$ to $(IMAX, JMAX, KMAX)$ for the 3D mode and from $(1,1)$ to $(IMAX, JMAX)$ for the 2D mode. $IMAX$, $JMAX$ and $KMAX$ are, respectively, the maximum number of grid lines in the x , y (or r) and z (or Θ) directions. For 2D computations, $KMAX$ is automatically set to 1. One-dimensional computations can be performed in a pseudo-2D mode where the gradients of all variables in the y direction are set to zero. A minimum of 3 nodes ($JMAX=3$) must be specified in the y -direction for one-dimensional computations.

5.4 SPECIFICATION OF A SUB-REGION OR WINDOW

A number of user input and output options require the selection and specification of a sub-region or "window." For example, the domain of interest may be composed of a number of distinct soil layers or types, or the tabular output of the state variables may be required only for a sub-region of the domain of interest. Each of these is defined by the user as a window and its grid-index coordinates are specified by an appropriate input command.

When PORFLOW is used in the 2D mode, a window is a rectangular region which is defined in terms of its lower-left (called starting node) and upper-right (called ending node) grid node indices. A window is then specified by a set of four numeric values which denote the lower-left and upper right (I,J) grid indices in the x and y direction. For example, the shaded sub-region of Figure 5-1 is specified by grid nodes $(3,3)$ to $(6,5)$. In the 3D mode, a window is defined in a manner similar to that for the 2D mode. In this case, it is a box-shaped region which is defined in terms of its lower-left and upper-right grid node indices by a set of six numeric values which denote the lower-left and upper right corner (I,J,K) grid indices in the x , y and z direction, respectively.

As mentioned in Section 5.3, the grid node indices vary from $(1,1)$ to $(IMAX, JMAX)$ for 2D and $(1,1,1)$ to $(IMAX, JMAX, KMAX)$ for 3D mode as specified by the **GRID** command. Therefore the valid set of window coordinates must lie in this range. If the values specified lie outside this range, then the input values are clipped to lie in the valid range specified by the **GRID** command.

5.5 INPUT AND OUTPUT FILE UNITS

PORFLOW employs nine I/O units; by default these units are assigned to be file units 11 through 19. The function and default assignments for these I/O units are defined in Table 5-3. The user is given an opportunity to attach these units to alternate files (or devices). The units 11 through 14, and the unit 17, may be redirected by the **READ**, **SAVE**, **HISTORY**, **FLUX** and **DEBUG** commands, respectively. The units 15 and 16, being the standard input and output devices, may be redirected by the operating system commands when PORFLOW is invoked.

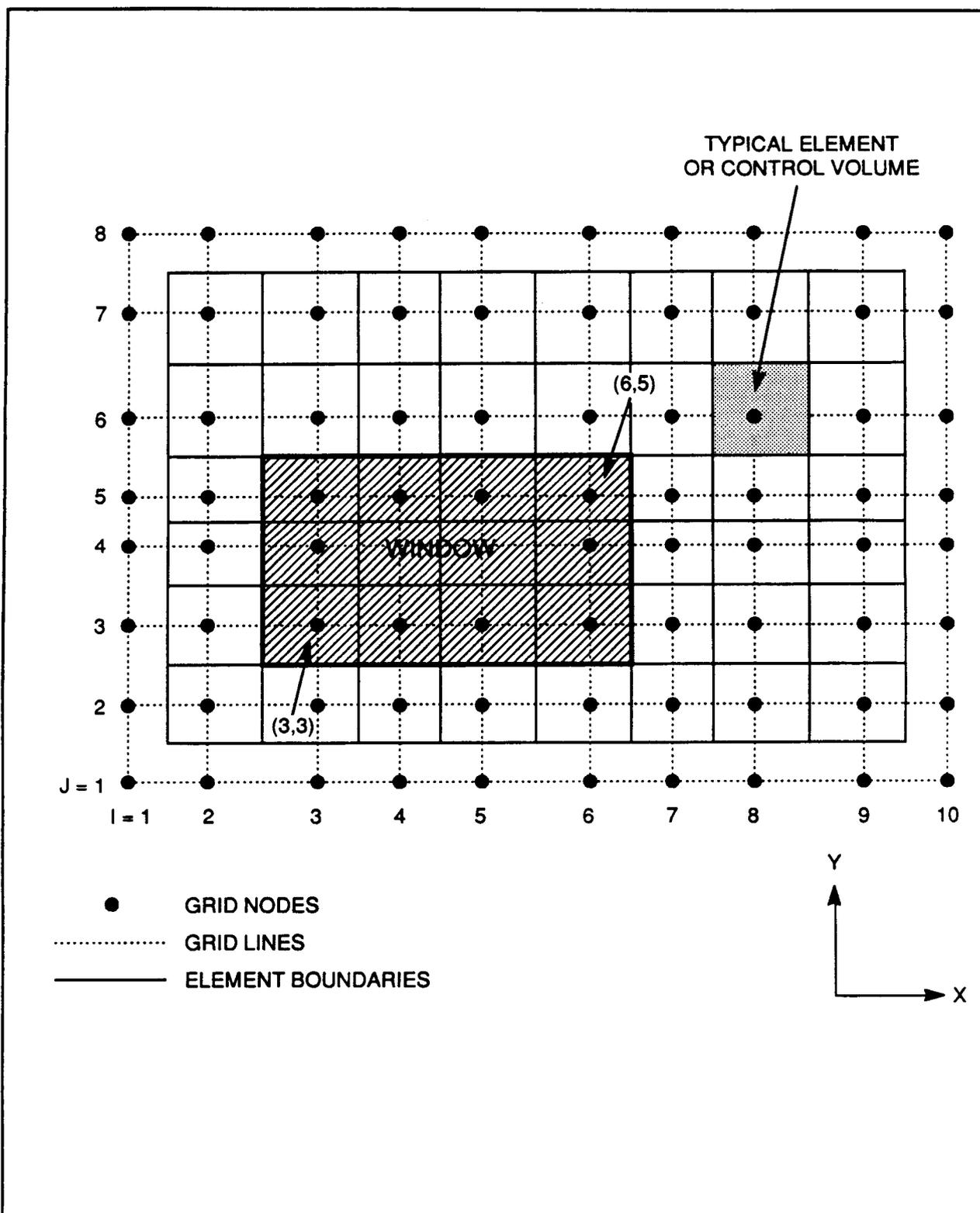


Figure 5-1. Subregion or window specification

TABLE 5-3. I/O FILE UNITS AND THEIR DEFAULT ASSIGNMENT

UNIT #	DEFAULT ASSIGNMENT		FUNCTION
	FILE NAME	DATA TYPE	
10	none	Formatted	Read input data from user specified commands.
11	RESTART	Formatted	Read input data for restart option.
12	ARCHIVE	Formatted	Write data file for restart, archiving and post-processing.
13	TIMEHIS	Formatted	Write time-history data.
14	FLUXBAL	Formatted	Write data for fluxes crossing a sub-region boundary.
15	Console	Formatted	Read user input commands.
16	Printer	Formatted	Write standard output.
17	USERIO	Formatted	User specific output.
18	TRACKS	Formatted	Tracks and elapsed time of particles released in the flow field.
25	SCRATCH	Formatted	Temporary Scratch file for input data.
26	ACRINIT	Formatted	ACRi Initialization file

5.6 UNITS OF PHYSICAL QUANTITIES

Any consistent set of units may be employed for input. However, all built-in default values for dimensional physical properties (such as the density of water) are in SI units. If other than SI units are used, then the user must specify these properties as part of the input data.

5.7 DIAGNOSTIC OUTPUT SPECIFICATION

PORFLOW provides five keyword commands to control the diagnostic output. These are the **DEBUG**, **DIAGnostic**, **FLUX**, **OUTPUT**, and **WINDOW** commands. The **DEBUG** command is useful for trouble-shooting. It provides trace-back and initiates diagnostic output from different modules of PORFLOW. The **DIAGnostic** command provides a means to monitor the time-history of the dependent variables at a particular node and the residuals of the governing equations from one iterative step to the next. The **FLUX** command provides output of convective and diffusive flux terms, and the residuals and errors in mass and energy balance in the numerical solution of the equations. The **OUTPUT** command allows the currently active variables to be written in a tabular format to the output file unit (IWR). The **WINDOW** command, in conjunction with the **OUTPUT** command, allows for the output of only a subregion of the master arrays.

5.8 DEPENDENT VARIABLES OF PORFLOW

PORFLOW provides for the numerical solution of an arbitrary number of coupled transport equations. The user may elect to solve any subset of these equations. Table 5-4 lists the variables of the governing equations in the order in which they are solved.

TABLE 5-4. DEPENDENT VARIABLES OF PORFLOW

PORFLOW [®] NAME	MATHEMATICAL SYMBOL	DESCRIPTION OF THE VARIABLE
P	P ¹	Total hydraulic head at reference density for primary fluid phase
P2	P ²	Total hydraulic head at reference density for secondary fluid phase
P3	P ³	Total hydraulic head at reference density for tertiary fluid phase
T	T	Temperature
C	C	Mass concentration of 1 st species in fluid
C2,C3, ...,Cn	C ⁿ	Mass concentration of 2 nd through n th species

5.9 TABULAR OUTPUT OF FIELD VARIABLES

The user may obtain tabular output of all the state variables listed in Table 5-4 plus some auxiliary variables at various stages of the calculations. Table 5-5 lists these in the order in which they are written to the output file. The output file is written to the file unit IWR (see Section 5.5). 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 which output is generated.

5.10 ARCHIVE OUTPUT SPECIFICATIONS

An archive file consisting of basic problem specification and values of up to 30 variables (including those listed in Table 5-5) may be generated by PORFLOW. This file may be used to restart a problem or for post-processing such as to produce contour, raster, surface or vector plots on a console screen, printer or plotter. The archive file is self-documenting. It contains an identification and the problem title specified by the user. The time and date of creation, the basic grid information, and the names of variables stored on the file are also included in the information written to this file. The archive information is written to file unit NUNIT2 in either unformatted or formatted records, depending on user specification. By default, NUNIT2 is

TABLE 5-5. OUTPUT FIELD VARIABLES OF PORFLOW

PORFLOW® NAME	MATHEMATICAL SYMBOL	DESCRIPTION OF THE VARIABLE
U	U	Velocity component in x-direction
V	V	Velocity component in y or r-direction
W	W	Velocity component in z or Θ -direction
P	P ¹	Total hydraulic head at reference density for primary fluid phase
P2	P ²	Total hydraulic head at reference density for secondary fluid phase
P3	P ³	Total hydraulic head at reference density for tertiary fluid phase
T	T	Temperature
C	C	Mass concentration of 1 st species in fluid
C2,C3, ..., Cn	C ⁿ	Mass concentration of 2 nd through n th species
S	S ¹	Saturation fraction for primary fluid phase
S2	S ²	Saturation fraction for the secondary fluid phase
S3	S ³	Saturation fraction for the tertiary fluid phase
H	h ¹	Pressure head for the primary fluid phase
H2	h ²	Pressure head for the secondary fluid phase
H3	h ³	Pressure head for the tertiary fluid phase
MOIS	ϕ_E	Effective moisture in primary fluid phase

assumed to be unit 12, the file is given the name ARCHIVE and the data records are formatted.

This output is controlled by the SAVE command which selects the variables to be archived, the frequency of output, the file name, and the nature of data records (formatted or unformatted). The archive output consists of several records for each data set. Whenever these records are written on the archive file, diagnostic messages appear on the standard output file that identify the information being transferred to the archive file.

5.11 MODIFICATION OF INPUT DATA DURING SIMULATIONS

The simulation is initiated by the SOLVE keyword command. The total span of simulations, however, may be divided into segments, and a SOLVE command used for each

segment. Any time-dependent or sequential aspects of the input or output requirements may be changed between the calculation segments.

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

An example of a two-segment calculation sequence is given in Table 5-6. In this example, the output requirements for both the archive file and the tabular output are changed after 50 steps of calculations.

5.12 DIMENSIONING PARAMETERS

PORFLOW employs FORTRAN PARAMETER statements to set the dimensions of the various arrays. These parameters and the minimum required values are given in Table 5-7. The user must ensure that the dimensions thus set are equal to, or larger than, those required for the problem to be solved.

TABLE 5-6. ILLUSTRATION OF A TWO-SEGMENT SIMULATION SEQUENCE*

```

TITLE EXAMPLE OF A TWO SEGMENT CALCULATION WITH OUTPUT OPTION CHANGES
//
GRID 11 BY 12
COORDinate X: RANGE = 100, grid spacing increment ratio = 1.1
COORDinate Y: RANGE = 40, grid spacing increment ratio = 1.
/
ZONE = 1 from (1,1) to (12,12)
/
INITial P = 1. from (2,2) to (4,4)
INITial T = 0 everywhere
INITial T = 100 from (2,2) to (4,4)
/
ROCK density = 1., Porosity = 0.4
HYDRaulic properties: storativity 0.1; conductivity x = 1., y = 1.
OUTPut for P (pressure) at this stage $ Print initial values of P
/
// Comment. Start of first segment of calculations
SOLVE for 5 years in time step of 0.1 yr
/
OUTPut for variables P and T
SAVE variables U, V, P
/
// Comment. Start of second segment of calculations
SOLVE for 15 more years in time step of 0.5 yr
/
OUTPut for variables U, P and T
SAVE variables U, V, W, P and T
/
// Comment. Start of third segment of calculations
SOLVE for another 30 years in time step of 1 yr
/
OUTPut for variables U, V, W, P and T
SAVE variables U, V, W, P and T
/
END
    
```

* The keywords are shown in bold-face type for emphasis only. In the actual FORTRAN data file, these must be in ordinary type face.

TABLE 5-7. DESCRIPTION OF DIMENSIONING PARAMETERS

PARAMETER	DESCRIPTION	MINIMUM VALUE
L1	Maximum number of grid coordinates in any one direction	Maximum (IMAX,JMAX,KMAX); IMAX=N1, JMAX=N2, KMAX=N3 on GRID command
LBC	Maximum number of boundary nodes in the solution domain	$2 \{ (IMAX-2)*(JMAX-2) + (JMAX-2) * (KMAX-2) + (KMAX-2)*(IMAX-2) \}$
LBE	Maximum number of boundary condition specifications for all variables	Number of boundary nodes times the number of equations solved
LBN	Maximum number of boundary segments with time dependent boundary conditions	Number of BOUNDary commands with TIME modifier
LBT	Maximum number of elements in all the time-dependent boundary condition specifications	$3 * (\text{number of BOUNDary commands with COSine modifier}) + 2 * (\text{sum of N2 on BOUNDary command with TABLE modifier})$
LEQ	Maximum number of transport equations which can be solved	10 for current versions of PORFLOW
LFLD	Maximum number of grid nodes excluding the boundary nodes	$(IMAX-2)*(JMAX-2)*(KMAX-2)$
LFLX	Maximum number of sub-regions for output of fluxes	Number of FLUX commands
LFX	Maximum number of fixed value subregions	Number of FIX commands
LF1	Maximum number of non-zero elements in the inverse matrix	$(2*L23D+1)*LFLD$ for ADI and SOR; for other matrix solvers, varies from problem to problem
LMAX	Maximum number of grid nodes in the domain of interest	$IMAX*JMAX*KMAX$
LMF	Maximum number of elements in the tabular input for multi-fluid characteristic curves	Sum of specified characteristic curve elements (N1 on MULTiphase command in mode 1)
LSO	Maximum number of source elements in all the SOURce commands	Sum of number of specified source elements (N2 on SOURCE command)
LSS	Maximum number of source locations.	Number of LOCAt commands with SOURce modifier
LVAL	Maximum number of input numerical values for any command.	The largest number of numerical values on any input command
LZN	Maximum number of zones.	Largest zone number specified by the ZONE commands
L23D	Dimensionality of Problem.	3 if KMAX > 2; otherwise = 2

6 DESCRIPTION OF PORFLOW[®] KEYWORD COMMANDS

This chapter describes the keywords which comprise the user interface of the PORFLOW software package. This interface is based on the ACRI free-format command language FREEFORM. A knowledge of the structure and syntax of this language is essential for understanding the descriptions of keyword commands in this chapter. The FREEFORM command language is fully described in Appendix A of this report. Some hints on the preparation of input for PORFLOW are given in the previous chapters. Descriptive notation is explained at the beginning of this chapter.

6.1 KEYWORD COMMAND NOTATION

The descriptive notation employed for input commands is described below. A detailed description of the user input is given in Chapter 6. The command language employed for this input, called FREEFORM[®], is described in Appendix A.

- BOLD** Upper-case characters in bold type-face denote keywords of PORFLOW. The keyword character string may be specified by the user in upper or lower case. Boldface is used in this manual for emphasis only; it must not be used as part of user input.
- CAPS** Upper-case characters in normal type-face denote modifiers of PORFLOW keywords which are *significant* for interpretation of user input. The character string shown may be specified by the user in upper or lower case.
- char** Lower-case characters denote information on keyword command which is *not significant* for interpretation of user input but improves the clarity or readability of the input. The character string shown may or may not be specified by the user, or may be replaced by other character strings.
- |** 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 each other 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.

N_n Denotes the *n*th numeric field on an input command denoted by a keyword.

fname Denotes the name of a file or device; see Section 6.2.2.

6.2 GENERAL INPUT FEATURES FOR FREEFORM COMMANDS

6.2.1 Interactive or Run Time Input

The FREEFORM command language used for PORFLOW[®] input allows interactive or run time data input for any keyword command. Any occurrence of a question mark (?) in the FREEFORM input is interpreted as a prompt for input by the user. The user may therefore insert a "?" for a numerical or character string in the input. The command interpreter will pause and prompt the user for input at this stage. Any input so specified is then inserted in the input command string starting with the location of the question mark symbol. The FREEFORM command interpreter is based on an 80-character input string for each input record (see Appendix A). Therefore, the number of characters that can be inserted after the question mark depends on the location of the question mark.

6.2.2 File Name Specification

Many of the input commands allow a part or whole of the input data to be read from a user specified file or device. The name of such a file or device, which is symbolically called "fname" in this Manual, is specified as a character expression which must be *enclosed in single or double quotes*. The file or device name may be up to 32 characters long, consisting of any characters accepted by the operating system as a valid I/O file name. Data is read from this file in free format mode according to the rules of FORTRAN 77.

6.2.3 Subregion Specification

Many of the input commands apply to a subregion of the domain of interest as described in Section 5.4. The starting and ending grid index coordinates of the subregion to which input applies are specified by four values in the 2D mode and six values in the 3D mode. In general, if such specification is required but is omitted by the user, then the subregion is defined to be the total domain of interest which is relevant for the keyword command (See Section 5.4 for subregion specification and valid input values).

PURPOSE

To print a banner page on the output file unit IWR (see Section 5.5). The banner page contains the PORFLOW version and date identification, time and date stamp, and user identification.

SYNTAX

BANN

EXAMPLES

BANNer page output at this stage

PURPOSE To specify boundary conditions on the external boundaries of the region of interest according to the boundary condition equations (2.5.46) through (2.5.48).

SYNTAX Mode 1: Dirichlet or Neumann Boundary Condition Fixed in Time

BOUN {symbol}, [NODE | INTE | FLUX | GRAD], {N1}, {N2}, [N3,..., Nn], [Nn+1, Nn+2, Nn+3]; n = 6 for 2D and n = 8 for 3D input mode.

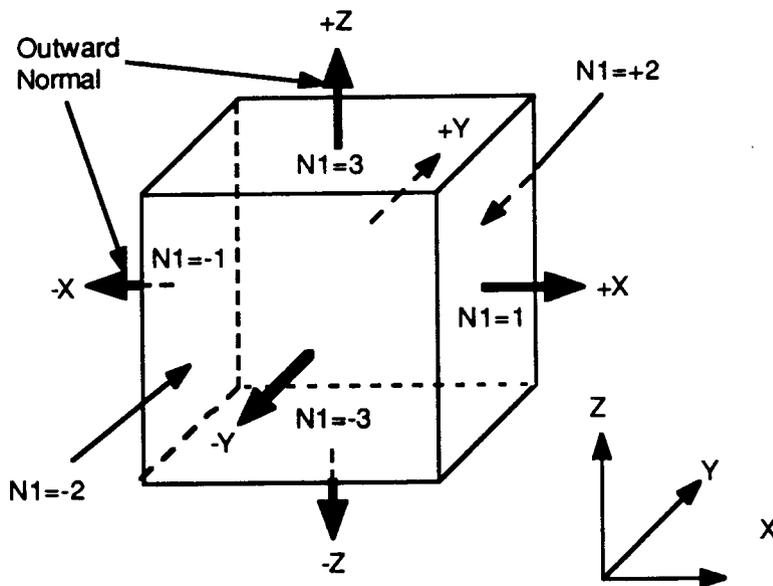
symbol: One of the character strings which denotes the dependent variable for which the boundary condition is specified. The valid symbols are listed in Table 5-4. One, and only one, character string must be specified for each command.

NODE: Value of the variable at the grid node is specified [Eqn. (2.5.46)]. This is the default option.

INTE: Value of the variable at the grid cell interface [Eqn. (2.5.46)] is specified.

FLUX: Flux of the variable [Eqn. (2.5.47)] at the grid cell interface is specified.

GRAD: Gradient of the variable [Eqn. (2.5.47) with $\Gamma = 1$] at the grid cell interface is specified.



S8812 085 001 GW

Figure 6-1. Illustration of the boundary index notation

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	<p>The orientation index of the external boundary (See Figure 6-1).</p> <p><i>When N1 = -1:</i> The outward normal at the boundary is along the negative direction of x. For example, the y-z plane at I=1.</p> <p><i>When N1 = 1:</i> The outward normal at the boundary is along the positive direction of x. For example, the y-z plane at I=IMAX.</p> <p><i>When N1 = -2:</i> The outward normal at the boundary is along the negative direction of y. For example, the z-x plane at J=1.</p> <p><i>When N1 = 2:</i> The outward normal at the boundary is along the positive direction of y. For example, the z-x plane at J=JMAX.</p> <p><i>When N1 = -3:</i> The outward normal at the boundary is along the negative direction of z. For example, the x-y plane at K=1.</p> <p><i>When N1 = 3:</i> The outward normal at the boundary is along the positive direction of z. For example, the x-y plane at K=KMAX.</p>
N2	<p>The boundary value for Dirichlet [F_0 of Eqn. (2.5.46)] or the boundary flux or gradient for Neumann [q_f of Eqn. (2.5.47)]. The input units for F_0 are the same as those for the dependent variable; the units for gradient are those of the variable divided by the distance; the units for flux are those of velocity for P, heat flux for T, and mass flux for C. <i>The default value is 0.</i></p>
N3 through Nn	<p>The subregion for which boundary conditions are specified. See Section 6.2.3 for interpretation of this input. If this input is omitted then the subregion is defined to be the whole of the boundary indicated by the index N1. Also see LOCAtE command for specification of an active non-rectangular or irregular subregion within the overall domain.</p>
Nn+1 Nn+2 Nn+3	<p>The gradients of the boundary value in the x, y and z directions, respectively. The specified N2 is modified for internal use according to the equation:</p> $N2_{in} = N2 + Nn+1 * x + Nn+2 * y + Nn+3 * z,$ <p>where $N2_{in}$ is the internal representation of N2, and x, y and z are the coordinates of the boundary nodes. <i>The default value is 0.</i></p>

EXAMPLES

```

BOUNDary for P: at -1 boundary, value = 0 $ Fixed value at all nodes: I=1 plane
BOUNDary for P: at +1: FLUX = 0.2 m/d          $ Velocity at I=IMAX plane
BOUNDary for P: at -3: GRAD = 1 $ Seepage boundary; specified pressure gradient
BOUNDary for P2: INTERface bndry -3, vel = 0   $ Dirichlet at interface K=1
BOUNDary for C: at +1; GRADient = 20          $ Neumann at I=IMAX plane
//      Next command specifies bi-linear Dirichlet condition (T = 1 + x/2 + y)
//      at K = 1 (x-y) plane for the sub-region (2,3,1) to (5,7,1).
BOUNDary T: -3, value=1., (2,3,1) to (5,7,1) xgrad=0.5, ygrad=1.
    
```

SYNTAX

Mode 2: Mixed Boundary Condition Fixed in Time

BOUN {symbol}, {MIXE}, [GRAD | FLUX], {N1}, {N2, N3}, [N4,..., Nn], [Nn+1, Nn+2, Nn+3]; n = 7 for 2D and n = 9 for 3D input mode.

symbol: See Mode 1 Specification.

MIXE: A combination of the variable value and its gradient or flux [Eqn. (2.5.48)] at the grid cell interface is specified. *By default it is assumed that the flux is specified.*

FLUX: Mixed boundary condition in terms of the flux of the variable [Eqn. (2.5.48)] at the grid cell interface is specified. *This is the default option.*

GRAD: Mixed boundary condition in terms of the gradient of the variable [Eqn. (2.5.48) with $\Gamma = 1$] at the grid cell interface is specified.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The orientation index of the external boundary. See Mode 1 specification.
N2	The equilibrium value for the variable [F_0 of Eqn. (2.5.48)]. The input units for F_0 are the same as those for the dependent variable. <i>The default value is 0.</i>
N3	The heat or mass transfer coefficient [h_F of Eqn. (2.5.48)]. In FLUX mode the input units are those of velocity, heat flux or mass flux divided by the units of P, T or C° . In GRADient mode, the input units are L^{-1} . <i>The default value is 0.</i>
N4 through Nn	The grid index coordinates for the subregion for which boundary conditions are specified. See Mode 1 specification for N3 through Nn.
Nn+1 Nn+2 Nn+3	The gradients of the boundary value in the x, y and z directions, respectively. See Mode 1 specification.

EXAMPLES

BOUNDary for T: at +2; MIXEd type: value=5 h=0.5

BOUNDary for T: at +2; MIXEd GRADient: value=1 h=0.1

BOUNDary for T: at +2; MIXEd GRADient: value=1 h=0.1 from (1,23) to (22,23)

BOUNDary T: +2; MIXEd GRAD: v=1, h=0.1 frm (1,23) to (22,23) gradx=0.1

SYNTAX

Mode 3: Boundary Condition as a Function of Time

BOUN {*TIME*}, {*symbol*}, {*N1, N2*}, {*N3, ..., Nm*}, [*Nm+1, ...,Nm+n*]
 $m = 2*N2 + 2$; $n = 4$ for 2D input mode; $n = 6$ for 3D input mode

TIME: The boundary condition varies as a function of time.

symbol: See Mode 1 Specification.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The orientation index of the external boundary. See Mode 1 specification.
N2	The number of sets of boundary information values which follow. <i>The default value is 0.</i>
N3	The time at which the boundary condition occurs. If the minimum time specified is greater than the start time of the simulation then the boundary values up to that time are taken to be constant at the value given at the minimum time. <i>The default value is 0.</i>
N4	The value of the boundary condition at time N3. <i>The default value is 0.</i>
N5 through Nm	Additional time, value pairs as dictated by N2. Any boundary values required beyond the specified maximum time are taken to be constant at the value given at the maximum time. <i>The default value is 0.</i>
Nm+1 through Nm+n	The grid index coordinates for the subregion for which boundary conditions are specified. See Mode 1 specification for N3 through Nn.

EXAMPLES

BOUNDary TIME dependent for T index -1: 3 sets (0,300) (100,325), (200,310)
 BOUNDary T index -1: TIME dependent 2 sets (0,300) (100,325) from (2,3,2) to (12,11,2)

SYNTAX

Mode 4: Boundary Condition as a Function of Time from a File

BOUN {*TIME*}, {*symbol*}, {*fname*}, {*N1, N2*}, {*N3, ..., Nn*}
 n = 6 for 2D input mode; n = 8 for 3D input mode

TIME: The boundary condition varies as a function of time.

symbol: See Mode 1 Specification.

fname: The name of the file which contains the boundary condition input. See Section 6.2.2 for specification of the file name. The structure of the data on this file is identical to that for Mode 3 where two values (time and boundary value) specify the data for each set.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The orientation index of the external boundary. See Mode 1 specification.
N2	The number of sets of boundary information values which are given on the 'fname' file. <i>The default value is 0.</i>
N3 through Nn	The grid index coordinates for the subregion for which boundary conditions are specified. See Mode 1 specification for N3 through Nn.

EXAMPLES

BOUNDary T index -1: TIME dependent: 57 sets on file 'BOUNDARY.DAT'
 BOUNDary T for +1: TIME mode 42 sets: (3,51) to (5,51) on file "BOUND.DAT"

SYNTAX

Mode 5: Boundary Condition as a Cosine Function of Time

BOUN {TIME}, {COSI}, {symbol}, {N1}, {N2, N3, N4, N5}, [N6, ..., Nn]
 n = 9 for 2D input mode; n = 11 for 3D input mode

TIME: The boundary condition varies as a function of time.

COSI: The boundary condition is a cosine function of time.

symbol: See Mode 1 Specification.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The orientation index of the external boundary. See Mode 1 specification.
N2	The amplitude of the cosine function which determines the boundary condition. <i>The default value is 0.</i>
N3	The period of the cosine function. <i>The default value is 0.</i>
N4	The phase of the cosine function. <i>The default value is 0.</i>
N5	A value to be added to the cosine function. <i>The default value is 0.</i>
N6 through Nn	The grid index coordinates for the subregion for which boundary conditions are specified. See Mode 1 specification for N3 through Nn.

EXAMPLES

- BOUNDary T; index 2: COSIne in TIME amp 20, period 365 days, phase 182 days, base 273
- BOUNDary T; index 2: COSI TIME (20, 365, 182), Ta = 273 from (1,12) to (17,12)
- BOUNDary T; index 2: COSI TIME (20, 365, 182), Ta = 273 from (1,12,1) to (17,12,11)

PURPOSE To specify the convergence criterion for solution of the system of equations.

SYNTAX CONV [symbol], [GLOB | LOCA], [SUM], [N1, N2, N3], [N4, N5]

symbol: One of the character strings which denotes the dependent variable for which convergence will be monitored. The valid symbols are listed in Table 5-4. *By default convergence is monitored for the P variable.*

For multiphase systems, if no symbol is specified, then the input is assumed to apply to the total flow system which consists of multiple pressure equations. In PORFLOW[®], the pressure fields are solved sequentially starting with the first pressure field. Since a given phase pressure also depends upon the other pressures through the capillary pressure relation for saturation, this check over the total flow system may be specified in addition to those for individual phase pressures to ensure that the total system converges to the specified tolerance.

GLOB: Convergence is judged on the basis of the global residual of the solution matrix [Eqn. (3.5.3)].

LOCA: Convergence is judged on the basis of the local changes in the value of the variable [Eqn. (3.5.4)]. *This is the default option.*

SUM: If the GLOBAL convergence mode is selected, and this modifier is present, then convergence is judged on the basis of the global sum rather than the mean value of the residual of the solution matrix; i.e., the division by N in Eqn. (3.5.3) is omitted. This modifier is ignored if GLOBAL modifier is not present.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The ϵ of Eqn. (3.5.3) or (3.5.4). <i>The default value is 0.001.</i>
N2	Maximum number of iterations for convergence. <i>The default value is 1.</i>
N3	The minimum value of the modulus of the variable for which the convergence criterion of Eqn. (3.5.4) is applied; if the modulus is less than N3, then its variations are ignored. This input is used only if the LOCAL convergence mode is invoked; otherwise it is ignored. <i>The default value is 1.E-7.</i>
N4, N5	This input is used only if the AUTOMATIC time step mode is selected by the SOLVE command. In that case, if the number of iterations required to reach convergence is below the value specified by N4, then the time step is increased by the N3 value specified on the SOLVE command. On the other hand, if the number of iterations to convergence is greater than N5 then the time step is decreased by the N6 value on the SOLVE command; otherwise the time step is maintained at its previous value. In case of multiple CONVERGENCE commands, the last specified non-zero values of N4 and N5 are effective. <i>If no value is specified, then N4 is set at one-third of N2 and N5 at two-thirds of N2.</i>

EXAMPLES

CONvergence criterion = 1.E-6
 CONvergence for P in LOCAL mode: value = 1.E-4
 CONvergence for P2 in LOCAL mode: value = 1.E-3, 20 iterations
 CONvergence for T in GLOBAL mode: value = 1.E-4
 CONvergence for T in GLOBAL SUM mode: value = 1.E-4
 CONV for C: LOCAL mode, value = 1.E-4, max iterations = 10, min value 1.E-5
 CONV for flow: LOCAL mode, epsilon = 1.E-2, max iterations = 5
 CONV LOCAL, eps = 0.001, max iter = 50, min F = 1.e-5; lower N = 10, upper N = 30

COMMENTS

This command is used in two modes. If the steady state-mode of solution is invoked by the SOLVE command, then the convergence criterion is used to check convergence to the steady state. However, if the transient solution mode is invoked, then this criterion is used to monitor the convergence of the solution at each time step. The latter is especially important for solution of the non-linear multi-phase or unsaturated flow equations in the transient mode.

PURPOSE To specify the grid locations for the coordinates in the cartesian (x,y,z) or cylindrical (x,r,θ) coordinate system.

SYNTAX COOR {dir}, [geom], [input], [DEGR], {N1}, [N2, ..., Nn], n ≤ NCMAX

dir: indicates the coordinate direction for which the input is specified. It must be one of the X, Y, Z, R or THETA modifiers which, respectively, denote the x, y, z, r or θ coordinates.

geom: indicates the nature of geometry; the available options are given below.

geom	INTERPRETATION
CART	The cartesian geometry is selected. <i>This is the default option.</i>
CYLI	The cylindrical coordinate system is selected.

input: denotes the nature of input. The available options are given below.

input	INTERPRETATION
USER	The coordinate values are explicitly specified by the user. <i>This is the default option.</i>
RANGe	Only the total range (total domain length in the corresponding direction) is specified. The coordinates are calculated internally with a geometric ratio between the successive grid intervals.
MINImum	The minimum and maximum values are specified. The coordinates are calculated internally with a geometric ratio between the successive grid intervals.
fname	The name of the file which contains the coordinate values. See Section 6.2.2 for specification of the file name. In this input mode, any specified numerical input is ignored.

DEGR: *By default, the angular input for θ is assumed to be in radians. However, if the modifier DEGRee is present, then the input values are taken to be in degrees.*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The 1 st coordinate value if the modifier USER or MINIMUM is present; the desired range if the modifier RANGE is present. <i>The default value is 1.</i>
N2	The 2 nd coordinate value if the modifier USER is present. The last coordinate value if the modifier MINIMUM is present. The geometric ratio by which the grid intervals between successive nodes change if the modifier RANGE is present. <i>The default value is 1.</i>
N3	The 3 rd coordinate value if the modifier USER is present. The geometric ratio by which the grid intervals between successive nodes change if the modifier MINIMUM is present. Otherwise this value is ignored. <i>The default value is 1.</i>
N4 through Nn	Successive coordinate values for 4 th node onwards, if the modifier USER is present. A total of NCMAX values must be specified (N1 through Nn) in an algebraically ascending order. NCMAX is the corresponding number of grid nodes (GRID command) in the selected direction.

EXAMPLES

COORDinate X values to be read from 'XVALUES.FIL'
 COORDinate Y: -5, 5, 15, 25, 35, 45, 55, 65, 75, 85, 95, 105
 COORDinate Z: RANGE = 6.28
 COORDinate X: MINIMUM = 0., maximum = 10.
 COORDinate R: RANGE = 10., ratio = 0.95
 COORDinate THETA: 0, 5, 15, 25, 35, 45, 60, 75, 90, 105, 120 DEGREes

COMMENTS

If multiple specifications of cartesian or cylindrical geometry exist (modifiers R, THETA, CARTesian or CYLIndrical), or are in conflict with each other, then the last specification is effective.

For cylindrical coordinates, the axis is taken to be coincidental with the x direction, the radial (r) direction is assumed to be co-directional with the y direction, and the angular (Θ) direction as coincident with the z direction. In this mode, an additional restriction is placed on the choice of r-coordinates: the interface radii (the element boundary "r" coordinates in Figure 3-2) must all be non-negative. This implies that:

$$r_n \geq -r_2; r_n > 0 : n = 2, 3, \dots, NCMAX.$$

For problems where the boundary at n=1 is to be the axis of symmetry, r₁ must equal -r₂ so that the first cell boundary in the r direction is located at r=0.

PURPOSE To specify datum coordinates, x_i^* , which are used to define the hydraulic head, P of Eqn. (2.1.6).

SYNTAX DATU {N1, N2, N3}

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1,N2,N3	The (x,y,z) or (x,r,θ) coordinate values, respectively, for the datum level which are used to define the hydraulic head. <i>The default value is 0.</i>

EXAMPLES

DATUm \$ set to zero since N1 is omitted
 DATUm coordinates for this problem are: x=0., y=1000, z=50.

COMMENTS The datum coordinates enter the computations only if multiphase flow option is used. *The default value for each coordinate is taken to be the maximum specified value of the coordinate in each respective direction.*

PURPOSE To obtain debug output and messages for diagnostics, trouble shooting or progress of the numerical solution.

SYNTAX *Mode 1: General Debug Output*

DEBU {N1}, [N2, N3, N4], [FINAL]

FINAL: If this modifier is present, then the debug output specified by N1 is obtained at the final step of the iterative procedure in addition to the output obtained from N2 through N4 as explained below.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	<p>An index for level of debug output. The default setting suppresses all debug output. <i>The default setting is 0.</i></p> <p><i>When N1 = 1:</i> A road-map (trace) of all subroutines called during execution is produced.</p> <p><i>When N1 = 2:</i> Matrix coefficients from the INVERT subroutine are printed.</p> <p><i>When N1 = 3:</i> Output of all active output variables (see the OUTPUT command) is obtained just before solution of the flow equations.</p> <p><i>When N1 = 4:</i> Output of all active output variables is obtained just before solution of the temperature equation.</p> <p><i>When N1 = 5:</i> Output of all active output variables is obtained just before solution of the concentration equation.</p>
N2	The first step of the iterative solution procedure at which the debug output specified by N1 is initiated. <i>The default value is 1.</i>
N3	The last step at which the debug output is obtained. If no value is specified, then a default value equal to N2 is assumed.
N4	The step increment, between N2 and N3, for output. <i>The default value is 1.</i>

EXAMPLES

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

SYNTAX

Mode 2: User Implemented Options

DEBU {USER}, [symbol], [fname], [N1]

USER: If the modifier USER is present, then the debug output is controlled by the user through specially written modules. These modules must be called from a subroutine called "USERIO". In some versions of PORFLOW[®] it is used to compute and print the maximum values of the Peclet and Courant numbers.

symbol: One or more of the character strings which denotes the dependent variable for which user specified debug output is printed. The valid symbols are: T, C, C2, C3 or C4 of Table 5-4. *If no symbol is specified then the output is obtained for all variables which are solved.*

fname: The name of the file on which the output is written. See Section 6.2.2 for specification of the file name. *By default, the output file is assumed to be named USERIO (see Section 5.5).*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The frequency, in step numbers, at which the output is obtained. The output will be obtained every N1 steps. <i>The default value is 1.</i>

EXAMPLES

DEBU output for USER specified options
 DEBU USER options: for T and C every 12 steps
 DEBU USER specified output: for T on 'MYFILE.DBG'

COMMENTS

This command may generate extensive output. It must therefore be used with due caution. Some types of output from this command, which produce a print out 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.

This command is not fully operational in all installations of PORFLOW.

PURPOSE To specify the chemical reaction or radioactive decay rate constants for the mass species, C.

SYNTAX DECA {symbol}, [FIEL], [N1, N2]

symbol: One of the character strings which denotes the species for which the decay or reaction rate constants are specified. The valid symbols are: C, C2, C3 or C4 of Table 5-4.

FIEL: If the modifier FIEL is present, then the decay or reaction is assumed to occur only inside the field and not at the boundaries. The boundary values are maintained at the specified conditions.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The half-life of radioactive decay or chemical reaction, $t_{1/2}$ of Eqn. (2.5.44), for the species specified by the symbol. The default value ensures that no decay occurs (provided the simulation time is much smaller than 1.E20). <i>The default value is 1.E20.</i>
N2	σ^{tr} of Eqn. (2.3.1). It represents the fraction (between 0 and 1) of the species specified by the symbol which is transformed into the next species in the decay chain. The chain-decay is assumed to be in the order C --> C2 --> C3 --> C4. If N2 is zero then, it is assumed that the species decays to another which is outside the decay chain. Also any specification of N2 for species at the end of the chain is ignored. For example, in a 4-chain species, the N2 for C4 is ignored. <i>The default value is 0.</i>

EXAMPLES

DECAY half life of C is 1.59E7 (I99)
 DECAY half life of C is 1.59E7; fraction transformed to next species is 0.7
 DECAY rate of C2 is 1.59E7 yrs; fraction transformed to next species is 0.1
 DECAY rate of C2 is 1.59E7 yrs; only for FIELd values

COMMENTS

The actual rate constant, λ^a of Eqn. (2.3.1), for the species C^a is calculated from the relation:

$$\lambda^a = 0.69314718 / N1,$$

where 0.69314718 is the negative of the value of the natural logarithm of 0.5.

PURPOSE	To define the value of a symbolic variable as numeric or character expression.
SYNTAX	DEFI {var}, {string N1}, [OFF]
	var: A symbolic variable to assist in interpretation of user input. Once a variable has been defined, any occurrence of this variable in the user input is replaced by the character expression or numeric value given by N1. <i>Only the first four characters are considered significant.</i>
	string: The character string which replaces every occurrence of the string defined by "var" in the user input. <i>Only the first four characters are considered significant.</i>
	N1: The numerical value which replaces every occurrence of the string defined by "var" in the user input.
	OFF: The previously defined variables are deactivated. New variables may be defined for input which follows.

EXAMPLES

```
DEFIne XXX = P in all input that follows
DEFIne PI = 3.1415
DEFInition OFF for all previous variables
```

COMMENTS

This command provides a powerful means of creating "prototype" data input files where symbolic variables may be used to denote problem-specific input data. These symbolic variables may then be defined at the beginning of the input or they can be replaced by character or numeric data at run time by the use of the screen input feature described in Section 6.2.1.

PURPOSE To specify the option and constants employed for calculation of fluid density as a function of pressure, temperature, or concentration of species.

SYNTAX *Mode 1: General Density Relations*

DENS {UNIF | POWE | POLY | LINE}, [SECO | THIR], [N1, N2, N3, N4]

UNIF: The fluid density is uniform and constant; *this is the default option.*

POWE: The fluid density varies according to power law Eqn. (2.5.1).

POLY: The fluid density varies according to the polynomial Eqn. (2.5.2).

LINE: The fluid density varies according to the linear Eqn. (2.5.3).

SECO: *By default the density specification is assumed to be for the primary fluid. If this modifier is present then specification is for the second phase.*

THIR: *If this modifier is present then specification is for the third phase.*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	Reference density, ρ^* of Eqns. (2.5.1) through (2.5.3). <i>The default value is 1 for the primary phase and 0 for other phases.</i>
N2	Coefficient a_1 of Eqns. (2.5.1) through (2.5.3). <i>The default value is 0.2 for Eqn. (2.5.1), and 0 otherwise.</i>
N3	The critical temperature, T_c , of Eqn. (2.5.1). The coefficient a_2 of Eqn. (2.5.2), the reference concentration C^* of Eqn. (2.5.3). <i>The default value is 374.15 for Eqn. (2.5.1), and 0 otherwise.</i>
N4	Coefficient a_3 of Eqn. (2.5.2) or the coefficient a_2 of Eqn. (2.5.3). <i>The default value 0.</i>

EXAMPLES

DENSITY constant and equal to 996.50

DENSITY by POWER law: $\rho^* = 1.$, Exponent = 0.25, $T_c = 374.15$ K

DENSITY POLYNomial law: $\rho^* = 1000.$, $a=1000.$, $b=0.05.$, $c=0.$, $d=3.E-5$

DENSITY LINEar function: 997., Beta=1.0E-4

SYNTAX *Mode 2: Gas Law Density Relation*

DENS {GAS}, [MULT], [SECO|THIR], [N1, N2, N3, N4]

GAS: The fluid density varies according to the gas law Eqn. (2.5.4).

MULT: *In the absence of this modifier, the gas may be composed of up to two species and the species concentration must be in units of density [ML⁻³]. If this modifier is present, then the gas may be composed of up to four species and the species concentration is in units of mass fraction.*

SECO: *By default the density specification is assumed to be for the primary fluid. If this modifier is present then specification is for the second phase.*

THIR: If this modifier is present then specification is for the third phase.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through N4	The molecular weights of the first through fourth species in the gas, respectively. <i>The default value is 29 for all gas species.</i>

EXAMPLES

DENSity from GAS law

DENSity from GAS law: M1 = 29 (air), M2 = 44 (for CO2)

DENSity: SECOnd phase; MULTi GAS: M1= 18 (H2O), M2= 44 (CO2), M3= 29 (air)

DENSity: THIRd phase; MULTi GAS: M1= 18 (H2O), M2= 29 (air), M3= 44 (CO2)

PURPOSE To disable built-in default options.

SYNTAX **DISA** *[FLOW]*

FLOW: By default, the flow (or pressure) equation is always solved. This command modifier must be used to disable flow calculations, if desired.

EXAMPLES

DISAble FLOW

PURPOSE To signify the end of a problem.

SYNTAX END

EXAMPLES

END
END of problem number 1

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

PURPOSE To fix the values of selected variables for a subregion within the domain of calculation.

SYNTAX **FIXE** *[symbol, ...,], [N1, ..., Nn]*
 n = 4 for 2D input mode; n = 6 for 3D input mode

symbol: One or more of the character strings which denotes the dependent variable for which the values are fixed for the subregion specified by N1 through Nn. The valid symbols are listed in Table 5-4. *If no symbol is specified, then the values are fixed for all the variables.*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through Nn	Grid index coordinates of the subregion for which the value of the variable are to be is fixed. See Section 6.2.3 for interpretation of this input. If this input is omitted then the subregion is defined to be total domain.

EXAMPLES

FIXEd P from (3,5) to (7,5)	\$ 2D mode
FIXEd T from (5,7,2) to (5,21,7)	\$ 3D mode
FIXEd values for P, T,C and C2 from (3,5) to 7,5)	\$ 2D Mode
FIXEd values from (5,7,2) to (5,21,7) for all variables	\$ 3D mode

COMMENTS

This command defines a subregion within the problem domain where the values of the variable are fixed. The values at the domain boundary can not 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 zone, such as a river passing through the domain of calculations. Multiple commands may be used to fix values in an arbitrary manner. The actual value to be assigned may differ from one grid node to another within the specified fixed value region. The fixed values, themselves, are specified by the **INITIAL** command. Once specified, they remain unchanged during calculations.

PURPOSE To compute, and obtain output of, convective and diffusive fluxes and source terms of a dependent variable for a subregion within the flow domain.

SYNTAX **FLUX** *[BALA], {symbol}, [NOW], [fname], [N1,..., Nn], [Nn+1]*
n = 4 for 2D input mode; n = 6 for 3D input mode

BALA: If the subregion specification (N1 through Nn) is that for a plane, then only the incoming or outgoing fluxes at the bounding planes of the subregion are written to the output file. However, if the modifier BALANCE is present, then the total flux balance, including cumulative and source terms, is written.

symbol: One of the character strings for which flux balance output will be obtained for the corresponding dependent variable. The valid symbols are listed in Table 5-4. *One, and only one, character string must be specified for each command.*

NOW: Fluxes are computed and output is produced as soon as the command is encountered.

fname: The name of the file on which the output is written. See Section 6.2.2 for specification of the file name. *By default, the output file is assumed to be named FLUXBAL (see Section 5.5).*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through Nn	Grid index coordinates of the subregion for which the flux computations are performed. See Section 6.2.3 for interpretation of this input. If this input is omitted then the subregion is defined to be total domain.
Nn + 1	The frequency (in terms of number of steps) at which the fluxes specified by the current command are written to the output file unit. For example, a specification of 10 will lead to output at the 10th, 20th, 30th, and so on, steps. A value of 0 is interpreted to be equal to 1. <i>The default value is 1.</i>

EXAMPLES

FLUX for P sub-region (2,2) to (11,15) print every 20 steps
 FLUX BALANCE for C for whole of region at every step
 FLUX for T at XY plane defined by (2,2,2) to (8,9,2) print every 10 steps
 FLUX BALANCE: T for region defined by (2,2,2) to (8,9,2) print every 100 steps
 FLUX output: C on 'FLUX.OUT' file for region (2,2,2) to (8,9,4) every 20 steps

COMMENTS

The maximum number of FLUX commands is limited by the LFLX parameter defined in Table 5-7.

PURPOSE To specify thermal and transport properties of the fluid.

SYNTAX *Mode 1: Specific Heat of the Fluid*

FLUI {SPEC}, [SECO | THIR], [N1, N2, N3, N4]

SPEC: Input is for the specific heat of the fluid.

SECO: Input is for the second phase of the fluid. This input is used only with the evaporation/condensation phase change option.

THIR: Input is for the third phase of the fluid.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	<p>The interpretation of this input is problem dependent.</p> <p>In the absence of the SECOnd modifier, it is the specific heat of the fluid.</p> <p>If the evaporation option is selected by the PROBLEM command, the second phase in PORFLOW[®] is taken to be a gas phase which may be composed of up to four different species (or components). The first gas species in this case is always taken to be the water vapor. If this case, in the presence of the SECOnd modifier, N1 is taken to be the specific heat of the water vapor which will be later replaced by the value computed dynamically from Eqn. (2.5.34).</p>
N2, N3, N4	<p>This input is used only for problems with evaporation if the SECOnd modifier is present. These values then taken to be the specific heats of the second, third, and fourth species of the gas phase, respectively. <i>The default value for all components is zero.</i></p>

EXAMPLES

FLUId SPECific heat for: 4.19
 FLUId SPECific heat for SECOnd fluid: 1.
 FLUId SPECific heat for SECOnd fluid: 0.24, 0.24, 0.24, 0.24

SYNTAX *Mode 2: Thermal conductivity or mass diffusivity of the fluid.*

FLUI {COND | DIFF}, [symbol], [SECO | THIR], [N1]

COND: The input is for the thermal conductivity of the fluid.

DIFF: The input is for the mass diffusivity of the fluid.

symbol: One of the character strings which denotes the dependent variable for which the input is specified. The valid symbols are: T, C, C2, C3 or C4 of Table 5-4. *The symbol is ignored if COND modifier is present. If DIFF modifier is present and no symbol is specified then the default is the first mass species (C).*

SECO: The input is for the second phase of the fluid.

THIR: The input is for the third phase of the fluid.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The thermal conductivity of the fluid or the diffusivity of the mass species in the fluid. <i>The default value for all components is zero.</i>

EXAMPLES

- FLUId thermal CONDuctivity = 4.10
- FLUId diffusivity for T = 4.10
- FLUId DIFFusivity for first species = 4.10
- FLUId DIFFusivity for C2 = 4.10
- FLUId DIFFusivity for C2 in SECOnd phase = 4.10

SYNTAX *Mode 3: Input for Fluid Enthalpy Relation*

FLUI {ENTH}, [N1, N2, N3, N4]

ENTH: Enthalpy-specific heat relation for phase are specified.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The latent heat of phase change; the constant c_0 of Eqn. (2.5.34). For the evaporation option, the default values is 3.9202E6 whereas for the freezing option, it is 1000.
N2, N3, N4	The specific heat-enthalpy constants, c_1 , c_2 and c_3 of Eqn. (2.5.34), respectively. For the evaporation option, the default values are $c_1 = 3681.$, $c_2 = -11.76$ and, $c_3 = 0.01772$. For the freezing option, the default values are $c_1 = 1.$ and $c_2 = c_3 = 0.$

EXAMPLES

FLUId ENTHalpy constants: 3.92017E6, cp= -2441 ! Bixler values
 FLUId ENTHalpy constants: 1000 (latent heat for freezing)
 FLUId ENTHalpy constants: 1000 (latent heat), c1 = 0.5

SYNTAX *Mode 4: Input for Fluid Vapor Pressure*

FLUI {VAPO}, [N1, N2, N3, N4]

VAPO: Constants for fluid vapor pressure relation are specified.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1, N2, N3, N4	The vapor pressure constants, a_0 through a_3 of Eqn. (2.5.36). The default values are $a_0 = 131.57894$, $a_1 = 18.3443$, $a_2 = 3841.1954$ and, $a_3 = 45.$

EXAMPLES

FLUId VAPOr pressure constants: 130, 20, 4000, 45

PURPOSE To select the soil or rock zones to which the property information following the FOR specification applies.

SYNTAX FOR {N1}, [N2, N3]

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The lowest zone number ($1 \leq N1 \leq LZN$) to which property specification applies. LZN is the dimensioning parameter (see Section 5.12). <i>The default value is 1.</i>
N2	The highest zone number ($N1 \leq N2 \leq LZN$) to which property specification applies. If N2 is not specified, then it is assumed to be equal to N1. <i>The default value is 1.</i>
N3	The interval in the zone number ($1 \leq N3 \leq LZN$) designation. The specification will be effective for N1 to N2 at increments of N3 in the manner of a FORTRAN DO loop. If N3 is not specified, then it is taken to be 1. <i>The default value is 1.</i>

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

COMMENTS

The zone numbers specified by this command must denote active zones; that is, these zone numbers must have previously appeared on a ZONE command. The property information to which this command applies, is specified through the HYDRauiic, MULTiphasE, ROCK, SOIL, THERmal and TRANsport commands. If the keyword command for the relevant property explicitly specifies the zones to which the information applies, then any previously specified FOR command is ignored. However, the input stays in effect for subsequential property commands until another FOR command is encountered.

PURPOSE To specify the components of the gravitational acceleration vector, g_j , of Eqn. (2.1.6).

SYNTAX GRAV {N1, N2, N3}

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The constant of gravitational acceleration along the direction of the x coordinate. A positive value implies that the acceleration vector is directed along the x-axis whereas a negative value implies that it is directed against the x-axis. <i>The default value is -9.81 for cylindrical and zero for cartesian geometry.</i>
N2	The constant of gravitational acceleration along the direction of the y or r coordinate. <i>The default value is -9.81 for cartesian geometry in 2D mode and zero otherwise.</i>
N3	The constant of gravitational acceleration along the direction of the z or Θ coordinate. <i>The default value is -9.81 for cartesian geometry in 3D mode and zero otherwise.</i>

EXAMPLES

GRAVity constants are: 0., -9.81	\$ Orientation against y-axis
GRAVity constants are: -6.937, -6.937, 0.	\$ 45 deg to x & y
GRAVity constants are: 0., 0., -9.81	\$ Orientation against z-axis
GRAVity constants are: 0., 0., 1	\$ Relative value: orientation against z-axis

COMMENTS

This command is required only if the multiphase flow option is selected or if fluid density variation is according to the gas law. The default values imply that for cylindrical geometry the gravitational vector is opposed to the X-direction whereas, for cartesian geometry the vector is directed against the Z-direction for 3D problems and against the Y-direction for 2D problems.

The absolute value of the gravitational acceleration is required only to compute pressure head, h , from the thermodynamic pressure, p . Otherwise it is only the ratio of the vector components, g_j , to the total gravitational acceleration, g , which appears in the equations. Therefore, for many problems, relative values of the three components of the vector may be specified.

PURPOSE To specify the number of grid lines in the (x,y,z) direction and the dimensionality of the problem.

SYNTAX GRID {N1, N2}, [N3]

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The number of grid nodes in the x direction. The specified value is denoted by IMAX in this document. The minimum permissible value is 3 and the maximum is L1, where L1 is the dimensioning parameter of Table 5-7. <i>The default value is 3.</i>
N2	The number of grid nodes in the y or r direction. The specified value is denoted by JMAX in this document. The minimum permissible value is 3 and the maximum is L1. <i>The default value is 3.</i>
N3	The number of grid nodes in the z direction. The specified value is denoted by KMAX in this document. If N3 is ≥ 3 , then PORFLOW is invoked in its 3D mode. If N3 is 1 or 2 then the 2D solution mode is invoked but it is assumed that all the subregion input specification of Section 5.4 (DIAGnostic, BOUNDary, FIXEd, FLUX, HISTory, INITial, LOCAtE, WINDow, and ZONE commands) is in the 3D mode. If N3 is 0 or is not specified, then the 2D solution mode is invoked and it is assumed that all subregion input specification is also in the 2D mode. The maximum permissible value is L1 and the minimum is 1. <i>The default value is 1.</i>

EXAMPLES

GRID is 31 by 25	\$ 2D problem with grid-index related input in 2D mode
GRID is 31 by 25 by 1	\$ 2D problem but grid-index related input in 3D mode
GRID is 31 by 25 by 12	\$ 3D problem with grid-index related input in 3D mode

PURPOSE To specify the reference hydraulic properties of the host porous matrix, or those of the planar or linear features.

SYNTAX HYDR [P | P2 | P3], [N1, N2, N3, N4], [N5, N6, N7]

P The values are specified for the primary fluid. *This is the default option.*

P2 The values are specified for the second phase fluid.

P3 The values are specified for the third phase fluid.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The effective fluid and matrix compressibility (≥ 0) to be used to compute effective storativity, S_e , according to Eqn. (2.1.17). The specified value is assumed to be the sum of the matrix and fluid compressibility ($\alpha_s + \Theta_E \alpha_f$) for a liquid and the matrix compressibility (α_s) for a gas. The α_f for a gas is computed from Eqn. (2.5.25). <i>The default value is 1.</i>
N2, N3, N4	The reference values (≥ 0) of the three components of the hydraulic conductivity tensor, K_{ij}^* of Eqn. (2.5.28) in the three principal directions, (x,y,z) or (x,r, Θ), respectively. All off-diagonal components ($i \neq j$) are assumed to be zero. <i>The default value is 0.</i>
N5, N6, N7	These three values select the zones to which N1 through N4 apply. Their interpretation is identical to that of N1, N2 and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command. <i>If no FOR command was previously specified, then the input is assumed to apply to zone number 1.</i>

EXAMPLES

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

PURPOSE To specify the initial values of a field variable in the domain of interest.

SYNTAX *Mode 1: Initial Conditions for a Subregion*

INIT {symbol}, {N1}, [N2, ..., Nn], [Nn+1, Nn+2, Nn+3]
 n = 5 for 2D input mode; n = 7 for 3D input mode

symbol: One of the character strings which denotes the field variable for which the initial conditions are specified. The valid symbols are listed in Table 5-5 (except H, H2, H3 and MOIS). *One, and only one, symbol must be specified.*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The base value for the variable, the constant F_0 of Eqn. (2.5.49). <i>The default value is 0.</i>
N2 through Nn	Grid index coordinates of the subregion for which the input is specified. See Section 6.2.3 for interpretation of this input. If this input is omitted then the subregion is defined to be total domain.
Nn+1, Nn+2, Nn+3	The coefficients a_1 , a_2 , and a_3 , of Eqn. (2.5.49). The coefficient a_3 is ignored for 2D mode. <i>The default value is 0.</i>

EXAMPLES

INITial P is 0.1 everywhere
 INITial T is 1.E-3 from (2,2) to (7,9) ! 2D input mode
 INITial T is 1.E-3 from (2,2,2) to (7,9,4) ! 3D input mode
 INITial P2 0.1 from (1,1) to (11,8); grads: x=0, y=0.2 ! 2D input mode
 INITial C 0.1 fr (1,1,1) to (11,8,5) grads: x=0, y=0.2, z=-0.2 ! 3D input mode

SYNTAX

Mode 2: Initial Conditions for a Predefined Zone

INIT {symbol}, {ZONE}, {N1}, {N2}, [N3, N4, N5]

symbol: See Mode 1 Specification.

ZONE: The input is for a zone number previously specified by the ZONE command.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The base value for the variable, the constant F_0 of Eqn. (2.5.49). <i>The default value is 0.</i>
N2	The pre-designated zone number of the subregion to be initialized. In this case, the zone number must have previously appeared on a ZONE command to identify the subregion.
N3,N4,N5	The coefficients a_1 , a_2 , and a_3 , of Eqn. (2.5.49). N5 is ignored for 2D mode. <i>The default value is 0.</i>

EXAMPLES

INITial C is 1.E-2 for ZONE 16

INITial T is 100 for ZONE 16, gradx = 0., grady = -0.5 !! 2D input mode

INITial T is 100 for ZONE 16, gradx = 0., grady = 0.2, gradz = -0.5 !! 3D input mode

SYNTAX *Mode 3: Initial Conditions for a Set of Nodes*

INIT *{symbol}, {NODE}, {N1, ..., Nn}, [Nn+1, Nm]; m ≤ LVAL.
n = 4 for 2D input mode; n = 6 for 3D input mode*

NODE: The input is on a node by node basis.

symbol: See Mode 1 Specification.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through Nn	Grid index coordinates of the subregion for which the input is specified. See Section 6.2.3 for interpretation of this input. <i>In this mode, this input must be specified.</i>
Nn + 1 through Nm	The values at the nodes of the subregion. The specification of values is in the manner of increasing I, J and K, in that order, for the subregion defined above. The maximum number of values which can be specified is LVAL-n (see Table 5-7 for definition of LVAL). <i>The default value is 0.</i>

EXAMPLES

INITial T on NODE basis: from (2,2) to (2,9); 1, 2, 3, 4, 5, 6, 7, 8
 INITial P on NODE basis: from (2,2,2) to (2,7,2); 0.1, 0.2, 0.3, 0.4, 0.5, 0.6

SYNTAX *Mode 4: Initial Conditions from a File*

INIT *{symbol}, {fname}*

symbol: See Mode 1 Specification.

fname: The name of the file from which the initial conditions are obtained. See Section 6.2.2 for specification of the file name. In this input mode, the total field of the variable must be specified.

EXAMPLES

INITial T from file 'INITIAL.T'

- PURPOSE** Choice of discretization scheme for integration of heat and mass transport equations.
- SYNTAX** INTE *{symbol}, {HYBR | EXPO | COND}*
- symbol: One of the character strings which denotes the heat or mass transport variable for which the profile specification will be effective. The valid symbols are: T, C, C2, C3 or C4 of Table 5-4. *If no symbol is specified, then the input is assumed to be effective for all variables.*
- HYBR: The hybrid scheme (Runchal, 1972) is employed for integration. *This is the default option.*
- EXPO: A tabulated version of the exponential scheme (Spalding, 1972) is employed for integration.
- COND: The CONDIF, a total variation diminishing scheme (Runchal, 1987), is employed for integration.

EXAMPLES

INTEgration for C by EXPOntial scheme
 INTEgration for T by profile: HYBRid (same as default)
 INTEgration for C2 by CONDif scheme

COMMENTS The default option should prove adequate for most applications. However, if the local grid Peclet number [Eqn. (3.2.1)] is significantly in excess of a value of 10, then the CONDIF or exponential scheme may be desirable. Further discussion is available in Sections 3.2 and 3.4.

The EXPOntial and CONDif options may not be available at some installations.

PURPOSE To locate a source region or boundary segment within the field of interest.

SYNTAX **LOCA** {*BOUN* | *SOUR*}, {*N1*}, {*N2*, ..., *Nn*}
 n = 5 for 2D input mode; n = 7 for 3D input mode

BOUN: Section of a domain boundary is to be moved to a location within the field of interest; that is the boundary conditions are to be applied at a boundary which is located within the field of interest rather than at the external edge of the domain.

SOUR: The location of a source is specified. The source may be located only within the field of interest and not at the domain boundary. Each source must be identified with a unique source identification number which is distinct from that for other sources.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The boundary orientation index for the boundary segment or the source identification number. Interpretation of the boundary orientation index is identical to that of N1 on the BOUNDary command. The source identification index must be a number between 1 and LSS where LSS is specified on the parameter statement (see Section 5.12).
N2, ..., Nn	The grid index coordinates of the boundary or source region. See Section 6.2.3 for interpretation of this input.

EXAMPLES

LOCAtE BOUNDary +1 from (11,1) to (11,7)	\$ 2D input mode
LOCAtE BOUNDary -3 from (1,1,5) to (7,7,5)	\$ 3D input mode
LOCAtE SOURce # 1 from (6,10) to (31,10)	\$ 2D input mode
LOCAtE SOURce 3 from (6,10,2) to (6,10,7)	\$ 3D input mode

PURPOSE To select the method of solution for the matrix of algebraic equations.

SYNTAX **MATR** *[dir], [symbol=N1, symbol=N2, ..., symbol=Nn], [Option]*

dir: One or more of the character strings: X, Y, Z. It denotes the direction in which the matrix sweeps will be conducted. For example, a specification of X will result in the matrix equations being solved along the x-direction nodes, in increasing order of the I grid index, for fixed values of the J and K indices. *By default, the matrix is swept along all three directions.*

symbol: One or more of the character strings which denote the variable(s) for which the N1, N2, ..., etc. and the specified option are effective. Valid symbols are listed in Table 5-4.

- option:**
- ADI** Matrix is solved by the alternating direction implicit method. *This is the default option.*
 - SOR** Matrix is solved by successive over relaxation method.
 - CONJ** Matrix is solved by Conjugate Gradient method.
 - GAUS** Matrix is solved by Gaussian Elimination method.
 - CHOL** Matrix is solved by Cholesky Decomposition method.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through Nn	Number of times per time step that the matrix is solved for the variable denoted by the symbol immediately preceding the value. This input is effective only for the ADI method. During this inner loop, only the values of the dependent variable change, the coefficients of the matrix stay constant. The value must be greater than 0. <i>The default value is 1.</i>

EXAMPLES

- MATR**ix sweeps in X direction only
- MATR**ix sweeps in X and Y directions: T=3 \$ Sweep temperature equation 3 times
- MATR**ix sweeps: P=3, T=1, C=2
- MATR**ix for P to be solved by SOR
- MATR**ix for T to be solved 3 times by the ADI method

COMMENTS

Limited options may be available in some installations of PORFLOW.

PURPOSE To select method of solution of the governing differential equations.

SYNTAX METH *[symbol], {HYBR | PICA | DELT}*

symbol: One or more of the character strings which denote the dependent variable for which the specified method of solution is selected. The valid symbols are listed in Table 5-4. *If no symbol is specified, then the input is assumed to be effective for all variables.*

HYBR: The equations are solved in a manner which leads to an unconditionally conservative solution method for transient problems. This relies on a hybrid formulation where the accumulation term in the governing equation is retained in its mass or energy conserved form [such as Eqn. (2.1.24) or (2.2.11)] rather than the linearized form [such as Eqn. (2.1.16) or (2.2.10)]. For steady state problems, the accumulation terms are zero and this method reverts to the Picard method. *This is the default option for transient problems.*

PICA: The Picard solution method based on the linearized accumulation terms [such as Eqn. (2.1.16) or (2.2.10)] is selected. This is the fastest solution method; however, for multi-phase flow problems it may require a small time step to ensure mass and energy conservation for transient problems. *This is the default option for steady state problems.*

DELT: The equations are solved in a "delta" formulation where the governing equations are recast in the form of differences of the dependent variable [such as Eqn. (2.1.25) or (2.2.12)]. For those problems where the changes in the variable are very small compared to the absolute value of the variable itself, this method provides a more accurate solution than other methods. However, if the initial values of the variable are not known accurately, then this method may be more prone to numerical instabilities.

EXAMPLES

METHod of solution for P and P2: PICARd
 METHod of solution for P: DELTα formulation
 METHod of solution for T: PICARd
 METHod of solution for P2: HYBRid

COMMENTS *The HYBRid and DELTα formulations may not be available for all variables in some installations of PORFLOW.*

PURPOSE To specify the nature of the characteristic curve and the values of the empirical characteristic constants for the multiphase or variably saturated flow. The presence of this command will automatically initiate multiphase algorithm of PORFLOW[®].

SYNTAX *Mode 1: Tabulated Data Input*

MULT [COND], [HEAD], {N1}, [N2, ..., Nn], [Nn+1, Nn+2, Nn+3]

COND: *By default, the tabulated data input mode specification is for the S- δh characteristic. If the modifier CONDUCTivity is present, then the specification is assumed to be for k_r vs. S.*

HEAD: *By default the relative conductivity characteristic is assumed to be specified as S vs. k_r . If the modifier HEAD is present, then the characteristic is taken to be specified as tabulated values of k_r vs. δh .*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The number of sets of tabulated values which follow.
N2	The first value of S^a [Eqn. (2.5.13)] for the (S-h) or (S- k_r) characteristic or the first value of the δh^a [Eqn. (2.5.17)] for the (δh - k_r) characteristic. The numerical value must be ≥ 0 .
N3	The first value of δh^a for the (S-h) or the first value of k_r^a for (S- k_r) or (δh - k_r) characteristic. The input value may be scaled internally by the SCALE command. The numerical value must be ≥ 0 .
N4 through Nn	The sets of values for S^a , δh^a or k_r^a in a manner similar to N2 and N3. The number of sets (including N2 and N3) must equal that specified by N1 above. The numerical values must be ≥ 0 .
Nn+1 through Nn+3	These three values select the zones to which N1 through Nn apply. Their interpretation is identical to that of N1, N2 and N3, respectively, of the FOR command. If these are omitted, then the input is assumed to apply to the zones specified by the most recent FOR command. <i>If no FOR command was previously specified, then the input is assumed to be for zone number 1.</i>

EXAMPLES

```
// Next command specifies tabulated input for (S-h) characteristic
MULTiphase flow: 4 sets: (0,1.E6), (0.1,1.E3), (0.9,1.E2), (1.,1.)
MULTiphase: COND: sets 4: (0,0), (0.2,0.4), (0.8,0.7), (1., 1.) for zone 4    $  $k_r$  vs. S
MULTiphase COND vs HEAD: sets 4: (100,0), (60,0.4), (40,0.7), (0, 1.)    $  $k_r$  vs.  $\delta h$ 
```

SYNTAX

Mode 2: Capillary Pressure Dependent Analytic Relationships

MULT {VAN | BROO}, [BURD | MUAL], [N1, N2, N3, N4], [N5, N6, N7]

VAN: The hydraulic properties are calculated according to van Genuchten (1978) relation given by Eqn. (2.5.19).

BROO: The hydraulic properties are calculated according to the Brooks and Corey (1966) relation given by Eqns. (2.5.20).

MUAL: The relative permeability, k_r , is derived according to Muallem (1976) predictive model. The exponents A and B of Eqns. (2.5.29) or (2.5.30) are 1/2 and 2, respectively. *This is the default option if the van Genuchten formula is specified for the S- δ h relation.*

BURD: The relative permeability, K_r , is derived according to Burdine (1953) predictive model. The exponents A and B of Eqns. (2.5.29) or (2.5.30) are 2 and 1, respectively. *This is the default option if the Brooks and Corey formula is specified for the S- δ h relation.*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	For van Genuchten option, the n of Eqn. (2.5.19) (> 0). For Brooks and Corey option, the λ of Eqn. (2.5.20) (> 0). <i>The default value is 2.</i>
N2	For van Genuchten option, the α^1 of Eqn. (2.5.19) (≥ 0). For Brooks and Corey option, the H^1 of Eqn. (2.5.20) (> 0). <i>The default value is 0.</i>
N3	The residual saturation, S_r of Eqn. (2.5.10) (> 0). <i>The default value is 0.</i>
N4	For van Genuchten option, the α^2 of Eqn. (2.5.19) (≥ 0). For Brooks and Corey option, the H^2 of Eqn. (2.5.20) (> 0). <i>The default value is 0.</i>
N5, N6, N7	These three values select the zones to which N1 through N4 apply. Their interpretation is identical to that of N1, N2 and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command. <i>If no FOR command was previously specified, then the input is assumed to apply to zone number 1.</i>

EXAMPLES

MULTiphase flow: BROOKs & CoreY: beta = 0.5; air entry p = 20

MULTiphase flow VAN Genuchten: n = 2.0, alpha = 0.5

MULTiphase: BROOKs with MUALem: beta=0.2, h* = 5.4, 2*0, zones: 1, 5, 2

MULTiphase flow: VAN GENUCHTEN: N=3.5; Aow=0.167, sr=0.067, Aao=0.090

SYNTAX *Mode 3: Temperature Dependent Analytic Relationship*

MULT {WHEE}, [N1, N2, N3, N4], [N5, N6, N7]

WHEE: Saturation relation is that of Wheeler (1973) given by Eqn. (2.5.22).

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The exponent n of Eqn. (2.5.22) (> 0). The default value is 10.
N2	The delay temperature, T _d of Eqn. (2.5.22) (≥ 0), for the freezing/thawing algorithm. The default value is 1.E-30.
N3	The residual saturation, S _r of Eqn. (2.5.22) (> 0). The default value is 0.
N4	The α ₁ of Eqn. (2.5.22) (≥ 0). The default value is set to be 1 - S _r .
N5, N6, N7	See Mode 2 specification.

EXAMPLES

MULTiphase flow: with WHEELer option: n=4, Td=0.1, sr=0.2

SYNTAX *Mode 4: Minimum Relative Hydraulic Conductivity Mode*

MULT {MINI}, {N1}, [N2,N3,N4]

MINI: The relative hydraulic conductivity, k_r, for multi-phase flow is computed by the tabulated input or analytic relationship. In general k_r can take any value between 0 and 1. However, it is sometimes preferable to set a lower limit for k_r.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The minimum value of k _r . Any computed value which is lower than N1 is set equal to N1. The default value is 1.E-10.
N2, N3, N4	Interpretation is identical to that of N5, N6 and N7 of Mode 2 specification.

EXAMPLES

MULTiphase MINIMUM relative CONDuctivity is: 1.E-5.

MULTiphase MINIMUM CONDuctivity: 1.E-5 for zones 2 through 8 in steps of 2.

PURPOSE To select the field arrays to be written to the output file unit, IWR, and to specify the manner and frequency of output.

SYNTAX **OUTP** *[symbol, ...], [plane], [NARR | WIDE], [NOW | OFF | ON], [N1]*

symbol: One or more of the character strings which represents a corresponding variable for which the output is desired. The valid symbols are listed in Table 5-5.

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

NARR: The output tables are produced in an 80-column (narrow) format.

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

NOW: Tabular output is produced as soon as the command is encountered.

OFF: Tabular output is completely suppressed.

ON: Tabular output is reactivated if it was previously suppressed.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The frequency index for tabular output. The output is obtained every N1 (≥ 1) steps; for example, a specification of N1 = 10 will lead to output at the 10th, 20th, 30th, etc., steps. <i>By default, tabular output is obtained automatically at the end of simulations for all active variables.</i>

EXAMPLES

OUTPut: U, V, W in NARRow tabular format
 OUTPut: U, V, C and P in WIDE tabular format NOW
 OUTPut: U, V, C, P, S by XZ planes in WIDE tabular format NOW
 OUTPut: U, V, P and T in NARRow format NOW and every 20 steps
 OUTPut tables for V, W, P and S and S2 by YZ planes every 15 steps
 OUTPut OFF for all variables
 OUTPut ON once again

COMMENTS

If no OUTPut command is specified, then output for all 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 fractions if the multi-phase option is invoked. Successive commands may be employed to accommodate changing output requirements.

PURPOSE To cause a temporary halt in the calculations.

SYNTAX PAUS

EXAMPLES

PAUSE and await operator action

COMMENTS Operator intervention is required to restart the calculation process. This command allows for operator action during interactive execution.

PURPOSE To select the periodic boundary option for boundary conditions in the x, y or z direction of the domain.

SYNTAX PERI [X, Y, Z], [OFF]

X: The boundary conditions for the x direction boundaries are determined automatically from the requirement of periodicity of the solution. Any boundary condition specification through the BOUNDary command (with boundary index -1 or +1) is ignored.

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

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

OFF: Periodic boundary condition option is deactivated.

EXAMPLES

- PERIodic boundaries in X
- PERIodic boundaries in Y
- PERIodic boundaries in X and Z
- PERIodic boundaries in X, Y and Z
- PERIodic boundary option OFF

PURPOSE To specify the general nature and type of the problem to be solved by PORFLOW[®].

SYNTAX **PROB** {type}, [N1], [N2]

type: indicates the nature and type of the problem to be solved by PORFLOW[®]. The valid modifiers are given below.

type	INTERPRETATION
SING	The fluid is single phase. <i>This is the default option.</i>
MULT	The multiphase, variable saturation, flow mode of PORFLOW [®] is selected. This option is also automatically selected if the command MULTiphase is present.
UNCO	Unconfined, free surface mode of PORFLOW [®] is selected.
SURF	If modifier FREE is also present then unconfined, free surface mode of PORFLOW [®] is selected; otherwise it has no effect.
FREE	In the SURFace modifier is not present, then the freezing/thawing phase change mode of PORFLOW [®] is selected; otherwise, the free surface, unconfined flow mode is selected.
EVAP	The evaporation/condensation phase change mode of PORFLOW [®] is selected.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The total number of phases for the MULTiphase option (<i>default value 2</i>); the normal direction to the bedding planes for FREE SURFace or UNCONfined mode (<i>default value 2 for 2D and 3 for 3D flow</i>); the evaporation coefficient, C_m of Eqn. (2.5.35), for the EVAPoration option (<i>default value 1</i>); and the freezing temperature, T_f of Eqn. (2.5.22), for the FREEzing option (<i>default value 0</i>).
N2	An empirical constant to determine the maximum rate of freezing or thawing from step to step. A small value leads to smoother freezing/thawing behavior whereas a large value leads to more abrupt changes from one time step to another. <i>The default value is 1000.</i>

EXAMPLES

- PROBLEM is MULTiphase
- PROBLEM is MULTiphase with 3 phases
- PROBLEM is UNCONfined
- PROBLEM with FREE SURFace; bedding plane normal to direction 2
- PROBLEM with phase change: EVAPoration constant = 2.
- PROBLEM with phase change: FREEzing at Temperature 32 F
- PROBLEM with phase change: FREEzing at $T_f = 32$ F, rate=500.

PURPOSE To specify the mode of interpretation and calculation of the properties of the host porous matrix or, planar or linear features.

SYNTAX **PROP** *[symbol, ...], [EFFE], [ARIT | GEOM | HARM]*

symbol: One or more of the character strings which represents a corresponding variable for which the input is effective. The valid symbols are listed in Table 5-4. *If no symbol is specified, then the input is assumed to be effective for all variables.*

EFFE: By default, the host media properties specified through the THERmal and TRANsport commands are assumed to be for the solid component of the matrix only. The input values of specific heats are interpreted to be in mass units [such as J/(kg K)] and the input value of N1 on the TRANsport command is taken to be the partition coefficient, k_d . The effective matrix properties are computed as weighted averages of solid properties and the fluid properties.

However, if the modifier EFFE is present, then the property input on the THERmal and TRANsport commands is assumed to be in the effective mode. In this mode, the input specific heats are assumed to be in terms of volume units [such as J/(m³ K)] and the input value of N1 on the TRANsport command is assumed to be the retardation factor, R_d . That is, it is assumed that the existence of fluid in the porous matrix has already been accounted for by the user. Any values specified with a FLUID modifier on the THERmal and TRANsport command are ignored.

ARIT: The mean value of the diffusion coefficient, Γ_{ij} of Eqn. (2.4.1), at a cell interface is computed as the arithmetic mean of the two nearest grid node values.

GEOM: The mean value of the diffusion coefficient, Γ_{ij} of Eqn. (2.4.1), at a cell interface is computed as the geometric mean of the two nearest grid node values. This mode is recommended for multi-phase or variably saturated flow.

HARM: The mean value of the diffusion coefficient, Γ_{ij} of Eqn. (2.4.1), at a cell interface is computed as the harmonic mean of the two nearest grid node values. *This is the default option.*

EXAMPLES

PROPerTy mode: equivalent matrix values directly specified.
 PROPerTy in EFFEffective mode; use GEOMETric means
 PROPerTy averages for T and C by GEOMETric means
 PROPerTy in EFFEffective mode for C

PURPOSE To read the archive file for basic problem information and initial conditions.

SYNTAX READ [N1], [fname], [fmt], [STAR]

fname: The name of the file from which the input is obtained. See Section 6.2.2 for specification of the file name. *By default, the input data file is assumed to be named RESTART (see Section 5.5).*

fmt: The modifier "FORMatted" or "UNFORMatted" which defines the nature of the data on the restart file. *If this specification is omitted, then the file is assumed to be formatted (see Section 5.10).*

STAR: If this modifier is present then the calculation step number for the current simulation is set to 0; otherwise it is computed by reference to the step number at which the data was archived.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The data set number (≥ 0) to be read from the archive file. If no data set number is specified, then the first set is read from the archive file. As explained in Section 5.10, a data set in this context consists of several records. <i>The default value is 1.</i>

EXAMPLES

READ from archive file
 READ record number 3
 READ from 'EXAMPLE1.SAV'
 READ record number 5 from 'EXAMPLE2.SAV' in FORMatted mode
 READ record # 5 from 'EXAMPLE2.SAV' and STARt step count from now

PURPOSE To specify the reference values of some constants and variables.

SYNTAX REFERENCE {P | T | GAS}, {N1}, {N2}

P: The reference value for pressure is specified.
 T: The reference values for temperature are specified.
 GAS: The universal gas constant is specified.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The temperature T* of Eqns. (2.5.1) through (2.5.7), or pressure p* of Eqn. (2.5.4) or the universal gas constant R _u of Eqn. (2.5.4). <i>The default value is 0 for T*, 101325 for p* and 8314 for R_u.</i>
N2	The base temperature for absolute temperature units [T _a of Eqns. (2.5.4) and (2.5.5)]. <i>The default value is 273.15.</i>

EXAMPLES

REFERENCE P = 2.5E5
 REFERENCE T = 30. deg C
 REFERENCE T = 60. F with base = 459.67 R
 REFERENCE GAS constant: 1545 ft lbf/lb-mole R

PURPOSE To specify the relaxation factors for iterative solution of the matrix of equations.

SYNTAX **RELA** { [symbol=N1, symbol=N2, ..., symbol=Nn], | [OFF] }

symbol: One or more of the character strings for which the relaxation parameters are specified. The valid symbols are all those listed in Table 5-4 plus KR, SE and S. KR denotes the relative conductivity [k_r of Eqn. (2.1.5)] and SE denotes the effective storativity [S_e of Eqn. (2.1.17)]. The concept of relaxation is extended in PORFLOW[®] to derived variables (KR, SE and S). For multi-phase flow, the equations are highly non-linear. The relaxation factors for these derived variables are used to compute applicable values as a weighted average of the values at the old and new time steps.

OFF: All relaxation parameters are set to unity. Any other input on the command is ignored. In essence, the relaxation feature is disabled.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through Nn	Relaxation factor [Θ of Eqn. (3.2.2)] for the variable denoted by the symbol immediately preceding the value. The numerical value must be greater than 0 and less than 2.

COMMENTS This command is effective in both steady and transient mode of solution. The relaxation factor affects the convergence of the numerical solution. If the solution shows instability, then a value less than unity may help in obtaining a stable solution. Alternatively, if the convergence rate is too slow, then a value greater than unity may result in more rapid convergence. A value less than 0 or greater than 2 will, almost always, lead to exponentially unstable growth of the solution.

In the steady state mode the relaxation factor affects the values of the variable during outer step-to-step iterations (N1 on SOLVe command). In the transient mode, it is used during the inner iteration loop where multiple iterations (N2 on CONVeRgence command) are used at each time step. A more complete discussion of the role of the relaxation parameter is given in standard text books (see, for example, Varga, 1962).

EXAMPLES

- RELAXation factor for P = 0.7
- RELAXation factors: T = 1.2, C = 0.9
- RELAXation factors: T = 0.7, C = 0.9, C2 = 0.7
- RELAXation factors: S = 0.5, SE = 0.5, KR = 0.5
- RELAXation OFF

PURPOSE To rename the output variables listed in Table 5-5.

SYNTAX **RENA** {symbol = name}

symbol: One of the character strings which define the output variables which is to be renamed. The valid symbols are listed in Table 5-5.

name: A character string which defines the new symbol and name for the variable denoted by the symbol. The name must be enclosed in single or double quotes and it must be a character string with a length of no more than 32 characters. The first four characters of this name will be then interpreted as the new symbol for all subsequent references to this renamed variable.

EXAMPLES

RENAme U = 'XDIR Velocity of fluid flow' ! symbol U will now become XDIR
 RENAME T = 'TEMPERATURE (THERMODYNAMIC)' ! Symbol T will become TEMP
 RENAME C = "TC99 Technitium 99 in Solution" ! Symbol C will now become TC99

PURPOSE To specify the density, porosity or tortuosity of the porous matrix, planar or linear features.

SYNTAX *Mode 1: Specification of Density and Porosity*

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

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The density of dry solid component, ρ_s (> 0). <i>The default value is 1.</i>
N2	The effective (or flow) porosity, Θ_E ($0 \leq \Theta_E \leq 1$). <i>The default value is 1.</i>
N3	The total porosity, Θ_T ($0 \leq \Theta_T \leq 1$). <i>The default value is 1.</i>
N4	The diffusional porosity, Θ_D ($0 \leq \Theta_D \leq 1$). <i>The default value is 1.</i>
N5 through N7	These three values select the zones to which N1 through N4 apply. Their interpretation is identical to that of N1, N2 and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command. <i>If no FOR command was previously specified, then the input is assumed to apply to zone number 1.</i>

EXAMPLES

- ROCK density = 1; porosities: effective = 0.1, total 0.2, diffusive 0.15
- ROCK density 2200, porosities: 3*0.15 for ZONE number 2
- ROCK density 2200, porosities: 0.2, 0.25, 0.21 for zones 1 through 5
- ROCK rho 2200, porosities: 0.10, 0.20, 0.15 for zone 1 to 5 in step of 2

SYNTAX

Mode 2: Specification of Tortuosity

ROCK {*TORT*}, [*N1*, *N2*, *N3*], [*N4*, *N5*, *N6*]

TORT: The input is specified for the tortuosity factor.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through N3	The x, y and z direction components, respectively, of the tortuosity factor [τ_{ij} of Eqn. (2.2.8) and (2.3.7)] of the porous matrix. Only the components in the principal directions are used. The numerical values must be between 0 and 1. <i>The default value is 1.</i>
N4 through N6	These three values select the zones to which N1 through N3 apply. Their interpretation is identical to that of N1, N2 and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command. <i>If no FOR command was previously specified, then the input is assumed to apply to zone number 1.</i>

EXAMPLES

ROCK TORTuosity factors: 0.7, 0.6, 0.9

ROCK TORTuosity factors: 0.7, 0.6, 0.9 for zones 3 through 6

PURPOSE To write the archive file for restart, plotting and archiving purposes.

SYNTAX **SAVE** [symbol], [fname], [fmt], [NOW | OFF | ON], [N1]

symbol: One or more of the character strings which represents a corresponding variable for which output is desired. The valid symbols are listed in Table 5-5. (See Section 5.9 for further information).

fname: The name of the file to which the output is written. See Section 6.2.2 for specification of the file name. If the specified file name is different than the file name specified on a previous command, then the previous archive file is closed and a new file is opened for subsequent output. *By default, the archive file is assumed to be named ARCHIVE (see Section 5.5).*

fmt: The modifier "FORMatted" or "UNFOrmatted" which defines the nature of the data on the archive file. *By default, the file is assumed to be formatted.*

NOW: Archive output is produced as soon as the command is encountered.

OFF: Archive output is completely suppressed.

ON: Archive output is reactivated if it was previously suppressed.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The frequency index for archive output. The archive output is obtained every N1 (≥ 1) steps. For example, a specification of N1=10 will lead to output at the 10th, 20th, 30th, etc., steps.

EXAMPLES

SAVE U, V, W on file 'DEMO.PLT' in UNFOrmatted mode
 SAVE U, V, P, THETA and C every 100 steps
 SAVE W, P and C NOW
 SAVE U, T and C NOW and every 20 steps
 SAVE OFF for all variables

COMMENTS

If no SAVE command is specified, then output for the active variables is automatically produced at the end of simulations. The active variables consist of all variables for which the equations are solved, the three velocity components (U, V, W) if the pressure equation is solved, and the saturation fractions if the unsaturated mode of PORFLOW is invoked. Successive commands may be employed to accommodate changing output requirements.

PURPOSE To allow internal scaling of the specified input according to the equation:

$$Q_{in} = a_1 * Q + a_2,$$

where Q_{in} is the internal representation of a quantity, Q is the value specified by the user, and a_1 and a_2 are user-specified constants.

SYNTAX SCAL [N1, N2]

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	Multiplier, a_1 , in the scaling equation. It is automatically set to 1 at the end of each application. <i>The default value is 1.</i>
N2	Addend, a_2 , in the scaling equation. It is automatically set to 0 at the end of each application. <i>The default value is 0.</i>

EXAMPLES

SCALE multiply by 3.3 and add 10.
 SCALE multiply by 0.3048

COMMENTS

This command can be used for internal scaling in conjunction with the COORDinate, INITial, MULTiphase, and SOURce commands.

PURPOSE To control echo of some of the diagnostic output obtained from the DIAGnostic command to the CRT device.

SYNTAX SCRE [OFF | ON]

OFF: The diagnostic output to the CRT device is turned off.

ON: The diagnostic output to the CRT device is turned on. *This is the default option.*

EXAMPLES

SCREen echo for diagnostic output to be turned OFF
 SCREen ON

\$ This is the default option

COMMENTS

By default echo of part of the diagnostic output produced by the DIAGnostic command is automatically printed to the CRT device. This allows the user to monitor the progress of the solution procedure on the CRT device. However, this echo to the CRT device may be turned off, if so desired. This command does not affect the diagnostic output to the output device (IWR unit).

PURPOSE To specify the density, porosity and tortuosity of the porous matrix, or planar or linear features.

SYNTAX *Mode 1: Density and Porosity*

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

Mode 2: Tortuosity

SOIL {TORT}, [N1, N2, N3], [N4, N5, N6]

EXAMPLES

See the ROCK command

COMMENTS This command is identical to the ROCK command.

PURPOSE To initiate solution of the governing equations and to select the transient or steady-state mode of solution.

SYNTAX *Mode 1: Transient Solution Mode*

SOLV *[symbol], [AUTO], [PASS], [MANU], [N1, N2, N3, N4, N5, N6, N7]*

symbol: *By default an appropriate set of governing equations is solved based upon the user specified input. However, the user may override this default selection by explicitly specifying one or more of the character strings to specify the corresponding dependent variable for which the governing equation is to be solved. The valid symbols are listed in Table 5-4.*

AUTO: *By default, it is assumed that the information about time step is specified by the user. If the modifier AUTO is present, then the time step is automatically determined with certain specified constraints (N2 through N7).*

PASS: *In the AUTO mode, the time step is adjusted both dynamically and passively. This modifier disables the dynamic mode; only passive adjustment takes place. The dynamic adjustment occurs when the process fails to converge to a specified tolerance in a specified number of iterations (see CONvergence command). In this case, the time step is decreased and the solution process is repeated from the previous time with the decreased time step. In passive adjustment, the time step is adjusted only from the next time step; the currently computed values are retained. In this case, the next time step is increased if the number of iterations to converge is less than N4 and decreased if iterations are greater than N5 on CONvergence command; the time step is left at its current value otherwise.*

MANU: *Manual time step mode is activated; time step is determined according to the current value of the time step and other specified constraints. Any automatic time step computation is disabled.*

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The incremental time period (≥ 0), additive to any previously specified value, for solution of the governing equations. <i>The default value is 0.</i>
N2	The time step (≥ 0) at the start of the current segment of calculations. The time step may be changed during calculations or by a subsequent SOLVe command. <i>The default value is set to N1/100.</i>
N3	The geometric ratio multiplier (> 0) for the time step in the transient mode. Each successive time step will be multiplied by this value until a maximum value specified by N4 is reached. <i>The default value is 1.1 if the AUTO modifier is present; otherwise it is 1.</i>
N4	The maximum permissible time-step value. <i>The default value is 1.E20.</i>
N5	The minimum permissible time-step value. With the AUTO modifier, it is very important to specify a reasonable lower bound for the time step. If too low a value is specified then computer resources may be wasted. On the other hand, too high a value may lead to unacceptable numerical errors. <i>The default value is 1.E-5.</i>
N6	The geometric ratio divisor (> 0) for the time step in AUTO mode. Each successive time step is decreased by this factor if the number of iterations to convergence is above the specified threshold on CONvergence command. <i>If no value is specified then the default value is set equal to N3.</i>
N7	The maximum number of time steps. This input proves useful in AUTOMATIC time step mode to limit the amount of computer resources which will be used. <i>The default value is 16000.</i>

EXAMPLES

SOLVe for 50 years in steps of 2
 SOLVe for 50 hours, initial step=0.2hr, increase by 1.1, max=10 hr
 SOLVe for 1.E6 yrs, DT=1, factor=1.1, max=1.E3, min=1, dfac = 1.1, max steps=1000

SOLVe for 10 days in AUTOMATIC mode
 SOLVe 10 days, AUTO: DT=0.2, fac=1.3, max=1, min=1.E-5, dfac=1.1, Nmax=1000
 SOLVe for 10 days, MANUAL mode from now on

SOLVe for T only for 10 days in steps of 0.2
 SOLVe for T only for 10 days in AUTO mode
 SOLVe for P2, T and C3 only for 10 days in steps of 0.2

SYNTAX *Mode 2: Steady State Solution Mode*

SOLV {*STEA*}, [*symbol*], [*N1*, *N2*]

STEA: The equations are solved in their steady-state mode. That is, the accumulation term, the first term in Eqn. (2.4.1), is set to zero.

symbol: Same as in Mode 1.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The maximum number of iterative steps for solution of the matrix. The default value in this case is 16000.
N2	The minimum number of iterative steps to be performed on the matrix. The default value is set to 10.

EXAMPLES

SOLV_e in STEADY state mode: maximum steps 200
 SOLV_e in STEADY mode: maximum steps 500; minimum steps 20

SYNTAX *Mode 3: Dummy Run Initial Condition Mode*

SOLV {*OFF*}

OFF: The actual solution of the equations is disabled; however a dummy run through the solution process takes place to compute any values of derived variables such as saturation for the given initial and boundary conditions. This mode is useful to check initial conditions and to create output or archive files of initial data and geometry for problem checking and verification of input.

EXAMPLES

SOLV_e OFF

COMMENTS

The SOLV_e command, in its various modes, initiates immediate solution process of the governing differential equations. It should therefore be specified only after complete input has been supplied for a solution to proceed. However, the sequence of calculations may be sub-divided into as many segments as desired and a SOLV_e command specified for each segment. See Section 5.11 for further information.

PURPOSE To specify the type and magnitude of the sources (or sinks) for fluid, heat or chemical species.

SYNTAX *Mode 1: Direct Generation or Disappearance*

SOUR {symbol}, [mod], {N1, N2}, [fname | N3, ..., Nn]

symbol: One of the character strings which denotes a corresponding dependent variable for which the source is specified. The valid symbols are listed in Table 5-4.

mod: One or more of the modifiers listed below which further define the nature of the source.

mod	INTERPRETATION
EXPO	<i>By default, the source rate is assumed to be constant or specified as a tabulated function of time. However, if this modifier is present then source input is assumed to be for the exponential multi-component decay function according to Eqn. (2.5.42).</i>
VOLU	<i>By default, the source units are assumed to be per unit time (e.g., m³/s for fluid, W (J/s) for heat and kg/s for chemical species). However, if the modifier VOLUMetric is present then the source units are taken to be per unit time per unit volume [e.g., m³/(m³ s) for fluid, W/m³ for heat, and kg/(m³ s) for chemical species]. This type of source occurs, for example, for radioactive species in which the decay heat is typically stated as per unit volume.</i>
SOLU	<i>If this modifier is present then the source 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 according to Eqn. (2.5.43). This type of source is allowed only for chemical species, C^a.</i>

fname: The name of the file from which the source input for N3 through Nn is to be obtained. See Section 6.2.2 for specification of the file name.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The location number ($1 \leq N1 \leq LSS$; See Table 5-7 for LSS) for the source which must have previously appeared on a LOCAtE command.
N2	Number of sets of source values (≥ 1) which follow. For SOLUbility limited source option, N2 is set to 2. <i>The default value is 0.</i>
N3	In the absence of the EXPO modifier, N3 (≥ 0) is taken to be the time at which the source becomes active (release time). If the EXPO modifier is present, then it is the first time constant, f_n of Eqn. (2.5.42). <i>The default value is 0.</i>
N4	The strength of source or s_n of Eqn. (2.5.42). The input value may be scaled internally by the SCALE command. <i>The default value is 0.</i>
N5 through Nn	N3 sets of source time and strength specifications in the manner of N3 and N4 above, except when the modifier SOLU is present. In the presence of the SOLU modifier, N5 is the saturation limit, C_n of Eqn. (2.5.43), and all values following N5 are ignored.

EXAMPLES

SOURCE # 1 for P: # sets = 1: time=0., value=100 cu ft/day
 SOURCE # 1 for T: set 1: time=10., S=10 W/per unit VOLUME
 SOURCE # 2 for T: EXPOntial type; 3 terms (.5,1)(.05,.1)(.001,.01)
 SOURCE # 3 for T: 5 sets: (0,50) (50,900) (100,1000) (500,1000), (5000,0)
 SOURCE 7 for C: # set 1: time=100, S=0.2 kg/day
 SOURCE 5 for C2: SOLUbility limited: 1 set: t=0., S=100kg; Cs=0.05
 SOURCE # 7 for T: 75 sets on file 'SOURCE.DAT'

SYNTAX

Mode 2: Flow Injection or Withdrawal

SOUR {FLOW}, [mod], {N1, N2}, [N3, ..., Nn],
 {symbol=Nn+1}, [symbol=Nn+2, ..., symbol=Nn+m]

FLOW: The source is assumed to be one in which the source variable (e.g. momentum, temperature, or species concentration) is accompanied by a fluid source.

mod: The EXPO or VOLU modifier as defined in Mode 1 specification. The SOLUbility limited source is not admissible with this type mode of input.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1, ..., Nn	Same as for Mode 1.
Nn+1, ..., Nn+m	These values represent an amount per unit volume of fluid of the variable denoted by the symbol immediately preceding the value.

EXAMPLES

SOURCE at 3: FLOW injection: 2 sets (0, 0), (100, 5.E3) T=50, C= 1.

SYNTAX

Mode 3: Flow Injection or Withdrawal with Input from a File

SOUR {FLOW}, {fname}, [mod], {N1, N2}, {symbol=N3}, [symbol=N4, ..., symbol=Nm]

FLOW: See Mode 3 Specification.

fname: The name of the file from which the source input is to be obtained. See Section 6.2.2 for specification of the file name. The structure of the input on this file is identical to that of the N3 through Nn in Mode 3 input.

mod: The EXPO or VOLU modifier as defined in Mode 1 specification. The SOLUbility limited source is not admissible with this type mode of input.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1, N2	Same as for Mode 1.
N3, ..., Nm	These values represent an amount per unit volume of fluid of the variable denoted by the symbol immediately preceding the value.

EXAMPLES

SOURCE at 3: FLOW injection: 20 sets from file 'SOURCE' with T=50, C= 1.

COMMENTS

The cumulative total values (each specified by N2) for all SOURCE commands must not exceed the value of the LSO dimensioning parameter (see Section 5.12).

PURPOSE To specify the thermal properties of the porous matrix, or the planar or linear features.

SYNTAX THER [N1, N2, N3, N4], [N5, N6, N7]

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	Specific heat of the solid, c_s , of Eqn. (2.2.3) (≥ 0). However, if a PROPerTy command with T and EFFEffective modifiers is specified, then the input is assumed to be the effective specific heat for the matrix, α_h , of Eqn. (2.2.6) (≥ 0). <i>The default value is 1.</i>
N2	Thermal conductivity of the dry solid, k_s , of Eqn. (2.2.8) (≥ 0). However, if a PROPerTy command with T and EFFEffective modifiers is specified, then the input is taken to be the effective matrix thermal conductivity which is equal to the sum of the first two terms on the right hand side of Eqn. (2.2.8) (≥ 0). <i>The default value is 0.</i>
N3	Longitudinal dispersivity, α_L , of Eqn. (2.5.37). <i>The default value is 0.</i>
N4	Transverse dispersivity, α_T , of Eqn. (2.5.37). <i>The default value is 0.</i>
N5, N6, N7	These three values select the zones to which N1 through N4 apply. Their interpretation is identical to that of N1, N2 and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command. <i>If no FOR command was previously specified, then the input is assumed to apply to zone number 1.</i>

EXAMPLES

THERmal properties cs = 26, kt = 45
 THERmal props cs = 26, ks = 45., alfa1 = 0., alfa2 = 0., for zones 1 to 3
 THERmal properties: ce = 26, ke = 45, alpha1 = 10, alfa2 = 2 for zones 4 to 9

PURPOSE To set the initial simulation time for a problem.

SYNTAX TIME {N1}

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The starting time (≥ 0) for simulations. <i>The default value is 0.</i>

EXAMPLES

TIME = 50 years at start of simulations

PURPOSE To specify the problem title.

SYNTAX **TITL** followed by character information

EXAMPLES

TITL ILLUSTRATIVE PROBLEM - DEFAULT SET UP - 01/02/92:ACRi/akr

COMMENTS The specification must be restricted to one 80-character record. Title specification is included in all output files generated by PORFLOW.

PURPOSE To compute particle tracks and their corresponding elapsed time in the flow field.

SYNTAX TRAC *[fname], [FREE], [dir], {N1, ..Nn}, [Nn+1, Nn+2, Nn+3]*

fname: The name of the file to which the output is written. See Section 6.2.2 for specification of the file name. *If no file name is specified, then output is written to a file called TRACKS (see Section 5.5).*

FREE: If this modifier is present, then the particle computation is halted when it reaches a free surface.

dir: The 'dir' must be *one* of the X, Y, or Z. if this modifier is present then the particle computation is stopped when the coordinate specified by 'dir' reaches the value equal to Nn+1.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1, ...,Nn	The coordinates of the starting location of the particle. Two values are required for 2D and 3 for 3D input mode.
Nn+1	The distance travelled by the particle before computation for this particular particle is stopped. If the modifier X, Y or Z is present, then this input is interpreted to be the coordinate value rather than the total travelled distance. <i>The default value is set to be a large number (1.E30).</i>
Nn+2	The time at which the computation of the track for this particle are started. <i>The default value is 0.</i>
Nn+3	The frequency index for writing the output on the particle track output file. The output is obtained every Nn+3 (≥ 1) steps. For example, a specification of 10 will lead to output at the 10th, 20th, 30th, etc.. <i>If no input is specified then the frequency is assumed to be 1.</i>

EXAMPLES

- TRACKs for particle start at: (35.0, 5.27) stop after 200.
- TRACKs for particle start at: (1.22, 10.0, 19.3) stop at X: 100. time = 20 years
- TRACKs for particle start at: (35.0, 5.27) after 200. start at 0 yrs; every 20 steps
- TRACKs for particle start at: (1.22, 10.0, 19.3) stop at FREE surface.
- TRACKs for particle at: (35.0, 5.27) after 100. on file "PARTICLE.TRK"

PURPOSE To specify the transport properties of the host porous matrix or, planar or linear features.

SYNTAX TRAN [symbol], [EXPO], [N1, N2, N3, N4], [N5, N6, N7]

symbol: One of the character strings which denotes the dependent variable for which the transport properties are specified. The valid symbols are: C, C2, C3 or C4 of Table 5-4. *By default the specification is assumed to be for the first species, C.*

EXPO: The diffusion coefficient is computed from the exponential formulation of Eqn. (2.3.9).

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The partition coefficient, k_d of Eqn. (2.3.4) (≥ 0). However, if a PROPERty command with appropriate symbol (C, C2, C3 or C4) and EFFEffective modifier is present, then it is taken to be the retardation factor, R_d of Eqn. (2.3.6) (≥ 0). <i>The default value is 0 for k_d and 1 for R_d.</i>
N2	Molecular diffusivity, D_M of Eqns. (2.3.7) and (2.3.9) (≥ 0), for the chemical species in water. <i>The default value is 0.</i>
N3	The coefficient α_1 of Eqn. (2.3.9) or the longitudinal dispersivity, α_L of Eqn. (2.5.37) (≥ 0). <i>The default value is 0.</i>
N4	The coefficient α_2 of Eqn. (2.3.9) or the transverse dispersivity, α_T of Eqn. (2.5.37) (≥ 0). <i>The default value is 0.</i>
N5, N6, N7	These three values select the zones to which N1 through N4 apply. Their interpretation is identical to that of N1, N2 and N3, respectively, of the FOR command. If these values are omitted, then the input is assumed to apply to the zones specified by any previous FOR command. <i>If no FOR command was previously specified, then the input is assumed to apply to zone number 1.</i>

EXAMPLES

TRANsport properties: kd=1, Dm=5.24, alpha L=10, alpha T=1
 TRANsport properties for C2: kd=1, Dm=5.24, alpha L=10, alpha T=1
 TRAN kd=0, dm=1.E-3, L=10, T=1, for ZONE 1
 TRANsport kd=1.1E-3, 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
 TRANsport EXPONential form: kd=1.1E-3, dm=1.2, a1=10, a2 = 5
 TRANsport EXPONential form: kd=1.1E-3, dm=1.2, a1=10, a2 = 5 Zone 1 to 7

PURPOSE To specify the user identification for the problem.

SYNTAX USER followed by character information

EXAMPLES

USER ACRI - AKR demonstration

COMMENTS The specification must be restricted to one 80-character record. User identification is included in all output files generated by PORFLOW.

PURPOSE To specify the option and constants employed for calculation of fluid viscosity as a function of temperature. The viscosity, in turn, is used to compute the hydraulic conductivity of the host matrix according to Eqn. (2.5.27).

SYNTAX

VISC {UNIF | POLY | EXPO}, [SECO], [N1, N2, N3, N4]

UNIF: The fluid viscosity is uniform and constant; *this is the default option.*

POLY: Polynomial variation in fluid viscosity according to Eqn. (2.5.6).

EXPO: Exponential variation in fluid viscosity according to Eqn. (2.5.5).

SECO: *By default the viscosity specification is assumed to be for the primary fluid. However, if this modifier is present then the input is taken to be for the second phase fluid.*

THIR: The specification is for the third phase of fluid.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	Reference viscosity, μ^* of Eqns. (2.5.6) and (2.5.7). The reference value is used only to determine the K_{ij}^a of the second and third phases from the reference value of K^* specified for the primary phase by the HYDRaulic command. For primary phase, it is only the viscosity ratio rather than the absolute value which is required [Eqn. (2.5.27)]. <i>The default value is 1 for all phases.</i>
N2	The coefficient a_1 of Eqns. (2.5.6) and (2.5.7). <i>Default value is 1436 K if modifier EXPOntial is present; otherwise it is zero.</i>
N3	The coefficient a_2 of Eqn. (2.5.6). <i>The default value is 0.</i>
N4	The coefficient a_3 of Eqn. (2.5.6). <i>The default value is 1.</i>

EXAMPLES

VISCosity UNIFORM for primary fluid: $\mu^* = 1.002E-3$ (water at 20 deg C)
 VISCosity UNIFORM for SECONdary phase: $\mu^* = 8E-2$ (Engine oil at 20 deg C)
 VISCosity EXPOntial option: $\mu^* = 0.544E-3$, $b = 1450$ K
 VISCosity POLYnomial option: $\mu^* = 8.0E-4$, $a=1.E-4$, $b=5.E-5$, $c=0$.
 VISCosity UNIFORM for THIRd phase: $\mu^* = 1.E-2$

PURPOSE To specify a window or subregion within the domain of simulations for which the output is desired.

SYNTAX WIND $[N1, \dots, Nn], [Nn+1, Nn+3]$
 $n = 4$ for 2D input mode; $n = 6$ for 3D input mode

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1 through Nn	The grid index coordinates of the window or subregion for output. See Section 6.2.3 for interpretation of this input. If this input is omitted then the subregion is defined to be the total domain.
Nn+1	The x-direction node interval (≥ 1) for output. For example, a specification of 3 will result in the print-out at I=1,4,7,10etc., grid nodes. <i>The default value is 1.</i>
Nn+2	The y-direction node interval (≥ 1) for output. <i>The default value is 1.</i>
Nn+3	The z-direction node interval (≥ 1) for output. <i>The default value is 1.</i>

EXAMPLES

WINDow is the total calculation domain
 WINDow from (2,4) to (10,9) \$ 2D input mode
 WINDow from (2,4,2) to (10,9,5) \$ 3D input mode
 WINDow from (2,4) to (10,9) skip I = 2, J = 3 \$ 2D input mode
 WINDow from (2,4,7) to (10,9,11) skip I = 2, J = 3, K = 2 \$ 3D input mode

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.

PURPOSE Define a zone or subdomain of the calculation domain that has unique hydraulic, thermal or transport properties, or linear or planar features.

SYNTAX *Mode 1: Direct Specification*

ZONE {N1}, {N2, ..., Nn+1}, [Nn+2, Nn+3], [FRAC | PLAN | BORE | LINE]
 n = 4 for 2D input mode; n = 6 for 3D input mode

FRAC: The zone designation is for a fracture.

PLAN: The zone designation is for a planar feature. The implementation of this modifier is identical to that for the FRACTure modifier.

BORE: The zone designation is for a borehole.

LINE: The zone designation is for a linear feature. The implementation of this modifier is identical to that for the BOREhole modifier.

NUMERIC FIELD	REMARKS & EXPLANATIONS
N1	The zone designation index ($1 \leq N1 \leq LZN$); LZN is a dimensioning parameter (see Section 5.12). <i>The default value is 1.</i>
N2 through Nn+1	The grid index coordinates of the zone or subregion. See Section 6.2.3 for interpretation of this input. If this input is omitted then the subregion is defined to be the total domain.
Nn+2	Width of the planer feature, if FRAC or PLAN is encountered; outer diameter of the linear feature, if BORE or LINE is encountered; otherwise this input is ignored.
Nn+3	Inner diameter of the linear feature, if BORE or LINE is encountered, otherwise this input is ignored.

EXAMPLES

ZONE 1 \$ total domain
 ZONE 3 from (1,1) to (11,7)
 ZONE 5 from (1,1,1) to (11,7,5) \$ 2D input mode
 ZONE 3 from (6,10) to (31,10) BORE hole in X-dir dia = 0.2 \$ 3D input mode
 ZONE 4 from (6,10) to (6,19) BORE in Y: D=0.2, Inner d=0.1
 ZONE 3 from (6,10,2) to (6,10,7) LINEar feature in Z dia = 0.1
 ZONE 3 from (6,10,2) to (31,10,7) FRACTure in XZ width = 0.1
 ZONE 5 from (6,10,2) to (6,19,7) PLANar feature in YZ: W=0.05

SYNTAX *Mode 2: Data Input from a File***ZONE** {fname}

fname: The name of the file from which the zone input is obtained. See Section 6.2.2 for specification of the file name. In this mode, the zone designation for the whole domain of interest must be read from the file in sequential order in the manner of increasing x, y and z grid nodes, in that order. Also this mode can only be used to provide input for the porous matrix zone designation. Any fractures, boreholes, planar or linear features must be explicitly defined by Mode 1 input.

EXAMPLES

ZONE information from 'ZONE.DAT'

COMMENTS

The **ZONE** command is used to divide the domain of interest into subdomains (see Section 5.4) each with its own distinct or unique properties. A non-rectangular or non-contiguous soil or rock zone may be specified by a series of **ZONE** commands with the same zone index (N1), but with different grid index values (N2 through Nn). However, each fracture (planar feature) or borehole (linear feature) must be specified by a distinct **ZONE** command. A fracture which is not oriented along the axis may be specified in a stair-step manner by its components along the axis (see Sections 4.1.1 and 4.2.6).

In 3D mode, a fracture may lie in the XY (N4=N7), YZ (N2=N5), or ZX plane (N3=N6). Similarly, a borehole may be in the X (N3=N6, N4=N7), Y (N2=N5, N4=N7), or Z (N2=N5, N3=N6) direction. In 2D mode only linear features may be present; they may be in the X (N3=N5) or Y (N2=N4) direction. The area of the linear element is calculated from:

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

where D and d are, respectively, the outer and inner diameters.

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APPENDIX A: ACri FREEFORM[®] COMMAND LANGUAGE

ACri FREEFORM[®] command language, developed by Analytic & Computational Research, Inc., provides a simple user interface for complex software packages through a set of conversational, English-like commands. These commands are free of any requirements of format or hierarchy except those naturally arising from the nature of the input. The modules which implement the commands are written in FORTRAN 77. These provide for interactive input or emulate the interactive input in batch mode.

A.1 THE FREEFORM INPUT RECORDS

The FREEFORM Input is specified through three types of records: **KEYWORD**, **CONTINUATION** and **COMMENT** records. These are described below.

A.1.1 The Keyword Record

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

Structure

- 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 all be separated from each other by comment, separator, or terminator fields.
- Any character or numeric data on a keyword record after the first occurrence of a terminator are ignored.

A.1.2 The Continuation Record

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

Structure

- 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 may only 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 on a continuation record after the first occurrence of a terminator is ignored.
- Any number of continuation records may follow a keyword record.

A.1.3 The Comment Record

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

Structure

- A comment record must begin with a back-slash (/), asterisk (*), dollar (\$) or exclamation (!) 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.

A.2 ELEMENTS OF INPUT RECORD

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

A.2.1 The Keyword

Function The keyword identifies the input group.

Structure

- The keyword may consist of any characters except separator (Section A.2.4) or terminator (Section A.2.5) characters. However, the first character of a keyword must be alphabetic ("A" through "Z" or "a" through "z"). To this extent, the concept of a keyword is similar to that of a variable name in FORTRAN.
- The keyword may be in upper or lower case.
- A keyword must begin in the first column of a record.
- The keyword is terminated with the first occurrence of a valid separator or terminator character.
- The keyword may consist of 1 to 80 characters. However, if there are more than four characters, only the first four are machine-identifiable.

Examples

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

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

Note that a specification of ABC) or ABC', ABC\$, although valid, is equivalent to that of ABC because the last character in all of these examples is either a separator (Section A.2.5) or a terminator (Section A.2.6).

A.2.2 The Modifier

Any character information on an input record following a keyword, except that embedded in a numeric or comment field (see Sections A.2.3 and A.2.6), is treated as modifier(s).

Function The modifier contains character data that helps in interpretation of the rest of the 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 a 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 A.2.1.

A.2.3 The Numeric Field

Any numeric characters on a keyword or continuation record following a keyword, except those embedded in a keyword, modifier or comment field (see Sections A.2.1, A.2.2 and A.2.6), are treated as numeric data.

Function A numeric field contains numeric data for input variables.

Structure

- A numeric field is a continuous string of characters that must begin with the numeric character set. In this context, the numeric character set consists of

the numerals (0-9), the decimal point (.), and the plus (+) and minus (-) operators.

- A numeric field must consist only of the numeric character set defined above, the asterisk (*), and the exponent in lower (e) or upper (E) case. It must not contain any other character.
- The plus (+) or minus (-) sign, if present, must immediately precede the numerical value without any intervening blank or other characters.
- The asterisk (*) or the exponent (E or e), if present, must be embedded; the numeric field must not begin or end with one of these characters.
- A numeric field must be separated from the keyword, modifiers and other numeric fields by a valid separator, terminator or comment field.
- 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., 9.99E2, 99.9E1)
- Successive, repetitive, identical numeric values may be specified by the asterisk (*) option. Thus, (30., 30., 30.) may be represented as (3*30. or 3*3.0E+1); embedded separators or non-numeric characters must not appear in such specification.

Examples

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

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

Note that a specification of 1.2)2. or 1.2=2, although valid, will be equivalent to a specification of two numeric fields, 1.2 and 2 because of the embedded separator (Section A.2.4) 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 A.2.5).

A.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 on an input record which 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 semi-colon (;), the pound sign (#), the apostrophe ('), the left parenthesis "(", and the right parenthesis ")" characters.

Examples

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

A.2.5 The Terminator

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

- Structure**
- The dollar (\$) and exclamation mark (!) characters are the only valid terminators.
 - The terminator terminates the input for the keyword or continuation record on which it occurs; input associated with that particular keyword may continue on a continuation record which follows.
 - The terminator may appear anywhere in a record.
 - Any characters following the terminator on that input record are not processed but are treated as user comments and are merely written to the output file.

Examples

The character sequences:

```

XYZ      $comments now
!      any comments here
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 complete sequence will

be treated as comments. In the third example, the numerical field 789.123 will be ignored, whereas 123.456 will be treated as numeric data.

A.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 one which occurs on a keyword or continuation record. It must begin with a terminator (\$ or !) character; any combination of characters may follow the terminator. The comment field is terminated at the end of the 80-th character in that record (Section A.2.5).
- A comment field on 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 (\$ or !) character as the first 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 the embedded comment on a keyword record. Input processing stops with the \$ character; all characters on that record following, and including, the \$ character are ignored.

As examples of comment records, the character strings:

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

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

A.2.7 The Prompt

Function The prompt allows for interactive or runtime input of a partial or entire input record.

- Structure**
- The user may insert a "?" in place of either an entire input record or numerical or character string in the input itself. The command interpreter will pause and prompt the user for input at this stage.
 - The input obtained by the prompt may be comprised of one or more of the elements of an input record described in Sections A.2.1 through A.2.6.
 - Any input specified by the prompt is inserted in the input command string starting with the location of the question mark symbol.
 - All input in the original command string following the prompt in that record will be disregarded.
 - The input for the prompt may consist of 1 to 80 characters depending on where the question mark symbol is located. The prompt will pause and display a message telling the user the maximum number of characters allowed.
 - It is possible to avoid the message, referred to above, from being displayed by placing two question mark symbols in succession (eg. "?"). The command interpreter will still pause and wait for input, however it will not display a message.

Examples

In the input record:

```
SOLVe ?                ! Prompt user for input
```

the character string "?" has the effect of pausing the command interpreter during run-time and displaying a message that asks the user for up to 74 characters of input, since the "?" appears in the 7th location of the input record. The comment "! Prompt user for input" will be overwritten by the input provided by the user at run-time or will be replaced by blank characters if the user input is less than 74 characters long.

Alternatively the user may choose to write:

```
SOLVe ??                ! Prompt user for input without a
                        message
```

this input record has the same effect as above except no message is displayed.

**APPENDIX B:
ERROR MESSAGES OF PORFLOW**

PORFLOW provides extensive checking of data input to ensure that the data specified by the user meets certain basic conditions of validity. The errors that may result from this data checking are described below. At this stage, no data checking to ensure that the values are physically realizable, or that they are within the experimental or theoretical bounds is provided. The user must ensure that the latter is the case for a given problem simulation.

<u>ERROR #</u>	<u>MEANING</u>
101	The keyword command or a modifier specified by the user is invalid. Check the User's Manual for a list of valid commands and modifiers.
105	The number of numerical input values following a keyword command exceeds the maximum permissible value (set by the LVAL parameter) that is printed out with the message.
111	The number of grid nodes in one of the directions (x, y or z) specified by the GRID command exceeds the L1 parameter.
114	The total number of grid nodes (product of N1, N2 and N3 on the GRID command) exceeds the LMAX parameter or is less than the minimum permissible value of 9.
115	The number of internal field nodes exceeds the LFLD parameter or is less than the minimum permissible value of 1.
116	The number of boundary nodes exceeds the LBC parameter or is less than the minimum permissible value of 6.
119	The number of boundary nodes multiplied by the active equations being solved exceeds the LBE parameter or is less than the minimum permissible value of 6.
121	Number of time dependent boundary segments exceeds the specified LBN parameter. See Chapter 5 in User's Manual.
123	Total number of time dependent boundary elements exceeds the specified LBT parameter. See Chapter 5 in User's Manual.

<u>ERROR #</u>	<u>MEANING</u>
131	Number of values through a tabular data input option exceeds the allocated array space. See Chapter 5 in User's Manual.
201	The time step specified for simulations of the SOLVe command is smaller than 1.E-20 or larger than 1.E+20.
215	The coordinate values specified by the COORdinate command are not increasing in a monotonic fashion, as required.
301	The density or the porosity of the porous matrix specified by the ROCK or SOIL command is less than zero.
305	The tortuosity factor for the porous matrix specified by the ROCK or SOIL command is less than zero.
311	The specific storativity or the hydraulic conductivity specified by the HYDRaunic command is less than zero.
321	The specific heat, the thermal conductivity or the dispersivity specified by the THERmal command is less than zero.
331	The distribution or retardation coefficient, the molecular diffusivity or the dispersivity specified by the TRANsport command is less than zero.
351	The soil characteristic exponent, the capillary pressure or the residual saturation, specified by the MULTiphase command is less than zero.
511	The total number of sub-regions with fixed variable values specified by the FIXEd command exceeds the LFX parameter.
551	The zone designation index of the ZONE command is less than unity or greater than the value of the LZN parameter.
711	The total number of active sources specified by the SOURce commands exceeds the LSS parameter.
715	The source number specified by the preceding input command was not previously defined by a LOCAte command.

- 717 Total number of input values in the **SOURCE** commands exceeds the specified LSO parameter. See Chapter 5 in User's Manual.
- 851 The fracture or borehole element geometry is incorrectly specified or is physically impossible.