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SAGUARO – A Finite Element Computer Program for Partially Saturated Porous Flow Problems

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ABSTRACT

SAGUARO is a finite element computer program designed to calculate two-dimensional flow of mass and energy through porous media. The media may be saturated or partially saturated. SAGUARO solves the parabolic time-dependent mass transport equation which accounts for the presence of partially saturated zones through the use of highly non-linear material characteristic curves. The energy equation accounts for the possibility of partially-saturated regions by adjusting the thermal capacitances and thermal conductivities according to the volume fraction of water present in the local pores. Program capabilities, user instructions and a sample problem are presented in this manual.

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Nomenclature

		Typical Units
c_p	- specific heat	J/kg•K
C^p	- specific moisture capacity ($\partial\theta/\partial\psi$)	1/m
D_{ij}	- themal diffusion tensor (Soret)	$m^2/s•K$
E_{ij}	- thermal dispersion tensor	J/s•m•K
g	- gravitational constant	m/s^2
h	- heat transfer coefficient	$J/s•m^2•K$
k_{ij}	- intrinsic permeability tensor	m^2
K	- hydraulic conductivity $\left(\frac{k\rho_o g}{\mu}\right)$	m/s
P	- effective pressure = $\rho_o g\ (\phi + z)$	N/m^2
p	- pressure	N/m^2
Q	- volumetric heat generation	$J/m^3•s$
t	- time	s
T	- temperature	°K
v	- Darcy velocity (Mean Specific flux, $m^3/s•m^2$)	m/s
V	- volumetric heat generation rate	$J/s•m^3$
x	- horizontal dimension	m
y	- vertical dimension	m
z	- vertical dimension	m
β	- coefficient of volumetric thermal expansion	$kg/m^3•K$
Δ	- increment	-
θ	- moisture content	-
λ_{ij}	- thermal conductivity tensor	J/s•m•K
ε	- emissivity	
μ	- dynamic viscosity	kg/m•s
ρ	- liquid density	kg/m^3
σ	- Stefan-Boltzmann constant	
ϕ	- porosity	-
ψ	- pressure head $\left(\frac{p}{\rho_o g}\right)$	m

Subscripts

eff - effective property
f - fluid
i,j - coordinate direction
o,r - reference condition
s - solid property

INTRODUCTION

Recent interest in the potential performance of a nuclear-waste repository located above the water table in tuff (a hard rock) has prompted the development of a computational code, SAGUARO.* SAGUARO is a general-purpose finite element code developed to solve problems of incompressible single phase water and energy transport through porous media which may be partially or fully saturated. The two transport equations (mass and energy), which model the flow, incorporate Darcy's law, the Boussinesq approximation, the Soret effect, conduction and convection. The resulting nonlinear parabolic equations are solved in finite-element form using an algorithm related to the standard Crank-Nicolson method. The matrix solution procedure used in SAGUARO is a form of Gauss elimination. Code results provide time and space distributions of hydraulic head, temperatures, velocities and moisture contents.

SAGUARO is the newest member of the family of codes NACHOS,[1] COYOTE,[2] and MARIAH[3] which employ a similar structure. SAGUARO represents a direct extension of MARIAH (which solves problems of fully saturated flow in porous media) in that the quasi-steady state continuity/momentum equation in MARIAH was replaced with a transient equation which allows some or all of the pore volume to be partially saturated with water. The resulting equation is

*The Nevada Nuclear Waste Storage Investigations Project, managed by the Nevada Operations Office of the U.S. Department of Energy, is examining the feasibility of siting a repository for high-level nuclear wastes at Yucca Mountain on and adjacent to the Nevada Test Site. This work was funded in part by the NNWSI Project. The ultimate use of this information will be used for system analysis and performance assessment of a nuclear waste repository in tuff.

similar to Richards equation[5] commonly used to solve near-surface isothermal hydrology problems. The general form of the energy equation remains the same except that coefficients now depend on the degree of saturation.

The structure of SAGUARO and MARIAH are identical in the areas of grid generation, element basis functions, quadrature schemes, solution methods and plot packages. Therefore, the layout of this manual closely parallels the report describing MARIAH. The user may refer to that manual for additional information regarding the general code structure and solution procedure.

MATHEMATICAL FORMULATION

The present analysis will be restricted to the flow of an incompressible Newtonian fluid through a homogeneous, rigid porous matrix. The mass transport equation used in SAGUARO is derived using the equation for the continuity of mass

$$\frac{\partial (\rho_f v_i)}{\partial x_i} + \frac{\partial (\rho_f \theta)}{\partial t} = 0 \qquad (1)$$

and the Darcy equation[4] to define velocity for laminar fluid flow,

$$v_i = \frac{-k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} + \rho g \frac{\partial z}{\partial x_j}\right) - D_{ij} \frac{\partial T}{\partial x_j} \qquad (2)$$

Substituting Equation (2) into (1) gives:

$$\frac{\partial}{\partial x_i}\left(\rho_f\left[-\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} + \rho_f\, g \frac{\partial z}{\partial x_j}\right) - D_{ij} \frac{\partial T}{\partial x_j}\right]\right) = \frac{-\partial (\theta \rho_f)}{\partial t} \qquad (3)$$

The indicies (i,j) range over the values (1,2) and summation is implied by repeated indicies. This equation is modified using the Boussinesq approximation

$$\rho_f = \rho_o\,(1 - \beta \Delta T) \quad . \qquad (4)$$

Substituting Equation (4) into (3) results in:

$$\frac{\partial}{\partial x_i}\left((1 - \beta\Delta T)\left[-\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} + \rho_o\, g \frac{\partial z}{\partial x_j} - \rho_o\, g\, \beta\Delta T \frac{\partial z}{\partial x_j}\right) - D_{ij} \frac{\partial T}{\partial x_j}\right]\right)$$

$$= -\frac{\partial}{\partial t}\left[\theta(1 - \beta\Delta T)\right] \qquad (5)$$

Defining $P = p + \rho_o gz$ and assuming the term $\beta\Delta T$ is much less than 1, Equation (5) becomes:

$$\frac{\partial}{\partial x_i}\left(\frac{k_{ij}}{\mu} \frac{\partial P}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(\frac{k_{ij}}{\mu} \rho_o\, g\, \beta\Delta T \frac{\partial z}{\partial x_j}\right) + \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial T}{\partial x_j}\right) = \frac{\partial \theta}{\partial t} \qquad (6)$$

Since the air is assumed to be free to escape at the surface, the air pressure is small in comparison to the liquid pressure p. Thus the liquid pressure is simply the negative of the capillary pressure P_c:

$$p = - P_c(\theta) \tag{7}$$

This can be inverted to yield a representation of the moisture content θ as a function of liquid pressure p or pressure head ϕ, whichever is desired, and its slope $C = \frac{\partial \theta}{\partial \psi}$ is the specific moisture capacity. Thus, using the chain rule, (6) and (7) yield the final form of the parabolic equation which is solved in SAGUARO

$$\frac{\partial}{\partial x_i}\left(\frac{k_{ij}}{\mu}\frac{\partial P}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(\frac{k_{ij}}{\mu}\rho_o g\,\beta\Delta T\frac{\partial z}{\partial x_j}\right) + \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial T}{\partial x_j}\right) = \frac{1}{\rho_o g} C \frac{\partial P}{\partial t} \quad . \tag{8}$$

In general, mass transport in partially saturated regions, resulting from bouyancy effects, is expected to be negligible. This fact is accounted for by setting $\beta \equiv 0$ when θ/ϕ is less 99%.

It is of interest to note two special cases of Equation (8). For saturated flows, the moisture content is constant ($\theta/\phi = 1$) therefore, $\frac{\partial \theta}{\partial \psi} \equiv 0$. Typically, mass transport resulting from temperature gradients, $\frac{\partial}{\partial x_i} D_{ij} \frac{\partial T}{\partial x_j}$, is much smaller than mass transport resulting from pressure gradients. For these conditions, the third and fourth terms in Equation (8) are neglected yielding an equation for flow through fully saturated media,

$$\frac{\partial}{\partial x_i}\left(\frac{k_{ij}}{\mu}\frac{\partial P}{\partial x_j}\right) = \frac{\partial}{\partial x_i}\left(\frac{k_{ij}}{\mu}\rho_o g\,\beta\Delta T\frac{\partial z}{\partial x_j}\right) \quad . \tag{9}$$

This equation, which is elliptic in nature, is the equation solved by MARIAH.

For isothermal flows, the second and third terms of Equation (8) vanish, leaving

$$\frac{\partial}{\partial x_i}\left(\frac{k_{ij}}{\mu}\frac{\partial P}{\partial x_j}\right) = \frac{1}{\rho_o g}\, C\, \frac{\partial P}{\partial t} \qquad (10)$$

This is the well-known Richards equation.[5]

For partially saturated flow, the properties k_{ij}, D_{ij} and C are strong functions of pore pressure. Thus Equation (8) is highly non-linear. Generally, the non-linear coefficients $k(\phi)$ and $C(\phi)$ are functions of ϕ similar to the typical curves shown in Figure 1. The curves show the significance of the hystersis effects on the $k(\phi)$ and $\theta(\phi)$ relationship. These curves account for the influence of capillary action.

Note $K(\phi) = k\rho g/\mu$.

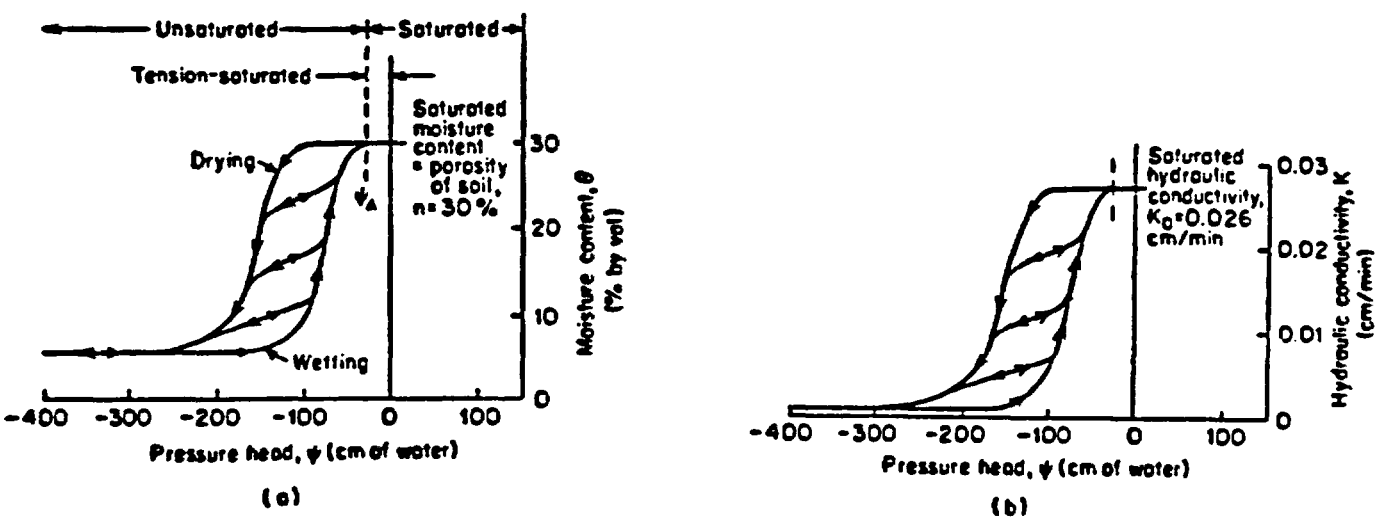


Figure 1: Characteristic Curves Relating Hydraulic Conductivity and Moisture Content to Pressure Head for Sand/Soil, see Reference 5.

The general form of the energy equation solved by SAGUARO is,

$$(\rho c_p)_{eff} \frac{\partial T}{\partial t} + \frac{\theta}{\phi} \rho_o (c_p)_f V_i \frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i} \left[(\lambda_{eff_{ij}} - \phi E_{ij}) \frac{\partial T}{\partial x_j} \right] - Q = 0 \quad . \quad (11)$$

This equation is an energy balance on a unit volume containing a porous matrix and liquid and neglects the heat capacity of the air. It is further assumed that the matrix and liquid are in thermal equilibrium. Both energy transport by convection (2nd term) and conduction/dispersion (3rd term) are included. However, the definitions of the coefficients of the terms must be defined to allow the possibility of partially saturated pores. These coefficients are therefore defined as follows:

$$(\rho c)_{eff} = \theta \rho_f (c_p)_f + (1 - \phi) \rho_s (c_p)_s \quad , \quad (12)$$

where $(\rho c)_{eff}$ represents the thermal capacitance of a unit volume with porosity (ϕ), saturation (θ/ϕ), and

$$\lambda_{eff_{ij}} = \phi \left[\frac{\theta}{\phi} \lambda_f + (1 - \frac{\theta}{\phi}) \lambda_{air} \right] + (1 - \phi) \lambda_s \, , \quad (13)$$

where λ_{eff} is the effective conductivity of the water, air, solid combination.

PROGRAM FEATURES AND ORGANIZATION

SAGUARO is restricted by the following limitations and assumptions.

(a) The geometric description of the problem is limited to two spatial dimensions, either plane or axisymmetric.

(b) The porous matrix is assumed to be homogeneous and rigid. The matrix material may be considered orthotropic in terms of thermal conductivity, permeability and thermal diffusion.

(c) The matrix material(s) is assumed to be saturated or partially saturated with a single, one-phase fluid (no vapor transport). The fluid is assumed to be incompressible and Newtonian.

(d) The fluid flow is assumed to be laminar. Inertia effects in the fluid are assumed negligible.

(e) For non-isothermal flows, the fluid and material matrix are assumed to be in local thermal equilibrium.

(f) Presence of air in momentum/continuity equation is neglected.

Despite these restrictions, SAGUARO has proved to be a useful tool in the solution of a wide range of transient porous flow problems. When considering flows with heat transfer, regions of solid body heat conduction are easily included in the analysis. Material properties such as fluid viscosity and thermal conductivity may be arbitrary functions of temperature; volumetric heat sources may be functions of time and/or temperature. Allowable boundary conditions on the hydrological and thermal parts of a problem are quite general and may include the specification of the fluid hydraulic head or hydraulic head gradient (fluid discharge), as well as specified temperatures, heat fluxes

or convective and radiative boundaries. All boundary conditions may be functions of time.

SAGUARO is a self-contained program with its own mesh generator, data analysis, and plotting packages. The mesh generator is based on an isoparametric mapping procedure[6] and allows very general meshes to be prepared easily and accurately. The data analysis portions of the code allow local heat fluxes as well as stream function values to be calculated. The plotting package provides graphic output of element meshes, nodal point locations, contour plots of temperature, hydraulic head, or stream function, profile plots, and time histories of any dependent variable.

Two other essential parts of the SAGUARO code are the element library and the solution procedures for the matrix equations. The elements included in SAGUARO consist of isoparametric and subparametric quadrilaterals and triangles as shown in Figure 2. Within each of these elements, the hydraulic head and temperature are approximated using biquadratic basis functions; the velocity components are expressed by a bilinear basis function. Transient problems are analyzed using a modified Crank-Nicholson procedure. The actual solution of the matrix equations is carried out by a specialized form of Gauss elimination.[7] These procedures are fully described in References 3 and 4.

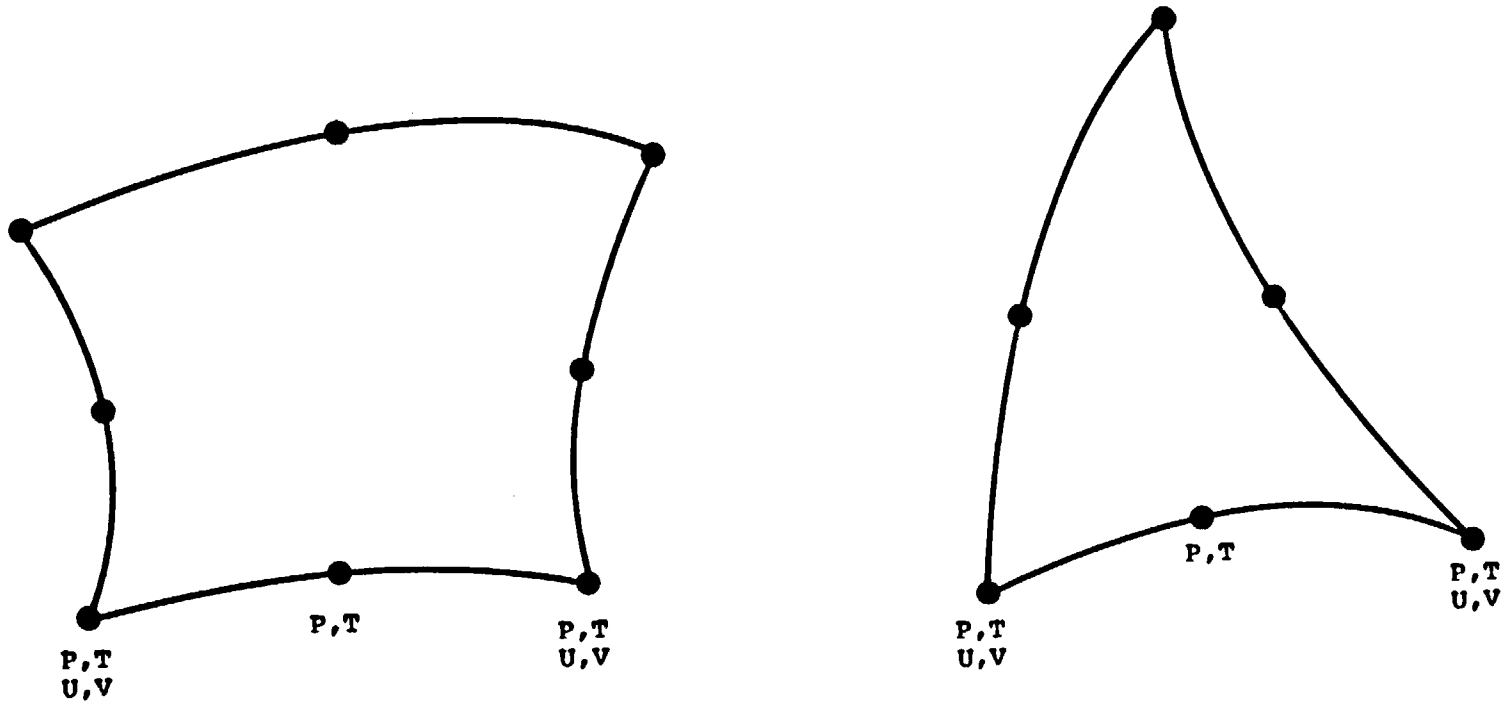


FIGURE 2. Isoparametric Quadrilateral and Triangle

INPUT GUIDE

The structure of an input data deck for the SAGUARO computer code directly reflects the steps required to formulate and solve a finite element problem. Through the use of a series of command and data cards, the program is directed to such functions as grid generation, element construction, solution of the matrix equations, and calculation of auxillary data. The actual sequence of commands to the program is quite flexible, although there are some obvious limits to the order in which operations can be specified. In the following sections, the command and data cards required by SAGUARO are described in roughly the order in which they would normally appear in an input deck. An example problem follows this section as an added aid to input format. Additional example problems for fully saturated cases can be found in Reference 1.

In the following section, the conventions listed below are used in the description of input cards:

(a) Upper case words imply an alphanumeric input value, e.g., FORMKF.

(b) Lower case words imply a numerical value for the specified variable, e.g., xmax.

(c) All numerical values are input in a free field format with successive variables separated by commas. All input data is limited to ten characters under this format for the CDC machine and eight for the CRAY version.

(d) [] indicate optional parameters which may be omitted by using successive commas in a variable list. If the omitted parameter is not followed by any required parameters, no additional commas need to be specified.

(e) <> indicates the default value for an optional parameter.

(f) The * character may be used to continue a variable list onto a second data card. When using this option the comma following the last variable and preceeding the * is omitted.

(g) The $ character may be used to end a data card allowing the remaining space on the card to be used for comments.

(g) The contents of each input card are indicated by underlining.

(i) All quantities associated with a coordinate direction are expressed in terms of the planar x-y coordinate system. The corresponding quantities for axisymmetric problems are obtainable from the association of the radial coordinate, r, with x and the axial coordinate, z, with y.

The description of the command cards are presented in the following order:

(a) Header Card

(b) SETUP Command Card

(c) FORMKF Command Card

(d) OUTPUT Command Card

(e) UNZIPP Command Card

(f) HEATFLUX Command Card

(g) PLOT Command Card

(h) RESTART Command Card

(i) Program Termination Card

Following the individual descriptions of the command cards are sections discussing input deck structure, user subroutines, initial conditions, error messages, and computer requirements for SAGUARO.

Header Card

The header card must be the first card in a deck for any particular problem. If two or more problems are run in sequence, the header card for each new problem follows the END, PROBLEM card of the previous problem. A $ symbol must appear in Column 1; the remaining 79 columns are available for a problem title. The header card is of the following form:

$ PROBLEM TITLE.

SETUP Command Card

The first task in formulating a finite element analysis of a problem involves the specification of the material properties and the definition of element mesh and boundary conditions for the problem geometry. These functions are accomplished through the SETUP command and its three sets of associated data cards.

The SETUP command card has the following form:

SETUP, [iprint], [maxi], [order], [grid plot]

where,

iprint <2>: determines the amount of printout produced during the setup operation. Output increases with the value of iprint and ranges from no printout for iprint = 1 to full printout for iprint = 4.

maxi <18>: is the maximum number of I rows to be generated in the grid. Maxi need only be specified if there are more than 18 I rows or more than 110 J rows. The limit on the maximum I's and J's is I*J < 4000 for the CDC version of SAGUARO and I*J < 5000 for the Cray version.

order < >: determines the numbering of the elements. For the default value (i.e., order left blank), the elements are numbered by increasing I,J values (e.g., (1,1), (2,1), (3,1) ... (1,2), (2,2) ...). For order = PRESCRIBED, the elements are numbered according to their order in the input list. The element ordering should be chosen such that the front width of the problem is minimized.

grid plot < >: determines if a grid point plot tape is written. If a plot of the grid points is to be made in a subsequent call to the plot routine, then grid plot = PLOT; if no plot of the grid points will be made, the grid plot parameter is omitted.

SETUP Data Cards

Following the SETUP command card, three sets of data cards are required for material property specification, grid point

generation, and element and boundary condition specification. Each of the data sets is terminated by an END card. The last END card (i.e., the third), ends the setup portion of the program and readies the program for the next command card.

Material Data Cards

The material data cards are of two types corresponding to the specification of fluid and matrix (solid) properties, respectively. For the specification of the fluid properties, the data cards are of the following form:

[Material Name], number, ρ_f, μ_f, c_f, λ_f,
β, g, temperature dependence, T_{ref}

where,

Material Name: is an optional alphanumeric material name for user reference.

number: is the internal reference number for the material. For the fluid property card, number must be set to 1.

ρ_f: is the fluid density.

μ_f: is the fluid dynamic viscosity.

c_f: is the fluid specific heat.

λ_f: is the fluid thermal conductivity

β: is the fluid volumetric expansion coefficient

$(= \rho[\partial(1/\rho)/\partial T]_p = -(1/\rho)[\partial\rho/\partial T]_p)$.

g: is the gravitational acceleration.

Temperature dependence <CONSTANT>: prescribes the dependence of the fluid properties on temperature. If all fluid properties (μ, λ, and β) are independent of temperature, this parameter is omitted or set equal

to CONSTANT. If one or more the indicated properties depend on temperature, this parameter is set equal to VARIABLE.

T_{ref} <0>: is the reference temperature for the buoyancy force, i.e., T_{ref} is the temperature at which the buoyancy forces are zero.

The material properties for the matrix are specified on data cards of the following form:

[Material Name], number ρ_S, c_s, λ_{11}, λ_{22}, α_λ,
ϕ, k_{11}, k_{22}, α_k, dispersion, temperature dependence
S, T_{int}, P_{int}
UNSAT, number, D_{11}, D_{22}, α_D, C, SAT, λ_{air}
.
.
.
END

where,

Material name: is an optional alphanumeric material name for user reference.

number: is the internal reference number for the material. SAGUARO will accept up to ten materials; the materials must be numbered such that 2 ≤ number ≤ 11.

ρ_s: is the material density.

c_s: is the material specific heat.

λ_{11}, λ_{22}<λ_{11}>: are components of the material thermal conductivity tensor (see below).

α_λ<0°>: is the angle in degrees between the principle material axes (for conductivity) and the coordinate axes (see below).

ϕ: is the material porosity. For ϕ set to zero, the material is treated as impermeable.

k_{11}, k_{22}<k_{11}>: are components of the material permeability tensor for the saturated state of the material.

α_k<0°>: is the angle in degrees between the principle material axes for permeability and the coordinate axes (see below).

dispersion <NONE>: prescribes the use of a model for hydrodynamic dispersion. If no dispersion is to be included in the analysis, this parameter is omitted or set equal to NONE. If a dispersion model is to be included, this parameter is set equal to VARIABLE.

temperature dependence <CONSTANT>: prescribes the dependence of the material properties on temperature time, location, etc. If all material properties (λ_{ii}, k_{ii}) are invariable, this parameter is omitted or set equal to CONSTANT. If one or more of the properties depend on temperature (or any other variable, e.g., hydraulic head or spatial location), this parameter is set equal to VARIABLE.

S<0>: is the volumetric heat source for the material. For no volumetric heating, this parameter is omitted; for constant volumetric heating, the parameter is set equal to the heating value. If the heat source varies with location, time or temperature, this parameter is set equal to VARIABLE.

T_{int}<0>, P_{int}<0>: specify the values of the initial temperature and effective pressure for the material. Note $P_{int} = p + \rho gz$ where p is the pore fluid pressure.

UNSAT: First word on current line of data. Inserting this data card implies that the user wishes to define constant values for D_{11}, D_{22}, α_D, C, SAT and λ_{air}. If temperature dependence is set equal to VARIABLE then the coefficients D_{11}, D_{22} , α_D, C, SAT and λ_{air} need to be defined in user supplied subroutines. If this card is omitted, D_{11}, D_{22}, α_D, and C will be initialized to zero. SAT will be set to one. If these values are appropriate for the calculation then this card can be omitted.

Number: This internal material reference number must agree with the material number on the preceeding material data card.

D_{11}, D_{22}<D_{11}>: Thermal mass diffusion coefficient (see equation 10).

α_D<0°>: is the angle in degrees between the principle material axis for thermal mass diffusion and the coordinate axis.

C: $\left[\frac{\partial \theta}{\partial \psi}\right]$ (Equation (10)) coefficient of time derivative term in the mass transport equation.

SAT: Saturation (moisture content/porosity); (unsaturated) 0 < SAT < 1.0 (fully saturated).

λ_{air}: Thermal conductivity of air (or any gas) in porous medium.

The material models allowed in SAGUARO include homogeneous matrix materials with either isotropic or orthotropic permeability and conductivity tensors. For isotropic materials ($k_{ij} = k$, $\lambda_{ij} = \lambda$), the permeability and conductivity are specified by setting $k_{11} = k$ and $\lambda_{11} = \lambda$, respectively; the parameters k_{22}, θ_k, λ_{22}, and θ_λ are omitted. For orthotropic materials ($k_{ij} = \delta_{ij}k_{ij} = k_{ii}$, $\lambda_{ij} = \delta_{ij}\lambda_{ij} = \lambda_{ii}$), the permeability and conductivity tensors are determined by specifying components of the tensor with respect to the principal material axes. Referring to Figure 3, the 1 and 2 axes indicate the principal material axes while θ specifies the orientation of the material with respect to the spatial reference frame. SAGUARO requires k_{11}, λ_{11}, D_{11} and k_{22}, λ_{22}, D_{22} to be specified for an orthotropic material; α_k, α_λ and α_D must be specified only if the material axes are not aligned with the coordinate axes. Note that α is measured from the positive x(r) axis and is positive in a clockwise direction.

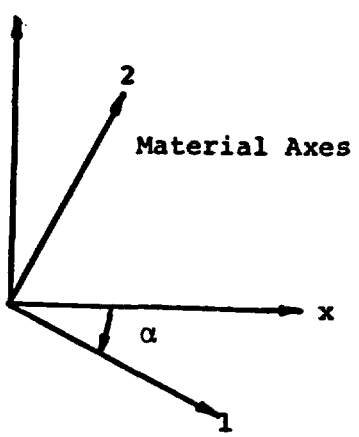


FIGURE 3. Notation for Orthotropic Materials

The variation of material and fluid properties with temperature, the specification of a hydrodynamic dispersion model and the variation of the volumetric heating with time and/or temperature is indicated by setting the parameters "temperature dependence," "dispersion," and "S" equal to VARIABLE, respectively. The actual variation of these quantities is specified by several user supplied subroutines. If temperature dependent properties have been specified, SAGUARO requires subroutines VISCOUS, ISOVOL, FLUIDC, DIF, PERM, FLAMBDA, and SLAMBDA to be supplied by the user. The inclusion of a dispersion model requires Subroutine DSPERSE to be provided; a variable heat source requires Subroutine SOURCE. Further details on these subroutines are given in a later section of this chapter. Note that when variable properties have been specified, all appropriate property values must still be supplied on the material data card. These values are used as initial estimates for the material properties when problems with material nonlinearities are being considered.

SAGUARO does not contain any dimensional constants and, therefore, the units for the material properties are free to be chosen by the user. For convenience, a table of consistent units is given in Appendix A.

Grid Data Cards:

Following the material specification, the grid points for the finite element mesh are generated. In contrast to many finite element codes, SAGUARO separates the generation of nodal points and the generation of elements into distinct operations. The calculation of nodal point locations is

accomplished by use of an isoparametric mapping scheme that considers quadrilateral parts or regions of the problem domain separately. For each part, a series of coordinates are specified which determine the shape of the region boundary. The node points within each part are identified by an I, J numbering system. The location of points in a region is controlled by user specification of the number of points along a boundary side and a local gradient parameter. These ideas are more clearly fixed through a description of the data cards required to generate points in a part.

For each part or region in the mesh, three data cards of the following form are required:

imin, jmin, imax, jmax, [g1], [g2], [g3], [g4], [POLAR], [xo], [yo]

x1, x2, x3, x4, [x5], [x6], ... [x12]

y1, y2, y3, y4, [y5], [y6], ... [y12]

.
.
.

END

where,

imin, jmin, imax, jmax: are the I, J limits for the region being generated as shown in Figure 4a. The difference between the maximum and minimum values determines the number of grid points generated in a particular direction.

g1<1>, g2<1>, g3<1>, g4<1>: specify the gradients for the node spacing along the four sides of the region. The gradients are defined by

$$g1 \text{ or } g3 = \frac{\text{node spacing at imin}}{\text{node spacing at imax}} = \frac{\Delta \text{imin}}{\Delta \text{imax}}$$

$$g2 \text{ or } g4 = \frac{\text{node spacing at jmin}}{\text{node spacing at jmax}} = \frac{\Delta \text{jmin}}{\Delta \text{jmax}}$$

and are illustrated in Figure 4a. The default values of unity give equal node spacing along a side. Gradients either larger or smaller than unity may be used to bias the spacing in either direction.

POLAR, xo<0>, yo<0>: specify the use of polar coordinates for describing the coordinates of the points defining the region. With POLAR specified, the x's and y's on the second and third data cards are interpreted as polar radii and angles referred to the local origin xo, yo. The polar angle is referenced to the positive x axis; positive angles are measured in a counterclockwise direction.

x1, x2, ... x12:
y1, y2, ... y12: define the coordinates of the four corner and optional side nodes for each part. If the region is bounded by straight lines, only the four corner coordinate (i.e., x1 to x4 and y1 to y4) need be specified. If any of the region sides are curved, then the appropriate side nodes, as shown in Figure 4b must be specified. If one side node is defined, a quadratic interpolation is used to define the boundary; specification of two side nodes allows a cubic interpolation. Side nodes should be located near the midside and one-third points for quadratic and cubic interpolation, respectively.

There are no limits on the number of parts which may be used to define a grid. The only restriction on the total number of grid points is that max (I*J) < 4000 for the CDC version of SAGUARO and max (I*J) < 5000 for the Cray version.

Node points may be generated for a triangular shaped region by allowing two adjacent corners of the quadrilateral part to coincide. However, when triangular meshes are created in this manner, the location of interior node points is generally unpredictable. The user is advised to verify the quality of such a mesh through use of a node point plot.

In generating mesh points for complex geometries, it is often convenient to be able to position an individual node point or a line of nodes. These situations are provided for in SAGUARO by use of the following data cards:

POINT, i, j, xl, yl, [POLAR], [xo], [yo]

where,

i,j: is the I, J name for the point.

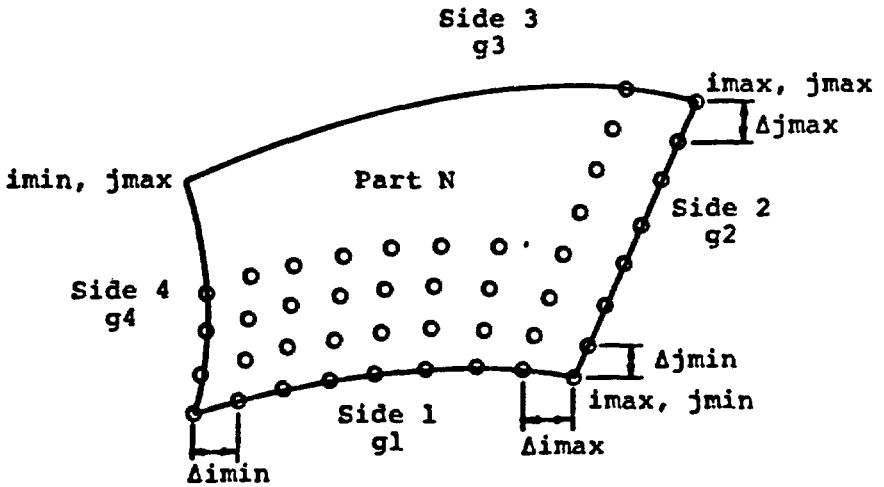
xl,yl: are the coordinates for the point.

POLAR, xo<0>, yo<0>: specify the use of polar coordinates as described previously.

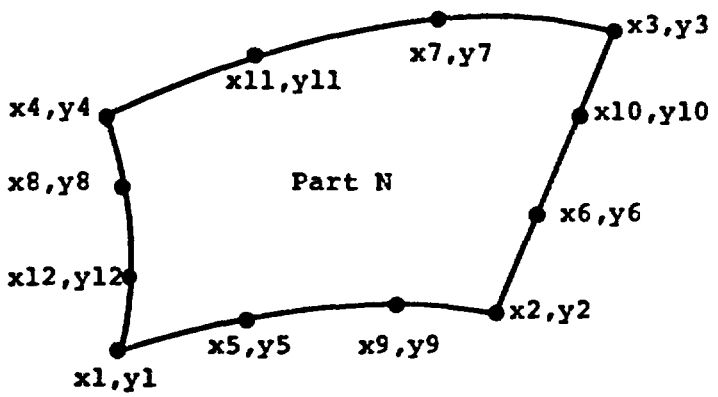
ARC, imin, jmin, imax, jmax, [gl], [POLAR], [xo], [yo]
xl, x2, [x3], [x4]
yl, y2, [y3], [y4]

where,

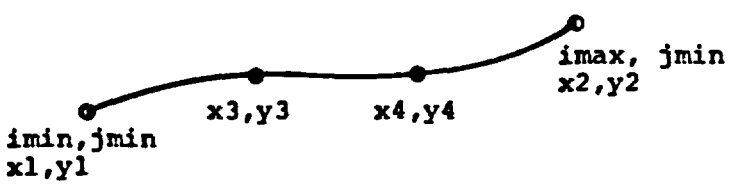
imin, jmin, imax, jmax: are the I, J limits for the arc as shown in Figure 4c. Since a one-dimensional array



(a) I, J Nomenclature



(b) Coordinate Nomenclature



(c) ARC Nomenclature

FIGURE 4. Grid Point Generation Nomenclature

of points is being generated, either imin = imax or jmin = jmax. The difference between the maximum and minimum values determines the number of grid points generated along the arc.

gl<1.0>: specifies the gradient for the node spacing along the arc.

The gradient is defined by

$$gl = \frac{\text{node spacing at ijmin}}{\text{node spacing at ijmax}} = \frac{\Delta ijmin}{\Delta ijmax}$$

and is illustrated in Figure 4c.

POLAR, xo<0>, yo<0>: specify the use of polar coordinates as described previously.

x1, x2, x3, x4:
y1, y2, y3, y4: define the coordinate for the ends of the arc and the optional intermediate points. If the arc is a straight line only the first two coordinates need be specified. The generation of a curved arc requires the specification of one or two intermediate points as shown in Figure 4c.

There are no limits on the number of POINT and ARC data cards that may be used in generating a mesh. Both types of cards may appear at any point within the grid point data section of the SETUP command.

EXTDEF

This data card causes the user supplied Subroutine EXTDEF to be called by the mesh generator. Within this subroutine, the user may create an arbitrary array of I, J labeled nodal

points. The EXTDEF data card may be used in conjunction with the standard nodal point generation schemes or may be used to create an entire mesh. The data card may appear at any appropriate point within the grid point data section of the SETUP command. Details on the form of Subroutine EXTDEF are given in a later section.

Element and Boundary Condition Data Cards:

Following the generation of the grid points, the program is ready to accept element and boundary condition data. Since the mesh points for the problem geometry are generated independently of the elements, the selection of nodes from which to construct a given element is very flexible. The actual construction process for an element consists of identifying an appropriate group of previously generated mesh points that will serve as the corner and midside nodes of the element. This concept is apparent from the form of the element data card.

element type, mat, i1, j1, [i2], [j2], ... [in], [jn]

where,

element type: is an alphanumeric name for the type of element. The element types used in SAGUARO are described below.

mat: is the matrix material number for the element. This number should be set to correspond to the matrix material number used on the material property card ($2 < mat < 11$).

i1, j1, [i2], [j2], ...: is the list of I, J values for the node points in the element. The nodes of an element are listed counterclockwise around the element starting with any corner as shown in Figure 5. In some situations, the list of I, J values may be significantly condensed. When only the first node, I, J values are specified for a quadrilateral element, the following values for the remaining nodes are assumed,

$$i4 = i8 = i1,\ i5 = i7 = i1 + 1,\ i2 = i3 = i6 = i1 + 2$$

$$j2 = j5 = j1,\ j6 = j8 = j1 + 1,\ j3 = j4 = j7 = j1 + 2$$

When I, J values are specified for only the corner nodes of any element, the midside I, J values are computed as the average of the corner values.

The specification of different types of elements is provided by the "element type" parameter on the previously described data card. The permissible element names for this parameter include the following:

(a) QUAD8/4 -- A subparametric quadrilateral with arbitrarily oriented straight sides.

(b) QUAD8/8 -- A general isoparametric quadrilateral with quadratic interpolation used to define the shape of the element sides.

(c) TRI6/3 -- A subparametric triangle with arbitrarily oriented straight sides.

(d) TRI6/6 -- A general isoparametric triangle with quadratic interpolation used to define the shape of the element sides.

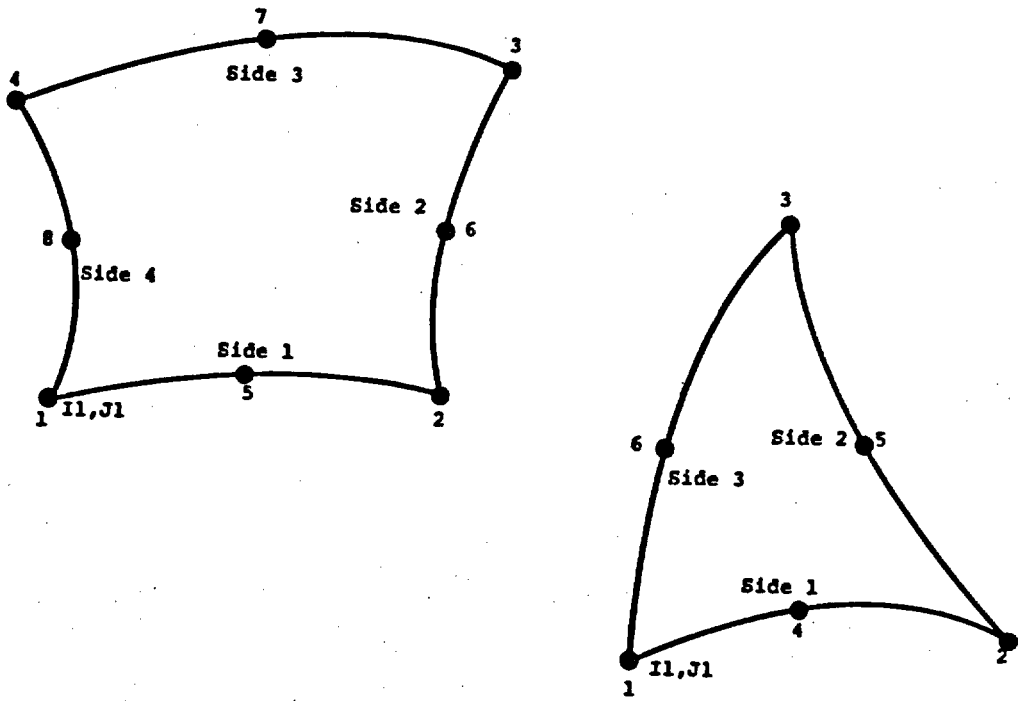


FIGURE 5. Element Node Numbering and Side Numbering

Note that in the generation of the subparametric elements, the physical coordinates (x, y) of the midside nodes need not lie precisely on the element side as these coordinates are not used in the element formulation. In all of the above elements, the fluid hydraulic head and temperature are approximated using quadratic shape functions over the element; the velocity components are approximated by linear shape functions.

During the construction of the element mesh, two points about the I, J identification scheme should be noted. Each element is identified internally by the I, J values for the first node named on the element data card, i.e., il, jl. Since any corner node may be named first, two or more elements may share the same internal designation or name. This situation must be avoided if any of the elements sharing names are to have boundary conditions imposed on them. A simple reordering

of the nodes in the appropriate elements remedies this situation. Secondly, during the generation of grid points, there is no requirement that adjacent parts of the grid have a continuous I, J numbering. When elements are constructed along boundaries of such adjacent parts of the grid, it is imperative that common nodes between elements have the same I, J values. Element connectivity is generated from the I, J values for each node and, therefore, common nodes with different I, J labels will not be properly connected. The generation of element meshes using node points with non-continuous I, J labels is illustrated in the example section.

The boundary conditions for the problem are specified by element and may appear at any point in the present data section after the element to which they apply has been defined. Boundary conditions are specified to have either a constant value along an element side or a particular value at a node. The boundary condition data card has the following form:

BC, b.c. type, il, jl, side/node, value/set no./time curve no.

where,

b.c. type: is an alphanumeric name for the type of boundary condition. The types of boundary conditions used in SAGUARO are described below.

il, jl: is the I, J identification of the element (i.e., the first I, J named on the element data card) to which the boundary condition applies.

side/node: identifies the side or node of the element

to which the boundary condition is to be applied. The numbering of nodes and sides begins with the identifying node (i.e., the first node named on the element data card) and proceeds counterclockwise as shown in Figure 5.

value/set no./time curve no.: is the numerical value of the applied boundary condition, the number of the boundary condition SET in the case of convective or radiative boundary condition, or the number of the time history curve for time dependent boundary conditions. For specified pressure, velocity, temperature, or heat flux boundary conditions, this parameter is set to the numerical value of the boundary condition. The specification of a set or time curve no. is explained below.

The permissible type of boundary conditions as specified by the parameter "b.c. type" include the following:

(a) P -- specifies the effective pressure at a node.

(b) PSIDE -- specifies the hydraulic head to have a constant value along an element side.

(c) PVARY -- specifies the hydraulic head along an element side to be a function of time.

(d) USIDE -- specifies the fluid velocity (volumetric flow/unit area) normal to the element boundary to have a constant value.

(e) UVARY -- specifies the fluid velocity (volumetric flow/unit area) normal to the element boundary to be a function of time.

(f) T -- specifies the temperature at a node.

(g) TSIDE -- specifies the temperature to have a constant value along an element side.

(h) TVARY -- specifies the temperature along an element side to be a function of time.

(i) QSIDE -- specifies a constant heat flux (energy/unit area/unit time) along an element side.

(j) QVARY -- specifies a time dependent heat flux along an element side.

(k) QCONV -- specifies a constant convective heat transfer process along an element side.

(l) QRAD -- specifies a radiative or temperature dependent convective heat transfer process along an element side.

(m) Impermeable surface -- no boundary condition need be applied.

(n) Adiabatic surface -- no boundary condition need be applied.

All of the above boundary conditions can be employed with any of the previously described elements.

The boundary condition options, PVARY, UVARY, TVARY, and QVARY permit hydraulic head, fluid velocity, temperature or heat fluxes along an element boundary to vary with time. The time histories of the boundary condition are input through a set of user supplied subroutines (Subroutine CURVEn). The association of a particular time history with the appropriate boundary condition is accomplished by use of the "time curve

no." which appears on the boundary condition data card and in the user supplied subroutine name. SAGUARO will allow a total of six different time histories to be input. The format for the time history subroutines is described in a subsequent section.

The use of convective and radiative boundary conditions requires the appropriate heat transfer coefficients (h_c, h_r) and reference temperatures (T_c, T_r) to be specified. These parameters are input through use of a SET data card which is of the form:

SET, b.c. type, set no., h, T

where,

b.c. type: is the alphanumeric name of the type of boundary condition for which data is being specified, i.e., either QCONV or QRAD.

set no.: is the number of the particular data set. The code allows up to ten data sets for each type of boundary condition. The set no. is used to identify the appropriate boundary condition set on the BC card.

h, T: are the parameters required for specifying a convective or radiative boundary condition. For convection, h = heat transfer coefficient = h_c and T = T_c. For fourth power radiation, h = emissivity, Stefan-Boltzmann constant = $\varepsilon \cdot \sigma$ and T = T_r. For generalized radiation/convection, h = VARIABLE and T = T_r. The generalized radiation/convection condition mentioned above has been provided to allow an arbitrary variation of h with temperature or time in the flux expression,

$$q = h(T, x, y, t)(T - T_r) \quad .$$

To incorporate such a boundary condition, the parameter "b.c. type" must be set to QRAD, "h" must be set to VARIABLE, "T" is set to the appropriate reference temperature, and the user supplied subroutine HTCOEF, which describes h(T, x, y, t), must be appended to the SAGUARO program. This subroutine is described in detail in a later section of this chapter.

The SET data cards may appear anywhere in the present data section; SET cards for both types of boundary condition may appear in the same problem.

Looping Feature:

In order to permit easy specification of elements and boundary conditions which appear in regular patterns in the mesh, a looping feature is incorporated in SAGUARO. This feature allows the definition of ILOOP's and JLOOP's (which are similar to FORTRAN DO loops) for incrementing data in the I and J directions. Nesting of the loops may be in any order but no more than one loop in a given direction may be used at one time. Note that within each loop all the I (or J) values are given the same increment. The looping commands are of the following form:

ILOOP, npass, inc.	or	JLOOP, npass, inc.
.		.
.		.
.		.
element or boundary condition data cards		element or boundary condition data cards

```
      .                                   .
      .                                   .
      .                                   .
      IEND                                JEND
```

where,

npass: specifies the number of passes to be made through the loop.

inc: specifies the increment to be added to the I or J values found within the loop. the "inc" parameter may be negative.

The looping commands may appear at any point within the element and boundary condition data section of the SETUP command. The use of the looping feature is illustrated in the example problem.

FORMKF Command Card

With the completion of the SETUP command, the next task in the analysis sequence is the formulation of the matrix equations for the individual elements in the mesh. This function is carried out by the command card:

FORMKF, [geometry], [type of flow], [vel. comp.]

where,

geometry: is an alphanumeric name to indicate the type of coordinate system desired. If geometry is omitted, the two-dimensional planar formulation is used; if geometry = AXISYM, the axisymmetric formulation is used.

type of flow: is an alphanumeric name to indicate the type of problem being considered. If type of flow is omitted, the problem is treated as an isothermal flow problem. Forced convection heat transfer problems are designated by setting type of flow = FORCED. Free convection or mixed convection problems are indicated by setting type of flow = FREE.

vel. comp.: is an alphanumeric name to indicate the type of velocity computation that will be used in the analysis. If vel. comp. is omitted, the velocity field will be computed on an element basis which results in a discontinuous velocity field. If vel. comp. = CONTINUOUS, the velocity field will be computed from a global matrix equation which results in a continuous velocity field.

OUTPUT Command Card

Prior to solution of the porous flow problem, it is sometimes convenient to limit the amount of printed output generated by SAGUARO. It may also be desirable to specify spatial locations within the mesh other than nodal points at which output of the dependent variables is required. Both of these functions may be invoked through use of the OUTPUT command card. The selective printing of the computed dependent variables may be set up through use of the following command card:

OUTPUT, delimiter type, n1, n2, n3, ...n50

where,

delimiter type: is an alphanumeric name to indicate how the subsequent element numers are to be interpreted in limiting the printed output. If delimiter type = SINGLE, individual element numbers are assumed to be listed in the following data. If delimiter type = STRING, the following data is interpreted as pairs of element numbers with each pair defining a sequence of elements.

n1, n2 ... n50: is a list of element numbers indicating which elements are to have flow field data printed during the solution process. A maximum of fifty individual element numbers or twenty-five element pairs may be specified on a single command card.

There is no restriction on the number of OUTPUT command cards that can be used in a SAGUARO input deck; OUTPUT cards with different delimiter types may be mixed in the same input deck. The OUTPUT command card(s) must precede the UNZIPP command card in the input deck. If no OUTPUT command is used in a SAGUARO input deck, the entire flow field data is printed at each output interval.

The specification of special output points for the dependent variables is achieved with the following form of the command card:

OUTPUT, POINTS, x_1, y_1, x_2, y_2, ... x_{25}, y_{25}

where,

x_1, y_1, ... x_{25}, y_{25}: is a list of the x, y (or r, z) coordinate locations for the special points. A maximum of twenty-five points may be specified on a single command card.

SAGUARO allows a maximum of fifty special points to be specified during any particular analysis. The OUTPUT command card in this form must precede the UNZIPP command card; OUTPUT command cards of both types may occur in the same input deck. The dependent variables at the special output points are printed at each normal output interval. The variables at these points are also stored for possible later plotting in history plots.

UNZIPP Command Card

The assembly and solution of the global system of matrix equations, for either steady state or transient problems is carried out by the following command cards:

UNZIPP, TRANS, [iprint],

$t_{initial}$, [t_{final}], Δt, [no. steps], [initial conditions]

.
.
.

END

where,

TRANS: the solution procedure available in SAGUARO is a transient modified Crank-Nicholson procedure.

iprint < 10 >: specifies how often the solution field is printed.

$t_{initial}$, t_{final}, Δt: specify the time limits ($t_{initial}$, t_{final}) and the time step (Δt) for the time integration procedure.

no. steps: indicates the number of time steps to be taken in the transient analysis.

initial conditions < >: specifies the source of the initial conditions for the problem. If this parameter is omitted, the initial hydraulic head and temperature fields are set from data on the material property card; The velocity field is assumed to be zero. If this parameter is set equal to TAPE, initial conditions may be input through a tape file as explained below.

One or more UNZIPP cards may be required depending on the need to change the time step (Δt) and/or the printout frequency (iprint) during the analysis. When using a sequence of UNZIPP cards, all information pertinent to the continued analysis of the problem must be specified on all cards following the first UNZIPP card (i.e., parameters iprint, $t_{initial}$, t_{final}, Δt and no. steps should be reset as required).

The control of the integration interval is accomplished by either of two methods--specification of a final time (t_{final}) or specification of the number of time steps to be taken (no. steps). When the running time reaches t_{final} or the specified number of time steps is equalled, the program checks for the presence of another UNZIPP command and the definition of a new integration interval. This process continues until an END card is encountered, thus ending the integration process.

When the initial condition parameter is set to TAPE, SAGUARO expects the initial velocity, hydraylic head, and temperature fields to be supplied from a disc (or tape) file called TAPE 19. Details on the required format for this file are given in a later section of this chapter.

STREAM Command Card

To aid in interpreting the solution obtained through the previous sequence of command cards, SAGUARO allows the calculation of the stream function field as a user option. The computation of the stream function is activated through the command card,

STREAM, [psi base], [iprint]

where,

psi base <0>: specifies the value of the stream function at the first node of the first element processed.

iprint <0>: specifies the amount of printout produced during the stream function calculation. If iprint is omitted, only the points of minimum and maximum stream function are printed; for iprint > 0, the stream function field is output by element.

The calculation of the stream function is carried out by considering line integrals of the velocity along element boundaries. If the element ordering is not sufficiently continuous (i.e., each successive element processed must have at least one corner node in common with a previously processed element), the entire stream function field cannot be calculated. SAGUARO provides a diagnostic message in this situation.

The stream function calculation is automatically carried out for each time step performed by UNZIPP beginning with the initial conditions. Though the actual numerical values

of the stream function do not provide much insight into the behavior of the flow field, subsequent commands to the plotting routines allow useful graphic representation of the flow field to be obtained.

HEATFLUX Command Card

To aid in interpreting and using the computed temperature solution, SAGUARO allows the computation of several heat flux quantities on an element basis. The computation of heat fluxes is initiated by the following command card:

HEATFLUX, time step no., location

where,

time step no.: is the number of the time step for which heat flux computations are desired. If time step no. = ALLTIMES, heat fluxes are computed for every element at every time step.

location: specifies where the heat flux calculations are to be made. For location = FULL, heat flux calculations are made for every element in the mesh. A second option allows fluxes to be calculated in up to twenty elements specified by the user. This latter option is specified by listing the required element numbers after the "time step no." parameter. This parameter is omitted if time step no. = ALLTIMES.

Within a given element, heat flux values are calculated on the element boundary midway between nodes. Calculations are made for the x and y (or r and z) components of the flux vector and also for the heat flux normal to the element boundary and the heat flux integrated over each side of the element (i.e. total energy transfered across the element boundary). When using the HEATFLUX command in conjunction

with a transient analysis note that the time steps are numbered continuously from 1 to n beginning with the initial conditions (i.e., solution at time = Δt is step number 2). Heat flux calculations can thus be made at any particular time step by appropriately setting the "time step no." parameter. Note that the use of the "time step no. = ALLTIMES" option does <u>not</u> result in any heat flux data being printed by SAGUARO. This option should be used only to create the data file for the subsequent plotting of flux histories (see HISTORY option under PLOT command). There is no limit to the number of HEATFLUX command cards that can be used in a SAGUARO input deck.

PLOT Command Card

The SAGUARO program contains a plotting package to facilitate the interpretation of data obtained from a solution and to aid in setting up element meshes. There are seven basic types of plots which are available in SAGUARO and are obtained with the following command card,

PLOT, plot type, xmin, ymin, xmax, ymax, [imin, jmin, imax, jmax], [xcale], [yscale], [number], [special pts]

where,

plot type: is an alphanumeric name which specifies the type of plot desired. The permissible parameter values are catalogued below.

xmin, ymin, xmax, ymax: specify the range of coordinates for the area to be plotted in a line drawing or define the range of the ordinate and abscissa for a graph. For line drawings (e.g., element plots, outline plots, contour plots) the xmin, ••• ymax parameters define a rectangular window; only elements and their associated data that fall entirely within the window will be plotted. For graphs (e.g., time histories or profiles), the xmin, ... ymax may be used to set the maximum and minimum values for the ordinate (ymin, ymax) and abscissa (xmin, xmax) of the plot. If these parameters are omitted, the axes for the graph are set by SAGUARO.

imin, jmin, imax, jmax: is an optional specification of the limits of the region to be plotted. If the I, J limits of the region are specified, the xmin ... ymax parameters are used to set the border for the plot. These parameters are omitted for graph plots.

xscale <1.0>, yscale <1.0>: specify magnification factors for the x and y coordinates of the plot. The default values produce a correctly proportioned plot of the largest possible size consistent with the plotting device. The use of a scale parameter produces a non-proportional plot.

number < >: specifies if the element numbers are to be displayed on the element plot. If number is omitted, element numbers are not plotted; if number = NUMBER, the element numbers are plotted at the element centroid.

special pts < >: specifies if the location of the special output points (see OUTPUT command) are to be displayed on the element plot. If special pts is omitted, special point locations are not plotted; if special pts = SPECIAL, the special point numbers are plotted at the appropriate location on the element plot.

The second parameter on the PLOT command card, denoted "plot type" may be set to any of the following values as required:

(a) POINTS -- generates a plot of the grid points generated by the SETUP command. The "grid plot" parameter on the SETUP command card must be set to PLOT to obtain this type of plot.

(b) ELEMENT -- generates a plot of the element mesh.

(c) CONTOUR -- generates contour plots of the stream function, pressure, or temperature.

(d) OUTLINE -- generates an outline plot of the problem domain with material boundaries indicated.

(e) HISTORY -- generates time history plots of any of the dependent variables.

(f) PROFILE -- generates plots of the dependent variables versus position with time as a parameter.

Following the command cards for the CONTOUR, HISTORY, and PROFILE plot options, a series of data cards are required.

Contour Data Cards:

For the CONTOUR plot option, the required data cards are of the following form:

contour type, time step no., no. contours, c1, c2, ... c20

.
.
.

END

where,

contour type: is an alphanumeric name indicating the variable to be contoured. This parameter may have the value STREAMLINE, PRESSURE, MOISTURE or ISOTHERMS.

time step no.: is the number of the time step for which a plot is required.

no. contours: specifies the number of contours to be plotted. A maximum of twenty contour lines is allowed on each plot.

c1, c2, ... c20: are optional vaues that specify the value of the contour to be plotted. If these parameters are omitted, the plotted contours are evenly spaced over the interval between the maximum and minimum values of the variable.

Note that when the contour values are left unspecified, the maximum and minimum values used to compute the contour levels are those for the entire mesh. This procedure may produce an unsatisfactory (or blank) plot in the event only a small portion of the mesh is plotted and the number of contours specified is small. This situation may be avoided by specifying the contour values to be plotted. When using the contour option with a transient analysis, note that the time steps are numbered continuously from 1 to n beginning with the initial conditions (i.e., solution at time = Δt is step number 2). A contour plot can thus be made at any particular time step by appropraitely setting the "time step no." parameter.

Any number and/or type of contour data cards may follow a CONTOUR command card; the sequence is terminated by an END card. To simplify the plotting of a series of contour plots for a transient analysis, a looping feature is available. The looping command has the following form:

PLOTLOOP, No. plots, plot inc

contour type, time step no., no. contours, c1, c2, ... c20

PLOTEND

.
.
.

END

where,

no. plots: specifies the number of plots to be generated.

plot inc: indicates the frequency at which a plot is generated, i.e., every "plot inc" time steps a contour plot is produced beginning with the "time step no." indicated on the contour data card.

There is no limit to the number of PLOTLOOP data sets that may follow a CONTOUR command card; the sequence is terminated by an END card. Within any given PLOTLOOP, only a single contour data card may be defined. PLOTLOOP's and individual contour data cards may be mixed under a single CONTOUR command.

History Data Cards:

For the HISTORY plot option, the required data cards are of the following form:

location, no. points, time step 1, time step 2,

elem no., node no., elem no., node no., ...

.
.
.

END

where,

location: is an alphanumeric name indicating the variable to be plotted as a function of time. For location = PLOCATION, effective pressure are plotted versus time; location = ULOCATION or VLOCATION implies that velocity components are to be plotted; location = TLOCATION specifies that temperatures will be plotted; location = MLOCATION plots moisture content versus time. The MLOCATION option is only available on the CRAY version.

no. points: specifies the number of histories to be plotted. A maximum of ten time histories per plot is allowed.

time step 1, time step 2: indicate the time step numbers at which the time histories are to begin and end, respectively. The maximum difference allowed between time step 2 and time step 1 is 400, i.e., only 400 time steps may be represented on a given plot.

elem no., node no.: are pairs of numbers indicating the element and node number for which a time history is required. A maximum of ten such pairs per data card is allowed. When plotting histories for special output points, pairs of numbers are not required. In this latter case, the numbers of the special points to be plotted are listed in sequence. A maximum of ten such numbers per data card is allowed.

Note: $1 \leq$ node no. ≤ 8 for effective pressure, temperature and moisture, $1 \leq$ node no. ≤ 4 for velocities.

There is no restriction on the number or type of LOCATION data cards that may follow a HISTORY command card; the sequence is terminated by an END card. The numbering of the element nodal points is shown in Figure 5. Note that the numbering of heat fluxes in an element differs from the node numbering convention; fluxes are numbered sequentially (counterclockwise) around the element beginning with the point nearest the identifying node for the element. Also, the plotting of flux histories assumes that the HEATFLUX, ALLTIMES command was executed prior to the command for the history plot.

Profile Data Cards:

For the PROFILE plot option, the required data cards are of the following form:

TIMEPLANE, no planes, t1, t2, ... t10
location, delimiter type, no. pairs, elem no., side/node no.,
elem no., side/node no., ...

.
.
.

END

where,

no. planes: specifies the number of profiles (at different times) to be plotted. A maximum of ten profiles per plot is allowed.

t1, t2, ... t10: specify the time step numbers at which the profile is to be plotted.

location: is an alphanumeric name indicating the variable to be plotted as a function of position. Location

should be set to PLOCATION, ULOCATION, VLOCATION, TLOCATION and MLOCATION for profiles of hydraulic head, velocity (components), temperature, and moisture content, respectively.

delimiter type: is an alphanumeric name indicating how the profile geometry is to be specified. If delimiter type = SIDES, the profile geometry is described in terms of element sides. For delimiter type = NODES, the profile is given in terms of individual nodal points.

no. pairs: specifies the number of data pairs (elem no., side/node no.) needed to describe the profile geometry. A maximum of twenty such data pairs is permitted.

elem no., side/node no.: are pairs of numbers specifying the profile geometry in terms of an element number and a side or node number.

There is no restriction on the number of TIMEPLANE/LOCATION data cards that may follow a PROFILE plot command. However, TIMEPLANE and LOCATION data cards must occur in pairs with the TIMEPLANE card first. The data sequence for the PROFILE option is terminated by an END card.

With the delimiter type set to SIDES, the temperature profile is plotted along element sides with the spatial distance being measured along the element boundary. When delimiter type is set to NODES, the temperature profile is plotted by constructing the straight line path between

successive nodes. In both options, the input sequence of elements determines the profile path. There is no requirement that the profile have a continuous path, i.e., some elements along a path may be omitted. Multiple side/node specifications for an individual element are permitted. When the SIDE option is used, the profile path is directed along element sides with the direction of increasing path length determined by increasing corner node number. Thus, for a quadrilateral with side 1 specified, the path proceeds from nodes 1 to 5 to 2; with side 3 specified, the path is directed from nodes 3 to 7 to 4. If the path direction is inappropriate with this option, the NODES description may be used.

RESTART Command Card

The SAGUARO program allows a computed solution and its associated problem data to be conveniently saved for further post-processing through the use of a restart command. In order to save a previously computed solution, the following command card may be used,

RESTART, SAVE

In order to restart a previously saved solution, the following command card is used,

RESTART, RESET [nsteps]

where,

nsteps <0>: is a parameter to indicate at what time step number the solution file is to be positioned at during the restart process. If nsteps is omitted, the solution file is rewound. For nsteps > 0, the solution file is positioned after the nsteps time step. This allows restarting of the solution process with the nsteps + 1 time step.

The command to save a solution may occur at any point after the UNZIPP command sequence, that is after a solution has been obtained. In order to restart a solution, the RESET command should immediately follow the header card.

If the solution is to be continued in time following a restart, the FORMKF command must be executed prior to the UNZIPP command as the restart procedure does not save the

matrix equations for the problem. Also, the initial condition parameter on the UNZIPP command card should be set equal to TAPE. The solution file should be repositioned at the appropriate time step through use of the nsteps parameter.

The RESTART commands when executed from the data deck direct the program to collect (or distribute) pertinent element and solution information onto (or from) two files, TAPE 13 (MESH data) and TAPE 19 (Hydraulic head and Temperature data). To complete the restart process, these files must be saved (or attached) by the appropriate system control cards. Typically, these files would be saved on a magnetic tape or catalogued on a permanent file.

Program Termination Card

There are two modes of termination for a SAGUARO analysis. If two or more problems are to be run in sequence, then the appropriate termination for any particular problem is,

END, [iprint]

However, if the program is to be terminated with no further computational operations, then the following command card is used,

STOP, [iprint]

where,

iprint: is an optional alphanumeric parameter that allows the printing of the last solution obtained to be suppressed. If iprint is omitted, the solution field is printed; if iprint = NOPRINT, then printing is suppressed.

Input Deck Structure

As noted previously, the order of the commands to SAGUARO is dependent on the needs of the user. However, some limitations on the command sequence are obvious as some operations are necessary prerequisites to other computations. The following comments provide some guidelines to specific sequencing situations.

(a) The POINTS plot option must follow the SETUP command sequence as the file used to store the grid point coordinates is rewritten in later operations. Typically, a grid point plot is used in setting up a grid and is not generated during a complete solution sequence.

(b) The ELEMENTS and OUTLINE plot options can be located anywhere after the SETUP command sequence; the OUTLINE option should precede a call to the FORMKF command or follow the UNZIPP command.

(c) The remaining plot commands can occur at any point after the values to be plotted have been computed.

(d) The RESTART, SAVE command can only be executed after a solution has been obtained. No provisions are made in the restart process to retain the element coefficient matrices and thus the SAVE option has little meaning prior to obtaining a solution.

(e) If a solution is to be saved, the RESTART, SAVE command should generally be the last command

(except for STOP) in a data deck. The restart process uses several tape files that are also employed by other program operations. The execution of commands following a RESTART, SAVE command could result in a conflict in file usage.

(f) If a transient solution has been saved, it may be continued in time by use of the RESTART, RESET command. The RESTART command should be followed by the FORMKF command and the UNZIPP commands with the TAPE parameter indicated.

(g) The OUTPUT command must occur after the SETUP command and must precede the UNZIPP command.

User Supplied Subroutines

There are several instances which require the user to supply FORTRAN coded subroutines to SAGUARO; the use of variable material properties, the use of a temperature and/or time dependent volumetric heat source, the use of a dispersion model, the use of a general radiation/convection boundary condition, and the use of time dependent boundary conditions.

When the parameter EXTDEF is encountered during the generation of nodal points, MARIAH accesses SUBROUTINE EXTDEF which is supplied by the user. This subroutine allows nodal point locations to be defined in any appropriate manner by the user. This subroutine must have the following form:

```
SUBROUTINE EXTDEF (X, Y, MAXI)
DIMENSION X(MAXI, 1), Y(MAXI, 1)

.
.
.

FORTRAN coding to generate an array of nodal
point locations

.
.
.

RETURN

END
```

where the variables in the subroutine parameter list are:

X, Y: two-dimensional arrays containing the x, y (or r, z) coordinate locations of the nodal points. The indices for each two-dimensional array correspond to the I, J name for the nodal point (i.e., X(I, J), Y(I, J) for point I, J).

MAXI: an integer specifying the largest I value that can be defined in the mesh. This parameter corresponds to the maxi parameter specified on the SETUP command card.

When the "temperature dependence" parameter on the fluid material data card (i.e., material number = 1) is set equal to VARIABLE, SAGUARO expects SUBROUTINE VISCOUS, SUBROUTINE FLAMBDA, and SUBROUTINE ISOVOL (for free or mixed convection problems) to be supplied by the user. These three subroutines allow the user to conveniently specify the fluid viscosity, conductivity, and volumetric expansion coefficient as an arbitrary function of the temperature. In the event only one or two of the three indicated parameters are to vary with temperature, the remaining properties must still be set through use of the appropriate subroutine, i.e., SAGUARO expects all the subroutines to be present.

The required subroutines must have the following forms:

```
SUBROUTINE VISCOUS (AMU, T, NNODES)
DIMENSION AMU(1), T(1)

.
.
.

FORTRAN coding to evaluate the fluid viscosity

.
.
.

END


SUBROUTINE FLAMBDA (FK, T, NNODES)
DIMENSION FK(1), T(1)
```

```
      .
      .
      .
      FORTRAN coding to evaluate the fluid conductivity
      .
      .
      .
      RETURN
      END


      SUBROUTINE ISOVOL (BETA, T, NNODES)
      DIMENSION BETA (1), T(1)
      .
      .
      .
      FORTRAN coding to evaluate the fluid volumetric
      expansion coefficient
      .
      .
      .
      RETURN
      END
```

where the variables in the subroutine parameter lists are:

AMU(NNODES): an array containing the values of the fluid viscosity evaluated at the temperatures T(NNODES).

FK(NNODES): an array containing the values of the fluid conductivity evaluated at the temperatures T(NNODES).

BETA(NNODES): an array containing the values of the fluid volumetric expansion coefficient evaluated at the temperatures T(NNODES).

T(NNODES): an array containing the values of the temperatures at the element nodes.

NNODES: an integer specifying the number of nodes at which the material property is to be evaluated.

When the "temperature dependence" parameter on the matrix material data card (i.e., material number = 2-11) is set equal to VARIABLE, SAGUARO expects SUBROUTINE PERM and SUBROUTINE SLAMBDA, SUBROUTINE FLUIDC, SUBROUTINE DIF and SUBROUTINE SLAMAIR (for forced or free convection problems) to be supplied by the user. These five subroutines allow the user to conveniently specify matrix permeability, conductivity, moisture content, mass diffusion coefficient and air conductivity as an arbitrary function of the temperature (and other variables). In the event only one of the five properties is to vary, the remaining properties (if required) must still be set through use of the appropriate subroutine, i.e., SAGUARO expects all five subroutines to be present. Each subroutine is used to evaluate the appropriate material property for <u>all</u> matrix materials labeled as temperature dependent on the material data cards.

The required subroutines must have the following forms:

```
SUBROUTINE PERM (AK1, AK2, P, T, U, V, X, Y, NNODES, MAT
NELEM, TIME, PROP)
DIMENSION AK1(1), AK2(1), P(1), T(1), U(1), V(1), X(1), Y(1)
DIMENSION PROP (17,11)

.
.
.
```

```
FORTRAN coding to evaluate the principal components of
the permeability tensor for each matrix material

.
.
.

RETURN

END


SUBROUTINE SLAMBDA (SK1, SK2, T, X, Y, NNODES, MAT, NELEM,
TIME, PROP)
DIMENSION SK1(1), SK2(1), T(1), X(1), Y(1), PROP(17,11)

.
.
.

FORTRAN coding to evaluate the principal components of the
conductivity tensor for each matrix material

.
.
.

RETURN

END


SUBROUTINE FLUIDC (CM, ATHR, TH, P, T, X, Y, NNODES, MAT,
NELEM, TIME, PROP)
DIMENSION CM(1), P(1), T(1), X(1), Y(1), AC(1), PROP(17,11)

.
.
.

FORTRAN coding to evaluate the nodal moisture content (TH),
average element moisture content (ATHR) and derivative of

moisture content with respect to pressure head (∂θ/∂ϕ)
at element node locations.

RETURN

END
```

```
      SUBROUTINE DIF (DIF1, DIF2, P, T, X, Y, NHALF, MAT, NELEM,
     TIME, PROP)
      DIMENSION DIF1(1), DIF2(1), P(1), T(1), X(1), Y(1), PROP(17,11)

      .
      .
      .

      FORTRAN coding to evaluate the components of the mass dis-
      persion tensor for each matrix material (Soret effect)

      .
      .
      .

      RETURN

      END


      SUBROUTINE SLAMAIR (SLAMAIR, P, T, X, Y, NNODES, MAT, NELEM,
     TIME, PROP)
      DIMENSION SLAMAIR(1), P(1), T(1), X(1), Y(1), PROP(17,11)
     NELEM(1)

      .
      .
      .

      FORTRAN coding to evaluate the thermal conductivity of air

      .
      .
      .

      RETURN

      END
```

where the variables in the subroutine parameter lists are:

AK1(NNODES), AK2(NNODES): arrays containing the values of the principal permeabilities k_{11} and k_{22}. For isotropic materials, set AK2(NNODES) = AK1(NNODES).

ATHR: average moisture content divided by porosity ($0 < ATHR < 1$)

C(NNODES): array containing the values of the derivative of moisture content ($\partial\theta/\partial\psi$).

DIF1(NNODES) and DIF2(NNODES): arrays containing the values of the principal mass dispersion tensor for each material.

SLAMAIR(NNODES): array containing the thermal conductivity of air.

MAT: an integer specifying the matrix material number as set on the material data card.

NNODES: an integer parameter specifying the number of nodes at which the material property is to be evaluated.

P(NNODES), T(NNODES), U(NNODES), V(NNODES): arrays containing the values of the effective pressure, temperature, velocity components and spatial coordinates at the nodes.

SK1(NNODES), SK2(NNODES): arrays containing the values of the principal conductivities λ_{11} and λ_{22}. For isotropic materials, set SK2(NNODES) = SK1(NNODES).

TH(NNODES): array containing the values of moisture content/porosity, (0 < TH < 1.0).

x(NNODES), y(NNODES): arrays containing the x(r) and y(z) coordinates of the nodes.

TIME: time at current computation

PROP(I, MAT): various material properties for

2 < MAT < 11

I = 1 density

= 2 specific heat

= 3 thermal conductivity

= 4 " "

= 6 porosity

= 7 permeability

= 8 "

for the fluid MAT = 1

I = 1 density

= 2 viscosity

= 3 specific heat

= 4 condictivity

= 6 gravitational constant

When the "dispersion" parameter on a matrix material data card is set to VARIABLE, SAGUARO expects SUBROUTINE DSPERSE to be supplied by the user. This subroutine must have the following form:

```
SUBROUTINE DSPERSE (E1, E2, E12, U, V, NNODES, MAT)
DIMENSION E1(1), E2(1), E12(1), U(1), V(1)
.
.
.
FORTRAN coding to evaluate the components of the
dispersion tensor for each matrix material .
.
.
RETURN
END
```

where the variables in the subroutine parameter list are:

E1(NNODES), E2(NNODES): arrays containing the values of the dispersion components. E1 and E2 contain the dispersion coefficients taken along the global

coordinate directions; E12 is the off-diagonal (coupling) component of the dispersion tensor.

U(NNODES), V(NNODES): arrays containing the x and y velocity components at the nodes.

NNODES: an integer parameter specifying the number of nodes at which the dispersion coefficients are to be evaluated.

MAT: an integer specifying the matrix material number as set on the material data card.

When the volumetric heating parameter, S, on the material data card is set equal to VARIABLE, SAGUARO expects SUBROUTINE SOURCE to be supplied by the user. This subroutine must have the following form:

```
SUBROUTINE SOURCE (QVALUE, P, T, X, Y, NNODES, MAT,
NELEM, TIME)
DIMENSIONS Q VALUE(1), P(1), T(1), X(1), Y(1)

.
.
.

FORTRAN coding to evaluate the volumetric heat source
for each material with a variable heat source

.
.
.

RETURN

END
```

where the variables in the subroutine parameter list are:

QVALUE: the value of the volumetric heating rate.

TIME: the current value of the time.

P(NNODES), T(NNODES), X(NNODES), Y(NNODES): arrays containing the values of the effective pressure, temperature, and spatial coordinates at the nodes.

MAT: an integer specifying the material number as set on the material data card.

NELEM: element number

NNODES: an integer parameter specifying the number of nodes at which the material property is to be evaluated.

The use of a generalized radiation/convection boundary condition requires that the variation of the heat transfer coefficient with temperature and/or time be specified. When the "h" parameter on the SET data card is specified as VARIABLE, SAGUARO expects SUBROUTINE HTCOEF to be supplied by the user. The required subroutine has the following form.

```
SUBROUTINE HTCOEF (HT, TSURF, TREF, XSURF, YSURF, TIME,
NELEM, ISET)
.
.
.

FORTRAN coding to evaluate the heat transfer coefficient
for each set number

.
.
.

RETURN

END
```

where the variables in the subroutine parameter list are:

HT: the heat transfer coefficient.

TSURF: the local surface temperature of the material.

TREF: the reference temperature of the environment as specified on the set data card.

XSURF, YSURF: the x, y (or r,z) coordinates on the surface.

TIME: the current value of the time.

NELEM: an integer specifying the element number.

ISET: an integer specifying the "set no." as set on the BC and SET data cards.

Note that if more than one generalized radiation/convection boundary condition occurs in a problem, SUBROUTINE HTCOEF is used for the evaluation of all heat transfer coefficients that vary with time and/or temperature. The set no. (ISET) parameter is used to distinguish the different boundary conditions.

When the boundary condition options PVARY, UVARY, TVARY, and/or QVARY are employed, SAGUARO expects the appropriate time history subroutines to be supplied by the user. The correspondence between a particular boundary condition and its variation with time is established through the "time curve no." which appears on the BC data card and in the name of the subroutine providing the time history. The required subroutines have the following form:

```
SUBROUTINE CURVEn (NELEM, PSURF, TSURF, TIME, BCVALUE)
.
.
.
```

```
      FORTRAN coding to evaluate a boundary condition for
      a specified time history
      .
      .
      .

      RETURN

      END
```

where the variables are:

n: an integer specifying the "time curve no." as set on the BC data card ($1 \leq n \leq 6$).

NELEM: an integer specifying the element number.

PSURF, TSURF: effective pressure and temperature of element.

TIME: the current value of the time.

SETVALUE: the value of the boundary condition for the current TIME.

The subroutines described above, when required by SAGUARO should follow the main overlay in the loading sequence. The control cards necessary to implement user supplied subroutines are described in a subsequent section.

Initial Conditions

The analysis of transient flow problems require the specification of initial conditions for the dependent variables. For cases where the fluid is initially quiescent and the temperatures may be assumed uniform (or at least constant over each material), the initial conditions may be set through a parameter on the material data cards. For problems where the initial velocity, pressure, and temperature fields are more complex, SAGUARO accepts initial conditions from an external storage device (disc or magnetic tape file) denoted TAPE 19.

In order to be compatible with SAGUARO, the initial conditions must be written to unit 19 with the following unformatted FORTRAN write statement:

```
WRITE (19) TIME, TMAX, TMIN, PMAX, PMIN, NUMEL,
     ((US (J, I), I = 1, 32), J = 1, NUMEL),
          (AMOIST (J), J = 1, NUMEL)
```

where,

TIME: is the initial time.

TMAX, TMIN: are the maximum and minimum pressures in the field.

NUMEL: is the number of elements in the mesh (the present version of SAGUARO requires NUMEL < 500 and the Cray version requires NUMEL < 1000).

US (J, I): is the two-dimensional array containing the dependent variables (P, T, U, V, θ). The J index

indicates the element number; the I index indicates the degree of freedom number (see page 109).

AMOIST(J): array containing average moisture of element J. (0 < AMOIST ≤ porosity)

Note that the I index has an upper limit of 32 which corresponds to the number of degrees of freegom in a quadrilateral element. If triangular elements are present in the mesh, the I index must still run to 32; the extra locations in the US array are ignored by SAGUARO when a triangular element is encountered. The ordering of the element degrees of freedom is given in Appendix B.

When the file containing the initial conditions is attached to the job, the file name must be TAPE 19. It should be noted that the output format for SAGUARO is the same as described above; the output file for SAGUARO is also TAPE 19. Thus, solutions obtained from SAGUARO may be used directly as initial conditions for subsequent problems. The use of these features is demonstrated in the next chapter.

Error Messages

SAGUARO has been supplied with a number of error checks and tests for bad or inconsistent input data, overflow of storage, etc. When an error is encountered, an error number and message is printed and the program is terminated with a STOP 1 if the error is fatal. The error messages embeded in SAGUARO, and corresponding explanations are listed below according to overlay.

(0,0) OVERLAY

DRIVER-UNRECOGNIZED COMMAND -- a command instruction was expected but was not found or was misspelled.

FFLD-END OF DATA -- an end of file was encountered on the input file, check termination command.

FFLDSB-INPUT VARIABLE TOO LONG -- an input variable with more than ten characters was encountered.

RESTART-UNRECOGNIZED COMMAND -- a restart command was used with an incomplete or misspelled parameter list.

PRINTER-UNRECOGNIZED COMMAND -- an output command was used with an incomplete or misspelled parameter list.

(1,0) OVERLAY

ELDATA-UNRECOGNIZED COMMAND -- erroneous element, boundary condition, or looping specification, check spelling.

ELDATA-LOOP PREVIOUSLY DEFINED -- error in looping specification, check for third loop within two existing loops.

ELDATA-MAXIMUM NUMBER OF ELEMENTS EXCEEDED -- reduce number of elements used or re-dimension code.

ELDATA-UNRECOGNIZED DATA ON SET CARD -- a set data card was used with an incomplete or misspelled parameter list.

ELDATA-BC APPLIED TO AN UNDEFINED ELEMENT -- a boundary condition was applied to an element that has not yet been defined.

ELDATA-EXCESSIVE BOUNDARY CONDITIONS ON ELEMENT -- too many boundary conditions (i.e., > 6) have been applied to an element.

ELDATA-UNRECOGNIZED BOUNDARY CONDITION -- boundary condition type is in error, check spelling.

ELDATA-BC ON IMPROPER SIDE OF ELEMENT -- a boundary condition was specified for an improper side of an element (1 < side < 4).

NMESH-IJ MAX OR MIN EXCEEDS SPECIFIED VALUE -- during generation of the grid points, a part was found with an imax, jmax, imin, or jmin that exceeded the specified maxi on the SETUP command.

MATREAD-TOO MANY MATERIALS SPECIFIED -- more than ten materials were specified.

(2,0) and (10,0) OVERLAY

FORMKFP-BAD ELEMENT JACOBIAN -- a negative element area was found, check element coordinates and connectivity.

TRI-ZERO JACOBIAN -- a triangular element with a zero area was found, check element coordinates.

QUAD-ZERO JACOBIAN -- a quadrilateral element with a zero area was found, check element coordinates.

(3,0) OVERLAY

UNZIPP-UNRECOGNIZED COMMAND -- a solution command was used with an incomplete or misspelled parameter list.

UNZIPP-MAXIMUM STORAGE EXCEEDED -- maximum active storage exceeded, reduce problem size or re-dimension code.

UNZIPP-COMMAND CARD MISSING -- another solution command was expected but not found, check for termination command.

UNZIPP-ZERO PIVOT -- zero on the diagonal of the equation being eliminated, equation system is singular or element connectivity is in error.

BCTIME-TIME CURVE NUMBER TOO LARGE -- a time curve number greater than six was encountered, check data cards and time history subroutine names.

PRESOLN-INSUFFICIENT STORAGE -- or
PREFRNT-INSUFFICIENT STORAGE -- insufficient storage for element connectivity, reduce problem size or re-dimension code.

PRESOLN-INSUFFICIENT STORAGE -- or
PREFRNT-INSUFFICIENT STORAGE FOR FRONT WIDTH -- reduce problem size or re-dimension code.

(4,0) OVERLAY

STREAM-INSUFFICIENT STORAGE -- maximum storage for the stream function field exceeded, reduce problem size or re-dimension code.

(6,0) OVERLAY

PLOTZ-UNRECOGNIZED COMMAND -- a plot command was used with an incomplete or misspelled parameter list.

CONTOUR-UNRECOGNIZED COMMAND -- error in contour specification, check spelling on contour type, looping command, and termination.

TIMEPLT-UNRECOGNIZED COMMAND -- error in history plot specification, check spelling and termination.

SPLOT-UNRECOGNIZED COMMAND -- error in profile plot specification, check spelling and termination.

SPLOT-TIMEPLANE DATA CARD NOT FOUND

Computer Requirements and Control Cards

SAGUARO is a large code (approximately 7500 source statements) that requires a relatively high threshold level of computer resources in order to operate successfully. SAGUARO is designed primarily for execution on the CDC 7600/CYBER 76 computer system and the CRAY 1S computer. The following discussion of computer request parameters and control cards is specifically directed toward the use of SAGUARO on the SLA computer system.

The central processor time needed to run SAGUARO is directly dependent on the number of elements in the mesh and to a lesser extent on the front width of the problem. To roughly estimate the CPU time required for a typical job for isothermal problems, the following formula may be used,

$$\text{CPU} = (\text{Number elements}) \times (0.03) + (\text{Number elements}) \times (\text{Number time steps}) \times (.02).$$

For non-isothermal problems, the number of time steps or iterations should reflect the fact that two equations are being solved. Note that the constants in the above formula are accurate for problems of moderate size, but could increase by a factor of two for very large analyses. Also, the above estimate of CPU time does not include the time for post-processing the solution, i.e., computing heat fluxes, plotting, etc.

The amount of Large Core Memory (LCM) needed for a SAGUARO run is also directly related to the number of elements in the mesh and the problem front width. Unfortunately, the LCM required cannot be estimated a priori. The experience of the user is, thus, the best guide for setting this parameter. After completion of a solution, SAGUARO reports the total LCM required for the job allowing the user to adjust the requested value for future runs. No LCM request is needed for SAGUARO (CRAY version).

The SAGUARO program is maintained in an UPDATE form in the Sandia National Laboratories permanent file (PF) system and may be accessed by attaching the file with the following control card:

```
PFGET, OLDPL, SAGUARO, AU = RREATON.   (CDC version)
```

and

```
FILE, OLDPL, RT = 2.
PFGET, OLDPL, CSAG, AU = RREATON.   (CRAY version)
```

Before executing, the file attached with the above control card must be run through the UPDATE processor and then compiled. In the following sections, control card decks are listed for using SAGUARO in its standard modes of operation.

Run With Plotting:

The control card deck in Figure 6A allows the user to run SAGUARO and plot results using the RSCORS software package. The graphical output is post-processed and returned through a

Versatec plotter at the appropriate Remote Job Entry Terminal (RJET). Other options for processing and disposing of plotted output are given in References 8 and 9. To access the CRAY version of SAGUARO the control stream in Figure 6b should be executed.

Run With Restart:

Figure 7a shows a control card deck to run SAGUARO (CDC) and save the solution for later restarting. In this case, the solution and element data were saved on magnetic tapes; permanent file storage could also have been used. The listing in Figure 7 is also suitable for restarting a job if the STAGE commands are modified to cause files TAPE 13 and TAPE 19 to be PRE staged. The control cards needed to run SAGUARO (Cray) with restarting are shown in Figure 7b.

Run With Conditions:

The control cards shown in Figure 7a are also suitable for running a transient analysis with initial conditions provided from an external source. If the initial conditions are written on TAPE 19 (in the format discussed previously), then the listing in Figure 7a is immediately applicable if the request for TAPE 13 is deleted. The control stream for the Cray version of this procedure is shown in Figure 7b.

Run With User Subroutines:

The control cards required to execute SAGUARO (CDC) when user supplied subroutines are to be included are shown in

Figure 8a; the equivalent SAGUARO (CRAY) control stream is shown in Figure 8b.

In Figures 6b, 7b and 8b, the execution of SAGUARO (CRAY) is carried out through a set of procedure files (SLTLIB[10]). The use of these procedures simplifies the access to SAGUARO on the Cray though, in fact, the basic Cray Job Control Language can also be used to run the program.

```
SAGUARO, TXXXX, ECYYY.                          NAME    BOX NO.
USER .....
PFGET, FLNAME, SAGUARO, AU=RREATON.
UPDATE, P=FLNAME, N, F.
FTN, I=COMPILE, L=0.
PFGET, RSCOR76, AU=SLTHOMP.    *
PFGET, RSCDI76, AU=SLTHOMP.    *
LIBRARY, RSCOR76, RSCDI76.     *
RFL, L=YYY.
LGO, PL=777777B.
PFGET, POP76, AU=SLTHOMP.      *
POP76, TAPE10, POPOUT, HC1.    *
COMQ, POPOUT, HC1.             *
7-8-9
7-8-9
SAGUARO DATA
6-7-8-9
```

NOTES:

(1) For large jobs producing large quantities of output, consideration should be given to using a FICHE, OUTPUT command to divert the printed output to microfiche.

(2) Graphical output may also be generated via the SCORS soft ware system by appropriate substitution for the lines marked by * (see Reference 10). The above control statements assume plots will be generated on a Versatec hard-copy plotter; other options are available (see Reference 9).

Figure 6a. Control Card Deck (CDC) -- Run With Plotting

```
SAGUARO, TXXXX, STSCZ.                          NAME      BOX NO.
USER .....
SLTLIB.
UID.       NAME       BOX NO.
CUPDATE, P=CSAG, UN=RREATON, F.
CFT, I=COMPILE, L=0.
RSCORLB.                          *
ASSIGN, DN=POPIN, A=FT10.         *
LDR, LIB=RSCORS.                  *
POP, POPIN, POPOUT, HC1.          *
XCOMQ, POPOUT, HC1, CS=R7.        *
7-8-9
7-8-9
SAGUARO DATA
6-7-8-9
```

NOTES:

(1) For large jobs producing large quantities of output, consideration should be given to using a XFICHE, $OUT command to divert the printed output to microfiche.

Figure 6b. Control Card Deck (CRAY) -- Run With Plotting

```
SAGUARO, TXXXX, ECYYY.                          NAME      BOX NO.
USER .....
PFGET, FLNAME, SAGUARO, AU=RREATON.
UPDATE, P=FLNAME, N, F.
FTN, I=COMPILE, L=0.
LABEL, TAPE13, W, L=$$.
LABEL, TAPE19, W, L=$$.
STAGE, TAPE13, VSN=AAAAAA, HY, POST.
STAGE, TAPE19, VSN=BBBBBB, HY, POST.
REWIND, TAPE13, TAPE19.
RFL, L=YYY.
LGO, PL=777777B.
7-8-9
7-8-9
SAGUARO DATA
6-7-8-9
```

NOTES:

(1) The above listing uses (skeleton labeled) magnetic tapes to store the element data and solution fields. The permanent file system could also be used to save the data by replacing the STAGE and LABEL commands with the appropriate PFSAVE commands. Note that PFSAVE commands should follow the LGO card.

(2) The above listing is suitable for restarting a SAGUARO run from tape. When restarting, the POST parameter on both STAGE commands should be changed to PRE. When restarting from permanent file storage, the PFSAVE commands should be replaced by an appropriate set of PFGETE commands.

(3) The inclusion of plotting in the above run is accomplished through the addition of the appropriate commands from the control stream shown in Figure 6a (i.e., those with an *).

Figure 7a. Control Card Deck (CDC) -- Run to Create a Restart Tape

```
SAGUARO, TXXXX, STSCZ.                          NAME      BOX NO.
USER .....
SLTLIB.
UID.       NAME       BOX NO.
CUPDATE, P=CSAG, UN=RREATON, F.
CFT, I=COMPILE,L=0.
LDR.
XTAPEOT, FT13, L=($$), VSN=AAAAAA.
XTAPEOT, FT19, L=($$), VSN=BBBBBB.
7-8-9
7-8-9
SAGUARO DATA
6-7-8-9
```

NOTES:

(1) The above listing uses (skeleton labeled) magnetic tapes to store the element data and solution fields. The permanent file system could also be used to save the data by replacing the XTAPEOT commands with the appropriate XPFSAVE commands.

(2) The above listing is suitable for restarting a SAGUARO run from tape. When restarting, the XTAPEOT commands precede the LDR command. When restarting from permanent file storage, the XPFSAVE commands are replaced by XPFGET commands.

(3) The inclusion of plotting in the above run is accomplished through the addition of the appropriate commands from the control stream shown in Figure 6b (i.e., those with an *).

Figure 7b. Control Card Deck (CRAY) -- Run to Create a Restart Tape

```
SAGUARO, TXXXX, ECYYY.                          NAME      BOX NO.
USER .....
PFGET, FLNAME, SAGUARO, AU=RREATON.
UPDATE, P=FLNAME, N, F.
FTN, I=COMPILE, L=0.
RFL, L=YYY.
LGO, PL=777777B.
7-8-9
IDENT, USERSUB                  *
DELETE, USER.2, USER.58         *
FORTRAN CODED USER SUBROUTINES
7-8-9
SAGUARO DATA
6-7-8-9
```

NOTES:

(1) The inclusion of plotting in the above run is accomplished through the addition of the appropriate commands from the control stream shown in Figure 6a (i.e., those with an *).

Figure 8a. Control Card Deck (CDC) -- Run With User Subroutines

```
SAGUARO, TXXXX, STSCZ.                          NAME      BOX NO.
USER .....
SLTLIB.
UID.       NAME       BOX NO.
CUPDATE, P=CSAG, UN=RREATON, F.
CFT, I=COMPILE, L=0.
LDR.
7-8-9
IDENT, USERSUB                    *
DELETE, USER.2, USER.58           *
      FORTRAN CODED USER SUBROUTINES
7-8-9
SAGUARO DATA
6-7-8-9
```

NOTES:

(1) The inclusion of plotting in the above run is accomplished through the addition of the appropriate commands from the control stream shown in Figure 6b (i.e., those with an *).

Figure 8b. Control Card Deck (CRAY) -- Run With User Subroutines

A NOTE TO EXPERIENCED MARIAH USERS

The following discussion should be helpful to potential SAGUARO code users who have already "mastered" the operating features of MARIAH. SAGUARO is set up to accept data decks for transient problems which have been designed for MARIAH. When the UNSAT material input data cards or user subroutines, page 15, are not supplied, the following default values are used (see Equation (10))

$$D_{11} = D_{22} = \theta_D = C = \lambda_{air} = 0$$

$$\text{and SAT} = 1.0 \quad .$$

Thus, the general equation for unsaturated flow (Equation (10)) reduces to Equation (11). Consequently, under these conditions, the equations solved in SAGUARO and MARIAH are identical.

If the material card for a specific material sets temperature dependence to VARIABLE, then D_{ij}, C, λ_{air} and SAT in addition to λ_{ij} and k_{ij} must be defined through five user subroutines and the UNSAT card for that material may be omitted. This would be the most realistic mode for partially saturated flow analysis where the coefficients in Equation (11) would be highly nonlinear.

SAMPLE CALCULATION

A sample problem has been included in this section to demonstrate the use of the previously described command cards and some of the capabilities of the SAGUARO code. Though this example illustrates many of the salient features of the code, all possible combinations of capabilities could not be covered. Further understanding of code usage can be obtained from the examples given in the MARIAH manual.[4]

The sample problem involves the one-dimensional infiltration of rain and heat into hard rock consisting of several strata which is partially saturated at time zero, see Figure 9.

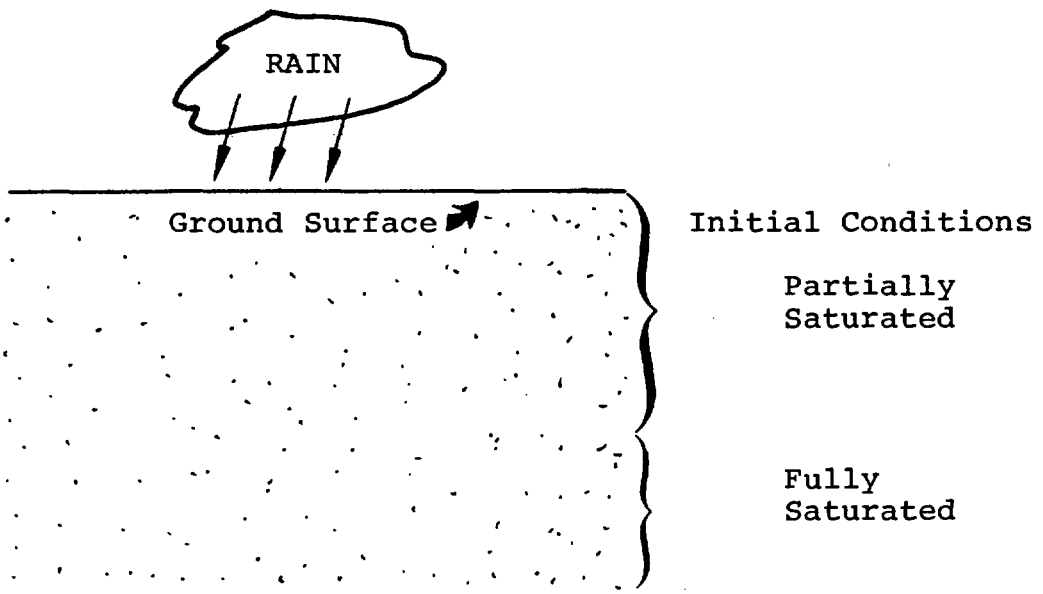


FIGURE 9. Geometry Used in Sample Infiltration Problem

In order to keep the sample calculations as simple as possible, the wetting portion of the characteristic curves similar to those shown in Figure 1 were used for a typical hard rock, Figure 10. These non-dimensional curves are used for all strata. The dimensional value of permeability and moisture content are obtained by multiplying the non-dimensional values by these respective saturated values given in Table 1.

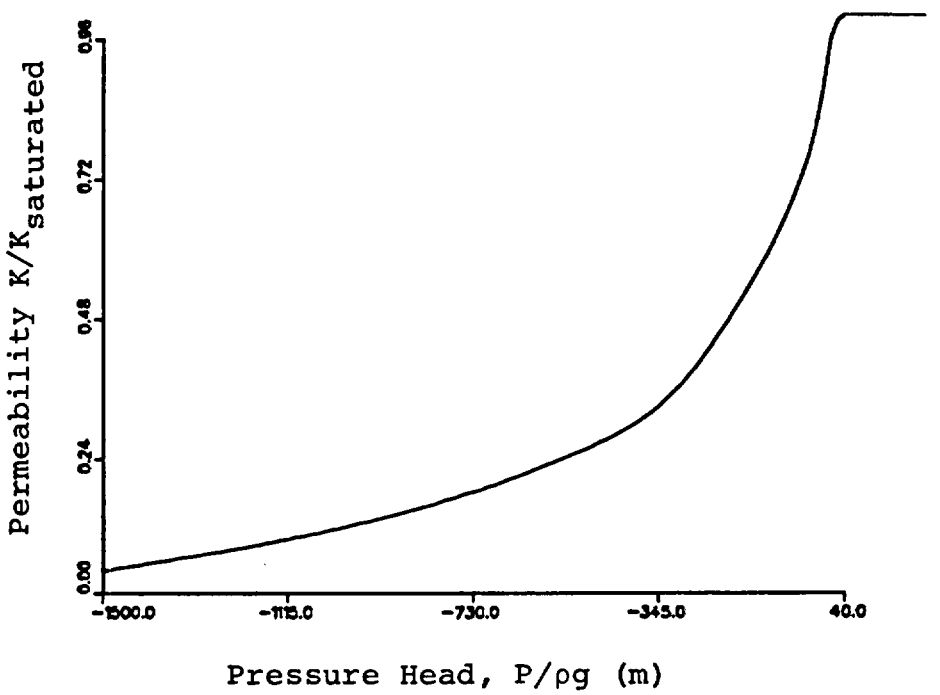


FIGURE 10a. Rock Permeability

Figure 10. Simplified Characteristics Curves for Sample Problem

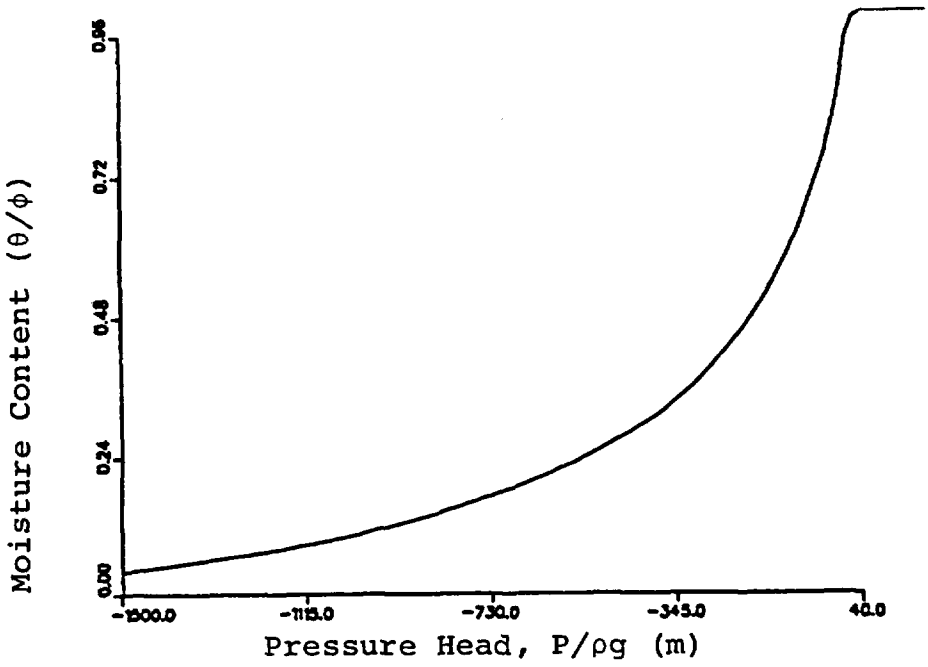


FIGURE 10b. Moisture Content

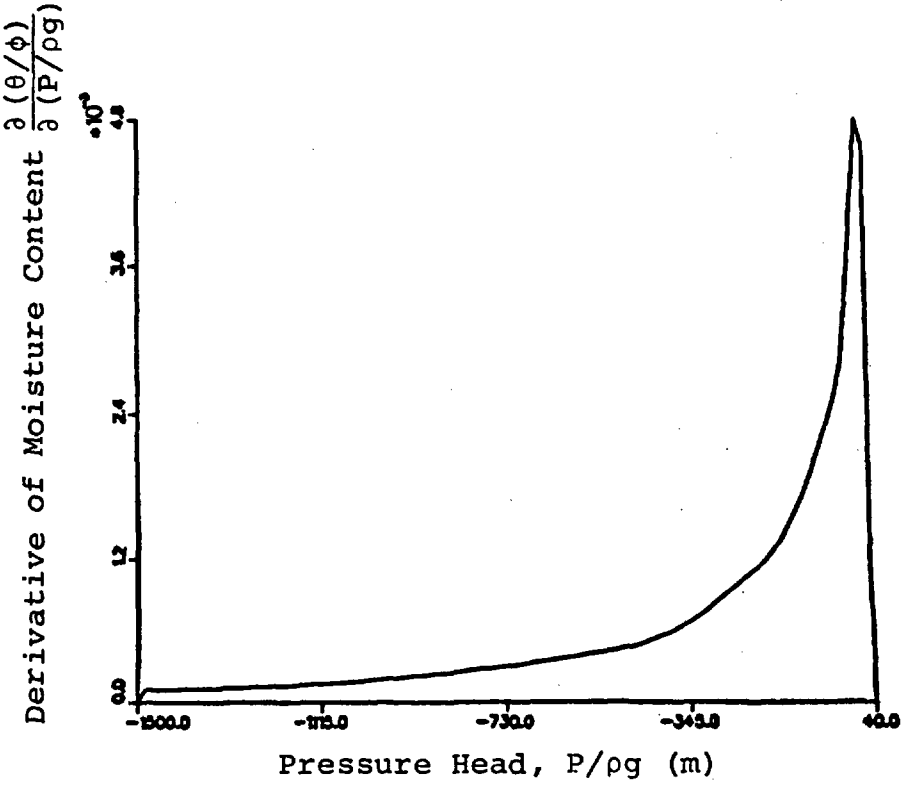


FIGURE 10c. Derivative of Moisture Content with Respect to Pressure Head.

TABLE 1

MATERIAL PROPERTIES

Strata (See Fig. 19)	Material No. (Fig. 13)	Saturation Permeability $k(m^2)$	Porosity ϕ	Rock Density (kg/m^3)
1 (bottom)	2	8×10^{-16}	.32	1700
2	3	8×10^{-15}	.10	2300
3	4	8×10^{-16}	.32	1700
4	2	1.6×10^{-14}	.23	1960
5	5	1.6×10^{-16}	.24	1840
6	7	8×10^{-15}	.24	1880
7	6	6.4×10^{-14}	.20	2140
8 (top)	7	1.6×10^{-16}	.24	1840

The boundary conditions for the test case are:

1. Rain is such that it feeds the soil at a rate of 1.0 m/yr.
2. Linear initial pressure head (ϕ) t = 0 (fluid velocity is zero everywhere).
3. No flow through bottom boundary.

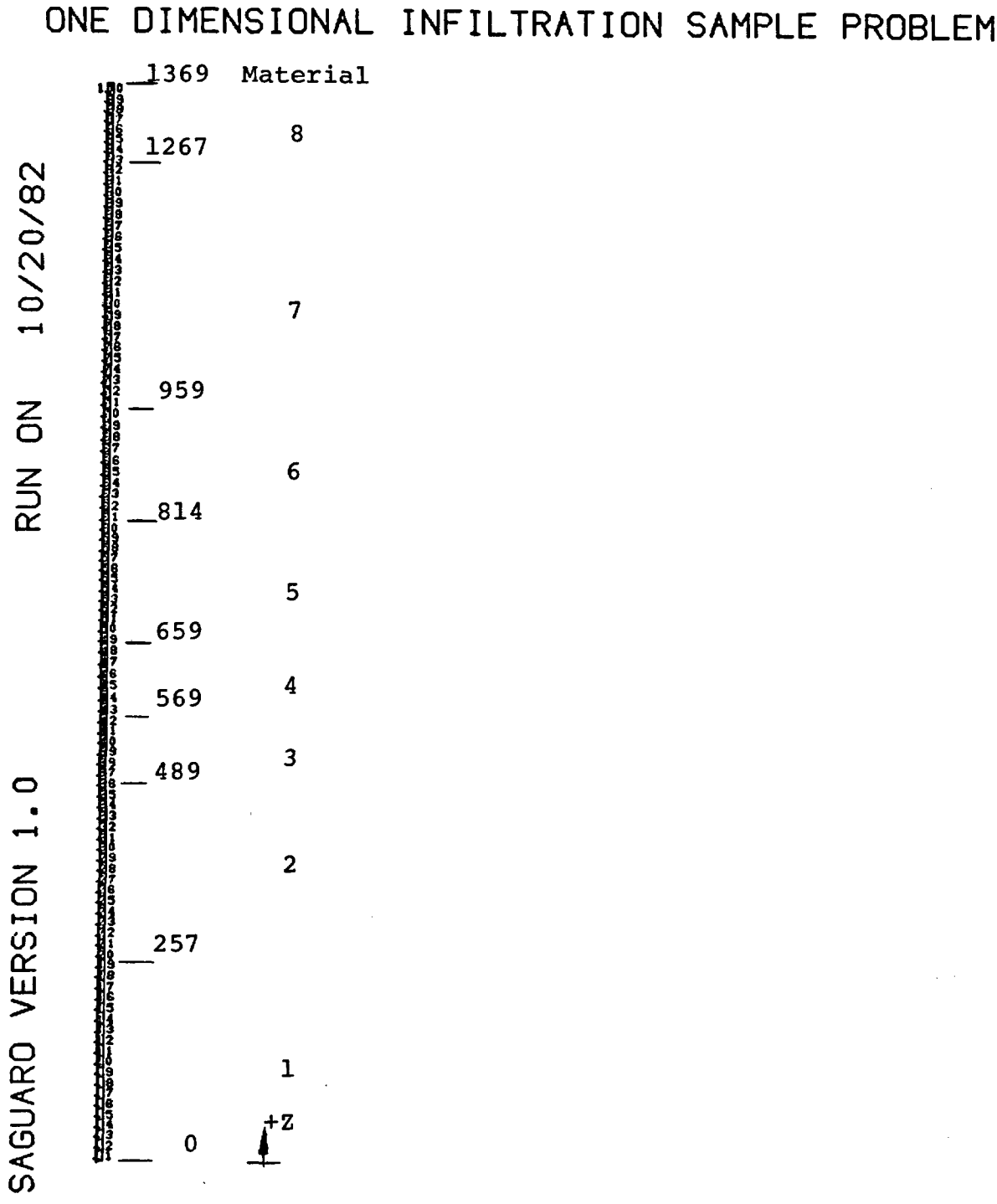


FIGURE 11. Finite Element Grid for Sample Infiltration Problem

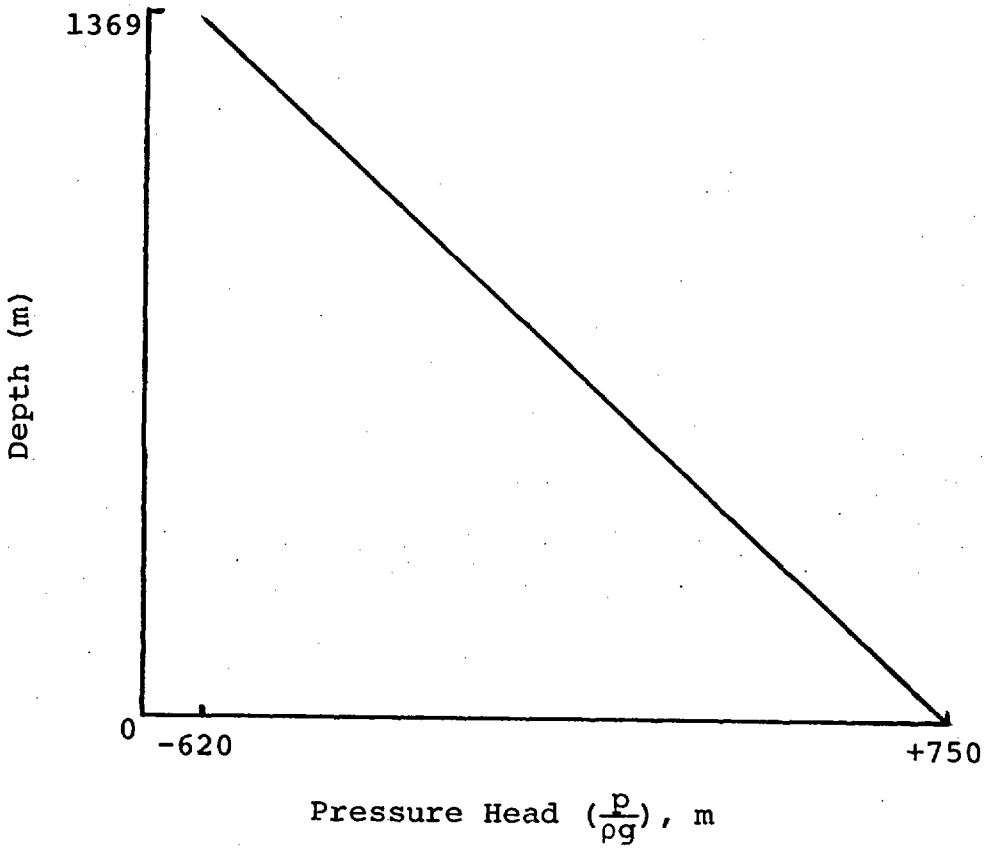


FIGURE 12: Initial Pressure Head

The computational mesh for this problem consisted of one-hundred elements, Figure 11, and the initial pressure distribution is shown in Figure 12. A listing of the input data and control cards is given in Figure 13. The units chosen for this problem are kg, m and seconds. The required users subroutines are listed in Figure 14. Figure 15 shows the output that can be expected from the input described above.

```
$ ONE DIMENSIONAL INFILTRATION SAMPLE PROBLEM
SETUP  ,  1  , 3  ,     ,  PLOT
WATER , 1 , 994.  ,7.8E-04 , 4190.  , 0.60, 0.0   , +9.8 , , 35.
STARTA1,2,1840.,1600.,2.5,,,.24,1.6E-16,,,,VARIABLE,,35.,7.301E6
STRATA2,3,2140.,1600.,2.5,,,.20,6.4E-14,,,,VARIABLE,,35.,7.301E6
STARTA3,4,1880.,1600.,2.5,,,.24,8.0E-15,,,,VARIABLE,,35.,7.301E6
STRATA5,5,1960.,1600.,2.5,,,.23,1.6E-14,,,,VARIABLE,,35.,7.301E6
STRATA6,6,2300.,1600.,2.5,,,.10,8.0E-15,,,,VARIABLE,,35.,7.301E6
TOP  ,7,1700.,1600.,2.5,,,.32,8.0E-16,,,,VARIABLE,,35.,7.301E6
END
1,1,3,39                    $ REG 1
0,10,10,0
0,0,257,257
1,39,3,73                   $ REG 2
0,10,10,0
257,257,489,489
1,73,3,85                   $ REG 3
0,10,10,0
489,489,569,569
1,85,3,97                   $ REG 4
0,10,10,0
569,569,659,659
1,97,3,121                  $ REG 5
0,10,10,0
659,659,814,814
1,121,3,141                 $ REG 6
0,10,10,0
814,814,959,959
1,141,3,185                 $ REG 7
0,10,10,0
959,959,1267,1267
1,185,3,201                 $ REG 8
0,10,10,0
1267,1267,1369,1369
END
JLOOP,19,2                  $ REG 1
QUAD8/4,2,1,1
JEND
JLOOP,17,2                  $ REG 2
QUAD8/4,3,1,39
JEND
JLOOP,6,2                   $ REG 3
QUAD8/4,4,1,73
JEND
```

FIGURE 13a. Input Data

Figure 13. Code Requirements for Sample Problem

```
JLOOP,6,2                    $ REG 4
QUAD8/4,2,1,85
JEND
JLOOP,12,2                 $ REG5
QUAD8/4,5,1,97
JEND
JLOOP,10,2                   $ REG 6
QUAD8/4,7,1,121
JEND
JLOOP,22,2                   $ REG 7
QUAD8/4,6,1,141
JEND
JLOOP,8,2,                    $ REG 8
QUAD8/4,7,1,185
JEND
BC,UVARY,1,199,3,1                  $BOUNDARY FLUX DEFINED IN SUB
BC,TSIDE,1,199,3,85.0               $BOUNDARY TEMPERATURE
END
PLOT,ELEMENTS, 0.0 , 0.0 , 10.0 , 1369.0,,,,,,,NUMBER
FORMKF ,, FORCED
OUTPUT,SINGLE,1,1,82,1,100,2
UNZIPP , TRANS , 10   , 0.0 , 3.15E8,3.15E7,10
END
PLOT ,HISTORY
PLOCATION,6,1,11,1,1,42,7,60,7,81,7,92,7,100,7
END
PLOT  , PROFILE
TIMEPLANE ,6 , 1 , 3 , 5 , 7 , 9 , 11
PLOCATION , NODES,20,1,5,20,5,30,5,40,5,50,5,60,5,70,5*
 80,5,86,7,88,7,90,7,92,7,93,7,94,7,95,7,96,7,97,7,98,7,99,7,100,7
END
PLOT ,HISTORY
VLOCATION,7,1,11*
37,1 , 42,1 , 48,1 , 60,1 , 82,1 , 92,1 , 100,3
END
PLOT  , PROFILE
TIMEPLANE ,6 , 1 , 3 , 5 , 7 , 9 , 11
VLOCATION , NODES,20,1,1,10,1,20,1,30,1,40,1,50,1,60,1,70,1*
 80,1,86,3,88,3,90,3,92,3,93,3,94,3,95,3,96,3,97,3,98,3,99,3,100,3
END
PLOT ,HISTORY
TLOCATION,7,1,10,90,7,92,7,94,7,96,7,98,7,99,7,100,7
END
PLOT  , PROFILE
TIMEPLANE , 6 , 1 , 3,5,7,9,11
TLOCATION , NODES,20,1,5,20,7,30,7,40,7,50,7,60,7,70,7*
 80,5,86,7,88,7,90,7,92,7,93,7,94,7,95,7,96,7,97,7,98,7,99,7,100,7
END
STOP
```

Figure 13a. continued

```
SYUCONE,T70,EC350.
USER(RREATON,    )
CHARGE,1286424)
PFGET,OLDPL,SAGUARO.
UPDATE,F.
FTN,I=COMPILE,L=0,PMD.
REWIND,TAPE12,TAPE19.
RFL,L=350.
MAP,PART.
PFGET,VTSCORS,AU=PLOTLIB.
ATTACH,FXMATH,AU=MATHLIB.
LIBRARY,FXMATH,VTSCORS.
LDSET(PRESET=NGINF)
LGO.
PFREPL,TAPE12,YODM,CT=PU.
PFREPL,TAPE19,PTOM,CT=PU.
REWIND,TAPE10.
LIBRARY,COMLIB.
COMQ,TAPE10,HC1.
REWIND,OUTPUT.
COPY,OUTPUT,DUMMY.
FICHE,DUMMY.
```

Figure 13b. CDC 7600 Control Cards

```
CSAG,T60,STSCZ.

USER(RREATON,(NOS PASWORD))
SLTLIB.
UID.     RR EATON BOX 1134
CUPDATE,P=CSAG2,UN=RREATON,F.
CFT(I=COMPILE,ON=Z,L=0)
RSCORLB.
ASSIGN,DN=POPIN,A=FT10.
ACCESS,DN=FXMATH,ID=MATHCRA.
LDR,LIB=RSCORS:FXMATH.
POP,POPIN,POPOUT,HC1.
XCOMQ,POPOUT,HC1,CS=R7.
REWIND,DN=$OUT.
COPYD,I=$OUT,O=FOUT.
XFICHE,FOUT,T='SAGUARO'.
EXIT.
DUMPJOB.
DEBUG.
REWIND,DN=$OUT.
COPYD,I=$OUT,O=FOUT.
XFICHE,FOUT,T='SAGUARO'.
```

Figure 13c. CRAY Control Cards with Updating Done on CDC 6600

```
      SUBROUTINE FLUIDC(CM,ATHR,PHI,T,X,Y,KUREL,MAT,NELEM,TIME,PROP)
C
C     THIS SUB CALC THE MOISTURE CONTENT AND DER OF MOISTURE CONTENT WRT PH(1/M)
C     UNITS - KG,M,SEC.
C
      DIMENSION CM(8),TH(8),PHI(8),PH(8),T(8),X(1),Y(1),PROP(17,7)
      DIMENSION PHD(20),WDAT(20),YP(20),YPP(20),W(60),YPI(1),YPPI(1)
      DATA RHOG/9.714E3/
      DATA(PHD(I),I=1,15)/-1500.0,-500.,-270.,-200.,-90.,-50.
     1,-40.,-30.,-20.,-10.,0.0,10.,20.,30.,40./
      DATA(WDAT(I),I=1,15)/0.04,0.256,0.398,0.470,0.635
     1,.725,.751,.78,.815,.855,.905,.961,.985,.997,1./
      DATA IFIRST/1/,W(1)/-1./ , EPS/-1./
      IMAX=15
      IF(IFIRST.EQ.1)
     1 CALL SPLIFT(PHD,WDAT,YP,YPP,IMAX,W,IERR,0,0,0,0,0)
      IFIRST=2
      DO 20 J=1,KUREL
      PH(J)=PHI(J)/RHOG - Y(J)
      IF(PH(J).GE.PHD(IMAX)) TH(J)=WDAT(IMAX)
      IF(PH(J).GE.PHD(IMAX)) CM(J)=0.0
      IF(PH(J).GE.PHD(1) .AND. PH(J) .LT. PHD(IMAX))
     1 CALL SPLINT(PHD,WDAT,YPP,IMAX,PH(J),TH(J),CM(J),YPPI,1,KERR)
      IF(PH(J) .LE. PHD(1)) TH(J)=WDAT(1)
      IF(PH(J) .LE. PHD(1)) CM(J)=0.0
      CM(J) = CM(J)*PROP(6,MAT)
   20 CONTINUE
      ATHR=-.25*(TH(1)+TH(2)+TH(3)+TH(4))
     1 +0.5*(TH(5)+TH(6)+TH(7)+TH(8))
C  GIVES THETA/THETA MAX
      RETURN
      END
```

Figure 14a. Moisture Content and Derivative of Moisture Content

```
      SUBROUTINE DIF(DIF1,DIF2,P,T,X,Y,NHALF,MAT,NELEM,TIME,PROP)
C
C  DIFUSION COEFICIENT FOR MASS TRANSPORT
C
      DIMENSION DIF1(4),DIF2(4),P(8),PH(8),T(8),X(8),Y(8)
      DIMENSION PROP(17,7)
      DO 10 J=1,NHALF
      DIF2(J)=1.E-8
      DIF1(J)=1.E-8
   10 CONTINUE
      RETURN
      END
```

Figure 14b.) Coefficient for Mass Transport (D_{11} and D_{22})

Figure 14. User Subroutines for the One-Dimensional Infiltration Problem

```
      SUBROUTINE PERM(COND1,COND2,PHI,T,U,V,X,Y,NHALF,MAT,NELEM,TIME
     1,PROP)
C
C     CALCULATES PERMEABILITY  (M**2)
C     UNITS - KG,M,SEC.
C
      DIMENSION COND1(1),COND2(1),PHI(8),PH(8),T(8),Y(1)
      DIMENSION PROP(17,7)
      DIMENSION PHD(20),HKD(20),YP(20),YPP(20),W(60),YPI(1),YPPI(1)
      DATA RHOG/9.714E3/
      DATA(PHD(I),I=1,15)/-1500.0,-500.,-270.,-200.,-90.,-50.
     1,-40.,-30.,-20.,-10.,0.0,10.,20.,30.,40./
      DATA(HKD(I),I=1,15)/0.04,0.256,0.398,0.470,0.635
     1,.725,.751,.78,.815,.855,.905,.961,.985,.997,1./
      DATA IFIRST/1/,W(1)/-1./ , EPS/-1./
      IMAX=15
      IF(IFIRST.EQ.1)
     1 CALL SPLIFT(PHD,HKD,YP,YPP,IMAX,W,IERR,0,0,0,0,0)
      IFIRST=2
      DO 20 J=1,NHALF
      PH(J)=PHI(J)/RHOG - Y(J)
      IF(PH(J).GE.PHD(IMAX)) COND1(J)=HKD(IMAX)
      IF(PH(J).GE.PHD(1) .AND.  PH(J) .LT.  PHD(IMAX))
     1 CALL SPLINT(PHD,HKD,YPP,IMAX,PH(J),COND1(J),YPI,YPPI,1,KERR)
      IF(PH(J) .LE.  PHD(1)) COND1(J)=HKD(1)
      COND1(J) = COND1(J)*PROP(7,MAT)
      COND2(J) = COND1(J)
   20 CONTINUE
      RETURN
      END
      SUBROUTINE SLAMBDA (SK1,SK2,T,X,Y,NNODES,MAT,NELEM,TIME)
      DIMENSION SK1(1) , SK2(1) , T(1)
      DO 10 I=1,NNODES
      SK2(I) = 10.0
      SK1(I) =  10.0
   10 CONTINUE
      RETURN
      END
      SUBROUTINE CURVE1 (NELEM,PSURF,TSURF,TIME,VALUE)
      VALUE=3.17E-8
      RETURN
      END
```

Figure 14c. Permeability

```
      SUBROUTINE SLAMBDA (SK1, SK2, T, X, Y, NNODES, MAT, NELEM, TIME)
      DIMENSION SK1(1) , SK2(1) , T(1)
      DO 10 I=1, NNODES
      SK2(I) = 10.0
      SK1(I) =  10.0
10    CONTINUE
      RETURN
      END
```

Figure 14d. Thermal Conductivity

```
      SUBROUTINE CURVE1 (NELEM, PSURF, TSURF, TIME, VALUE)
      VALUE=3.17E-8
      RETURN
      END
```

Figure 14e. Curve for Water Source

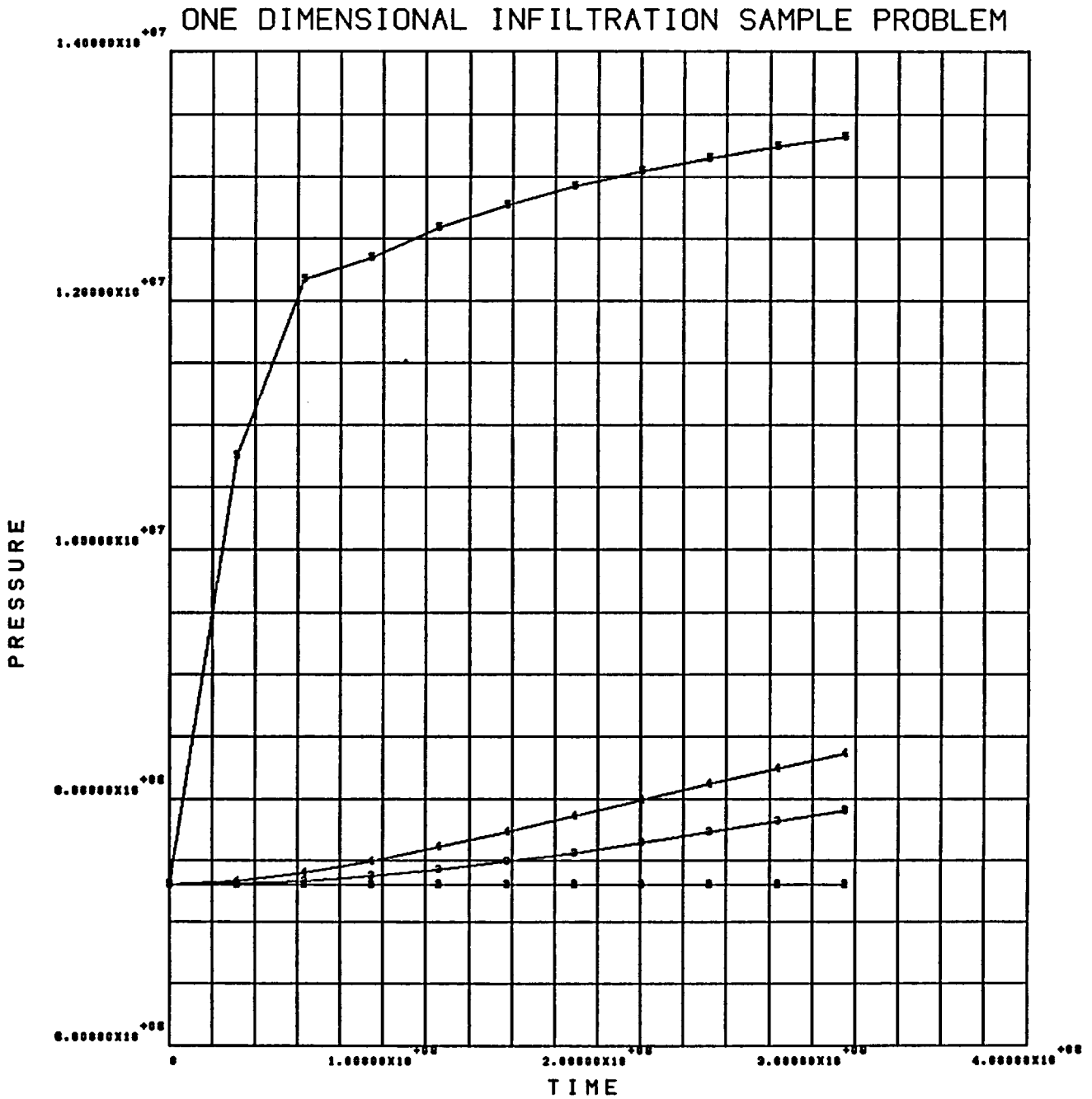


Figure 15a. Effective Pressure as a Function of Time for Z = 0, 569, 814, 1113, 1267, and 1369 m.

Figure 15. Graphics Output from Sample Infiltration Problem

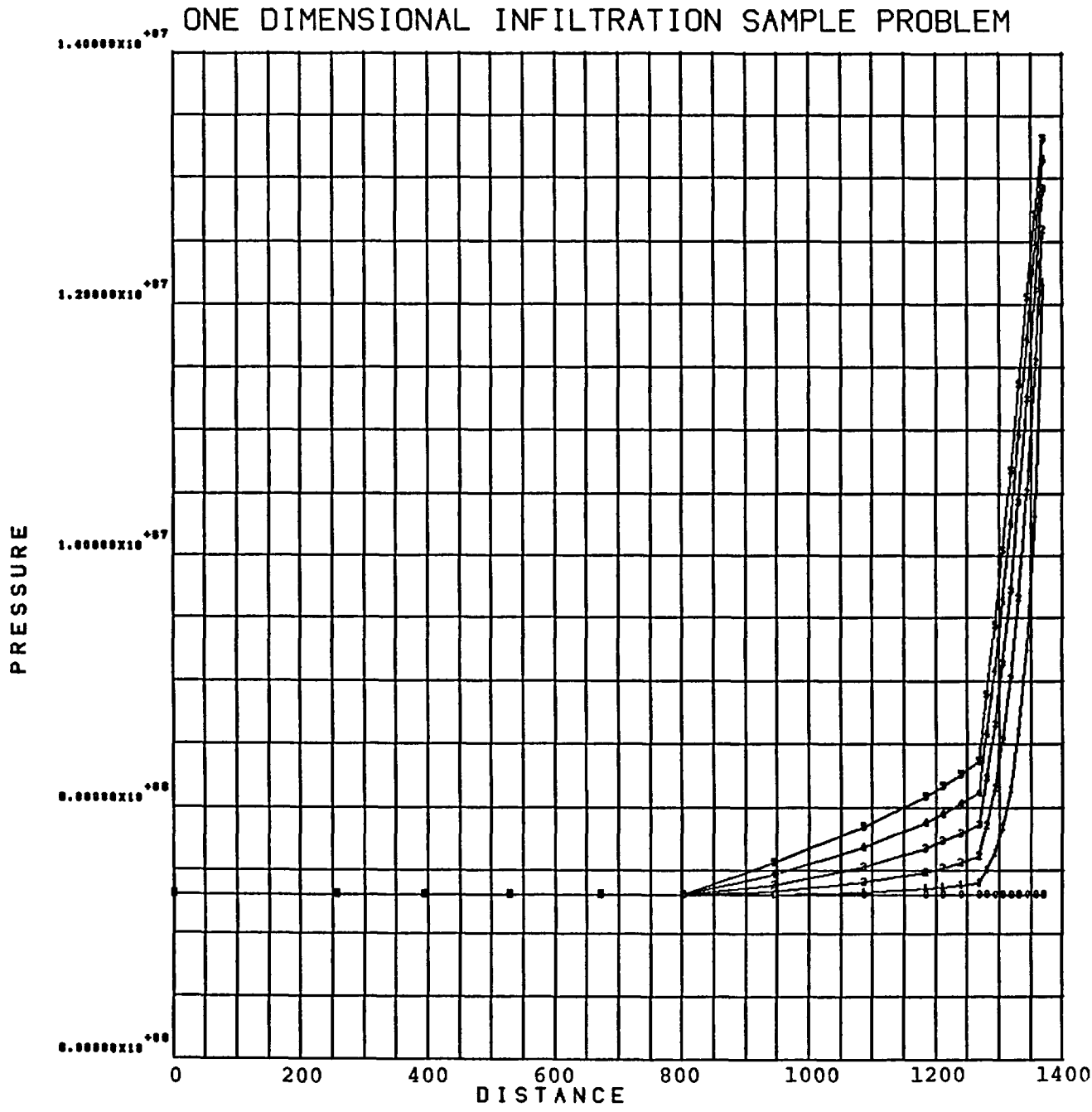


Figure 15b. Effective Pressure as a Function of Depth for Time = 0, 2, 4, 6, 8, and 10 yr.

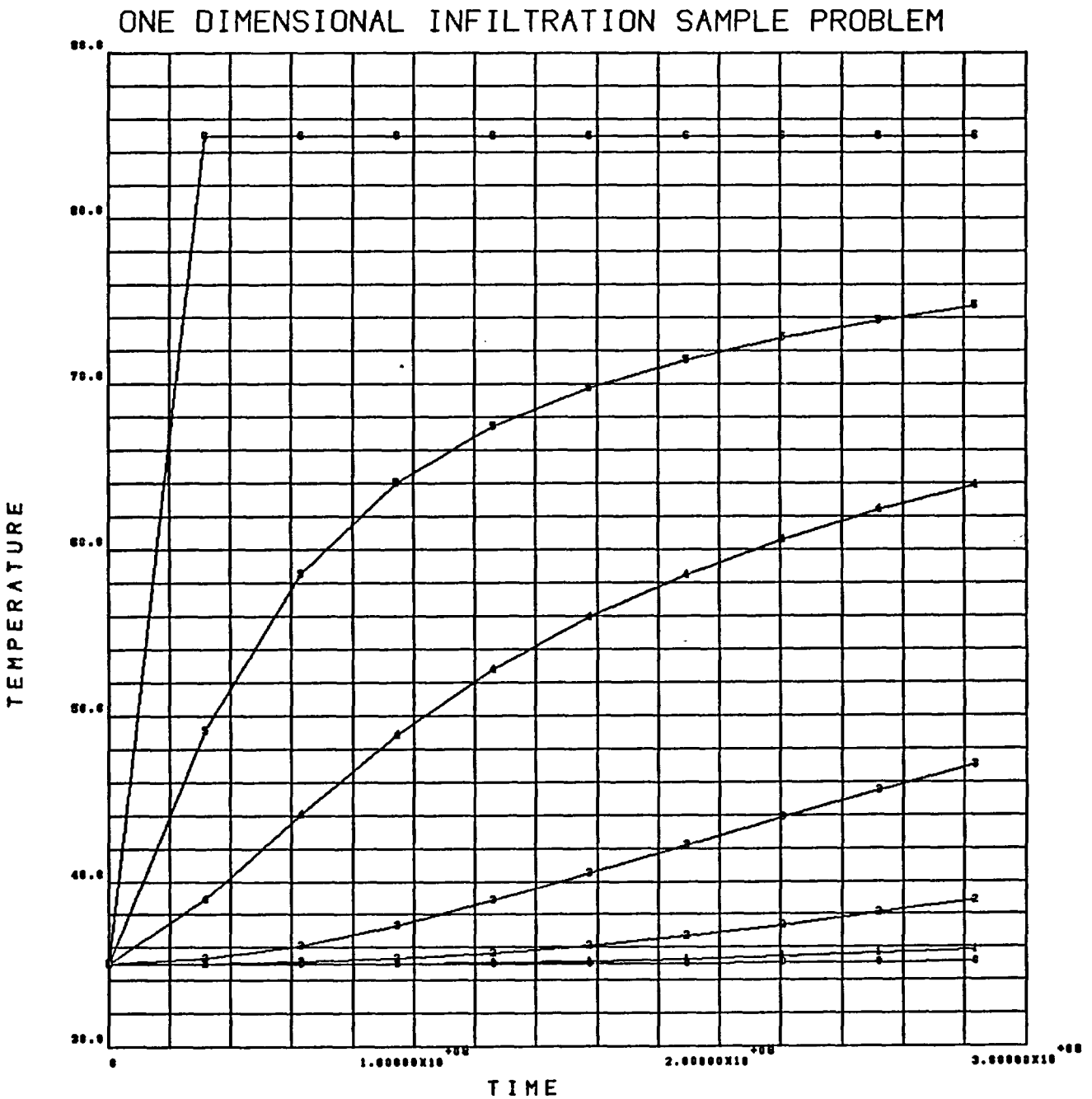


Figure 15c. Temperature as a Function of Time for Z = 0, 569, 814, 1113, 1267 and 1369 m.

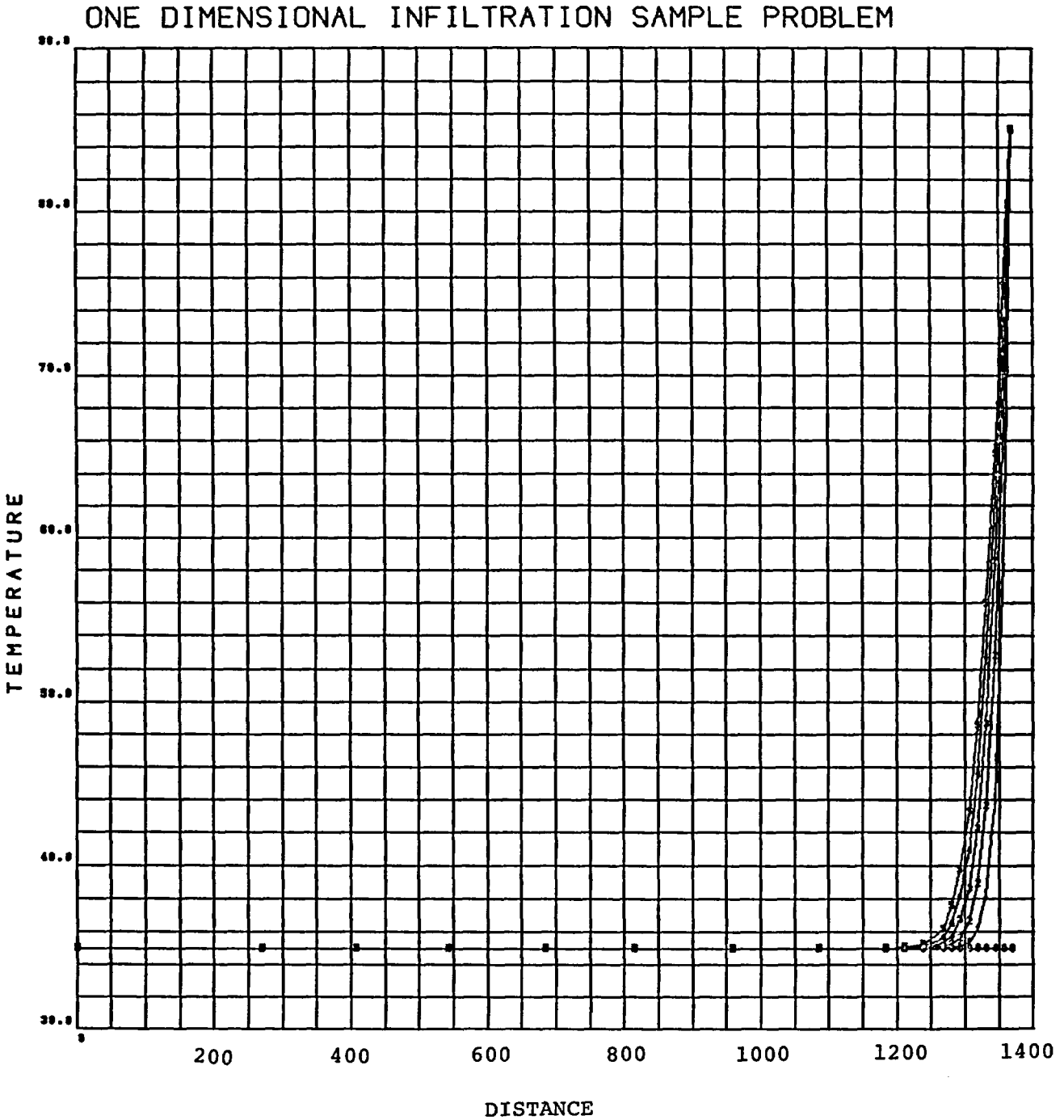


Figure 15d. Temperature as a Function of Depth at Time = 0, 2, 4, 6, 8, and 10 yr.

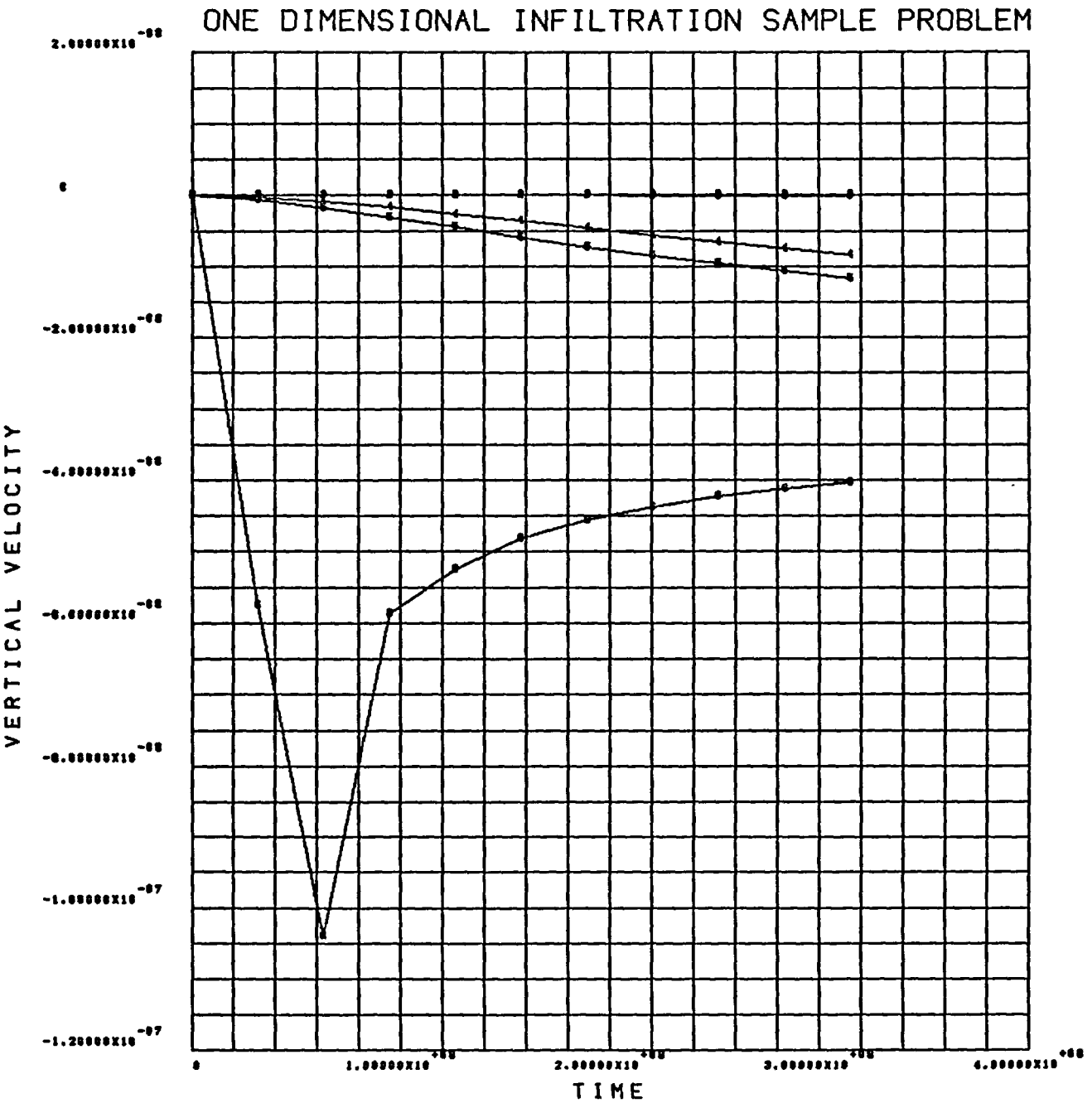


Figure 15e. Velocity as a Function of Time for Z = 0, 569, 814, 1113, 1267 and 1369 m.

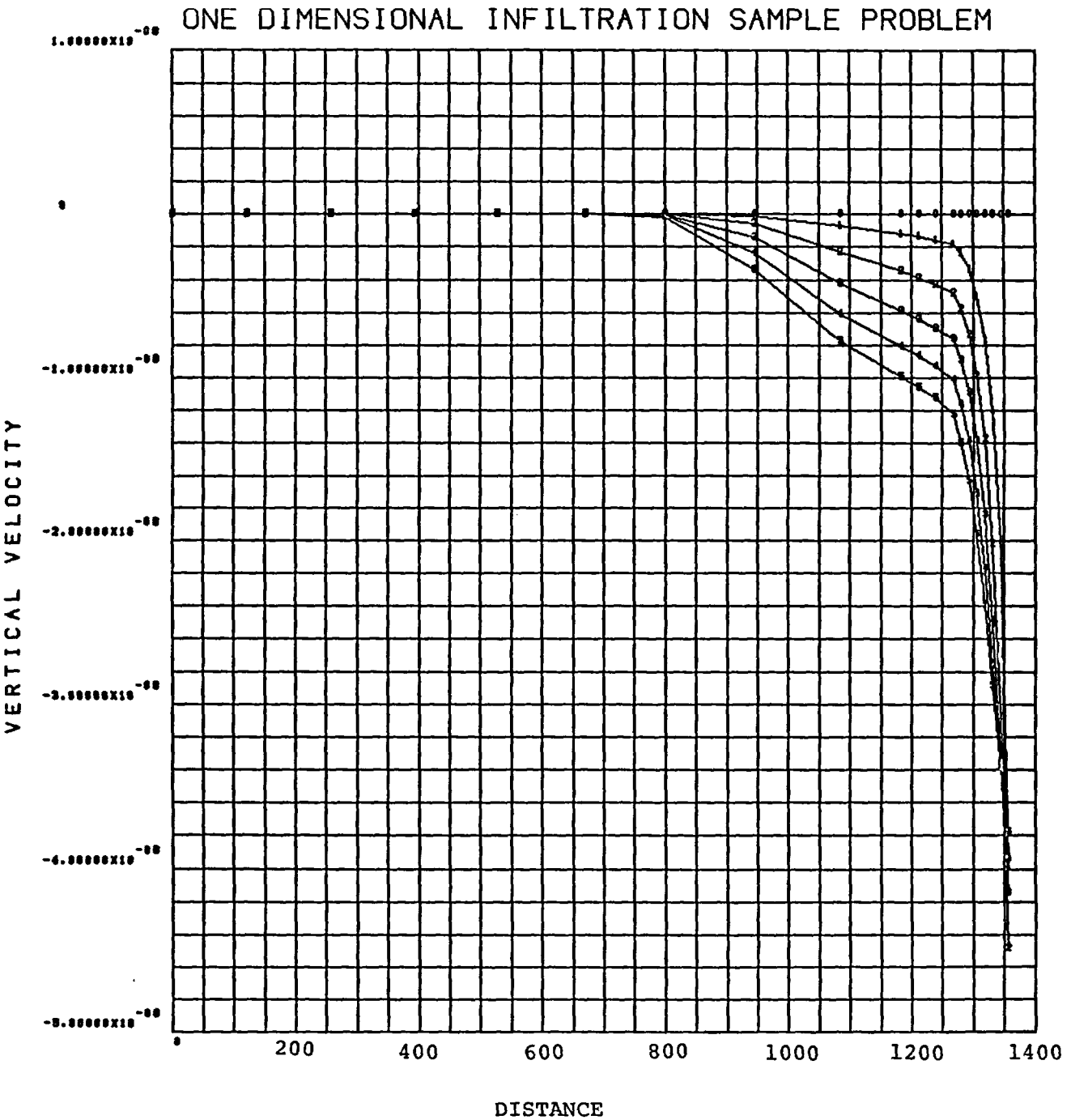


Figure 15f. Velocity as a Function of Depth at Time = 0, 2, 4, 6, 8 and 10 yr.

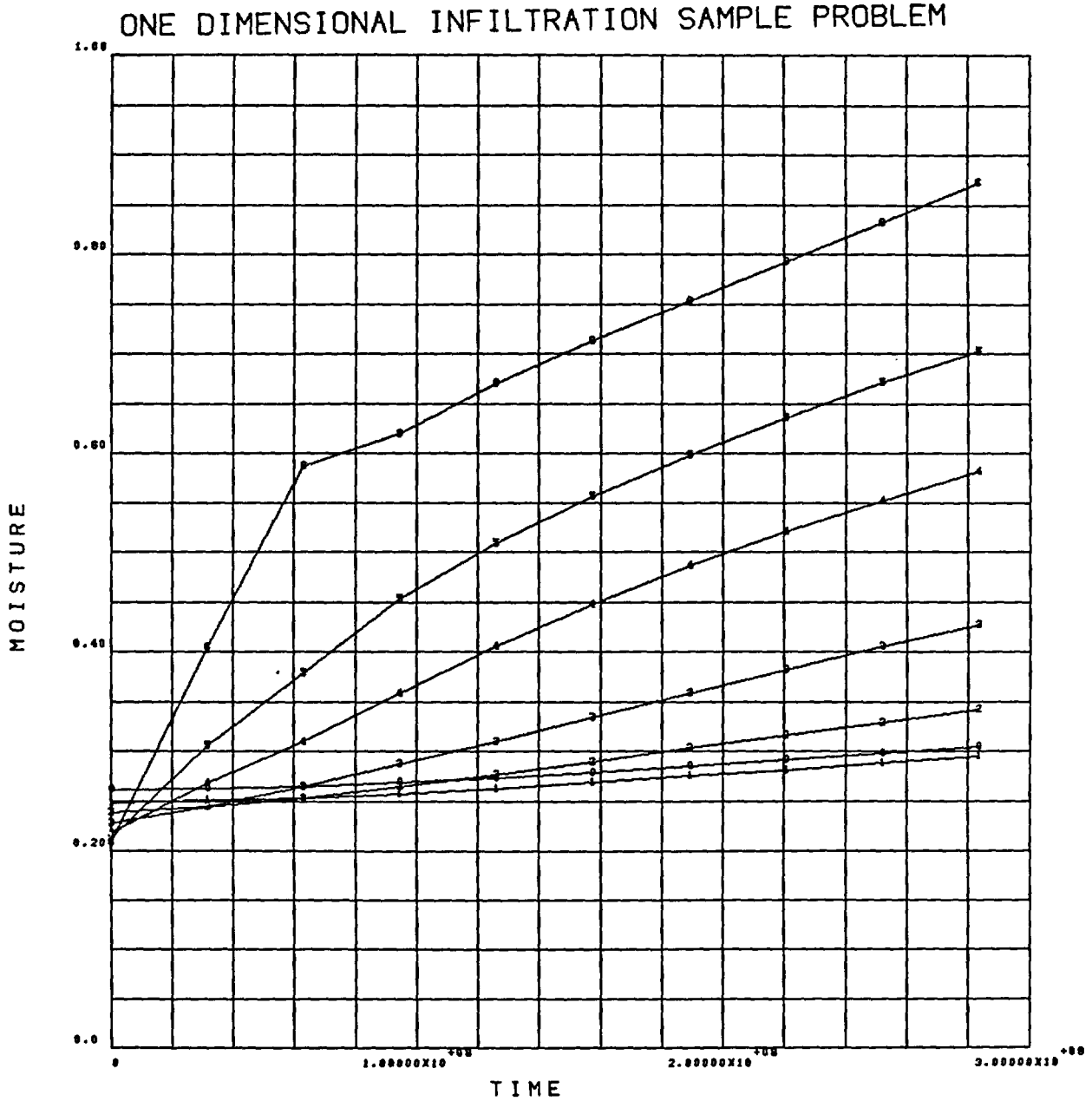


Figure 15g. Moisture Content as a Function of Time for Z = 0, 569, 814, 1113, 1267 and 1369 m.

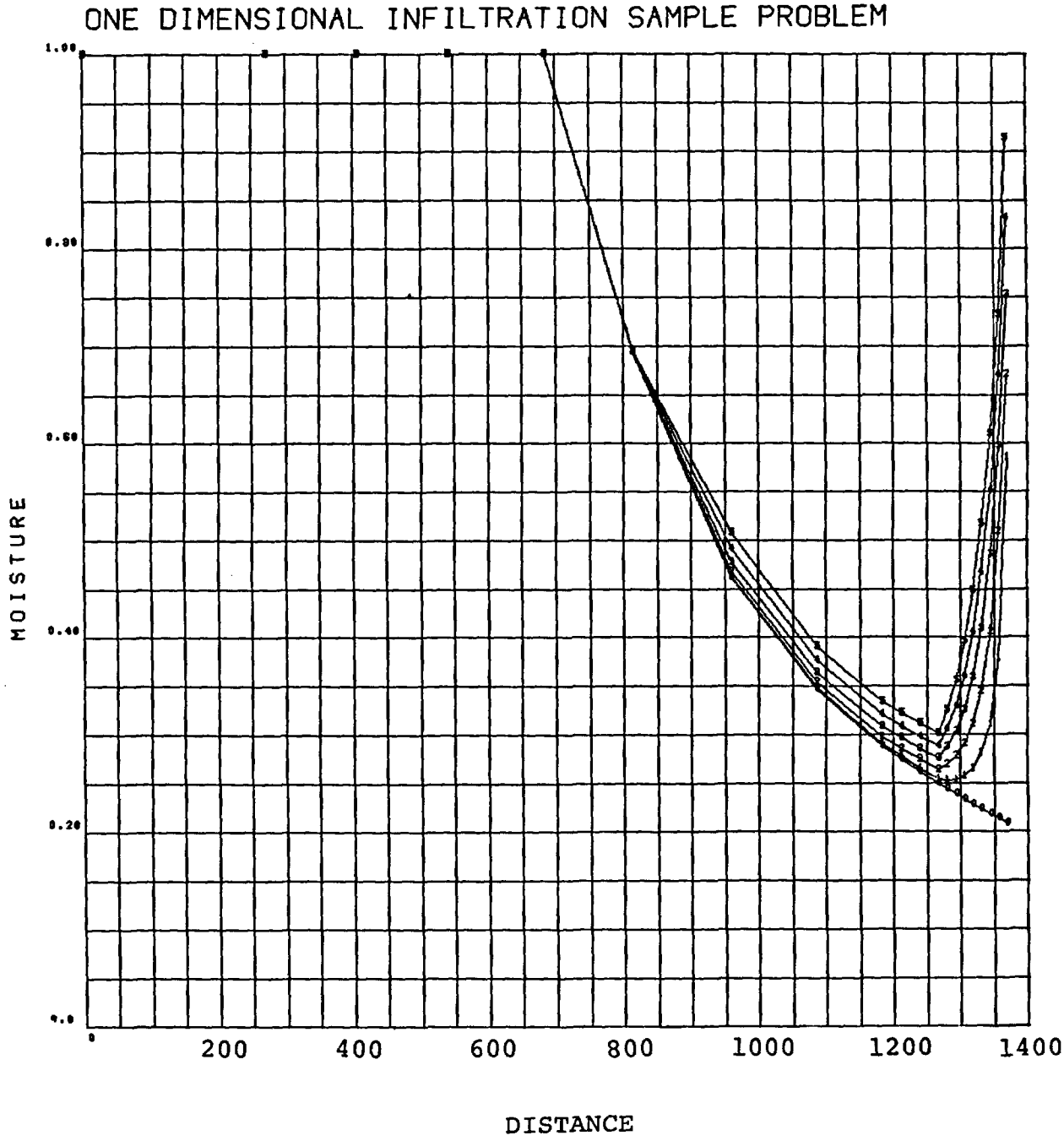


Figure 15h. Moisture Content as a Function of Depth at Time = 0, 2, 4, 6, 8 and 10 yr.

REFERENCES

1. D. K. Gartling, "NACHOS -- A Finite Element Computer Program, Part I -- Theoretical Background," SAND770-1333, Sandia National Laboratories, Albuquerque, NM, 1978.
2. D. K. Gartling, "COYOTE -- A Finite Element Computer Program for Nonlinear Heat Conduction Problems," SAND77-1332, Sandia National Laboratories, Albuquerque, NM, 1978.
3. D. K. Gartling and C. E. Hickox, "MARIAH -- A Finite Element Computer Program for Incompressible Porous Flow Problems: Theoretical Background, SAND79-1622, Sandia National Laboratories, Albuquerque, NM, Sept. 1982.
4. D. K. Gartling and C. E. Hickox, "MARIAH -- A Finite Element Computer Program for Incompressible Porous Flow Problems: User's Manual" SAND 79-1623, Sandia National Laboratories, Albuquerque, NM, Aug. 1980.
5. R. A. Freeze and J. A. Cherry, Groundwater, Prentice-Hall, Inc., 1979.
6. Womack, S. J., "Shape Function Techniques for Generating Finite Element Grids," TICOM Report 73-3, Texas Institute for Computational Mechanics, Austin, TX, 1973.
7. Irons, B. M., "A Frontal Solution Program for Finite Element Analysis," Int. J. Num. Meth. Engng., 2, 1970, pp. 5-32.

APPENDIX A

CONSISTENT UNITS

The following list provides examples of consistent units for quantities encountered in the use of the MARIAH program:

Quantity	English	Metric	SI
Length	foot (ft)	centimeter (cm)	meter (m)
Time	second (s)	second (s)	second (s)
Mass	lb_m	gram (g)	kilogram (kg)
Force	$lb_m ft/s^s$	$g\text{-}cm/s^2$	Newton (N)
Energy	Btu	calorie (cal)	Joule (J)
Temperature	Fahrenheit (F) or Rankine (R)	centigrade (C) or Kelvin (K)	Kelvin (K)
Gravitational Acceleration	ft/s^2	cm/s^2	m/s^2
Density	lb_m/ft^3	g/cm^3	kg/m^3
Velocity	ft/s	cm/s	m/s
Stress (Pressure)	$lb_m/ft\text{-}s^2$	$g/cm\text{-}s^2$	pascal (N/m^2)
Viscosity	$lb_m/ft\text{-}s$	g/cm-s	pascal-s
Specific Heat	$Btu/lb_m\text{-}F$	cal/g-C	J/kg-K
Power	Btu/s	cal/s	J/s (Watt)
Heat Flux	$Btu/ft^2\text{-}s$	$cal/cm^2\text{-}s$	$J/m^2\text{-}s$
Heat Transfer Coefficient	$Btu/ft^2\text{-}s\text{-}F$	$cal/cm^2\text{-}s\text{-}C$	$J/m^2\text{-}s\text{-}K$
Thermal Conductivity	$Btu/ft^2\text{-}s\text{-}F$	cal/cm-s-C	J/m-s-K
Thermal Dispersion	Btu/ft-s-F	cal/cm-s-C	J/m-s-K
Intrinsic Permeability	ft^2	cm^2	m^2

Quantity	English	Metric	SI
Porosity	---	---	---
Coefficient of Volume Expansion	1/F	1/C	1/K
Volume Heat Source	$Btu/ft^3\text{-}s$	$cal/cm^3\text{-}s$	$J/m^3\text{-}s$
g_c	$32.174 \frac{lb_m\text{-}ft}{lb_f\text{-}s^2}$	$1 \frac{g\text{-}cm}{dyne\text{-}s^2}$	$1 \frac{kg\text{-}m}{N\text{-}s^2}$
σ	4.755×10^{-13}	1.355×10^{-12}	5.6697×10^{-8}
	$\frac{BTU}{s\text{-}ft^2\text{-}R^4}$	$\frac{cal}{s\text{-}cm^2\text{-}K^4}$	$\frac{J}{s\text{-}m^2\text{-}K^4}$
θ	n.d.	n.d.	n.d.
D_{ij}	$ft/s\cdot°R$	$cm^2/s\cdot°K$	$m^2/s\cdot°K$

APPENDIX B

DEGREE OF FREEDOM NUMBERING

The following list provides the correspondence between the nodal point variables in an element and the degree of freedom numbering scheme used internally in MARIAH. The node numbers shown below refer to Figure 5.

Quadrilateral Element:

Node No.	Variable	Degree of Freedom Number
1	P	1
	T	9
	U	17
	V	21
	θ	25
2	P	2
	T	10
	U	18
	V	22
	θ	26
3	P	3
	T	11
	U	19
	V	23
	θ	27
4	P	4
	T	12
	U	20
	V	24
	θ	28
5	P	5
	T	13
	θ	29
6	P	4
	T	14
	θ	30
7	P	7
	T	15
	θ	31
8	P	8
	T	16
	θ	32

Triangular Element:

Node No.	Variable	Degree of Freedom Number
1	P	1
	T	9
	U	17
	V	21
	θ	25
2	P	2
	T	10
	U	18
	V	22
	θ	26
3	P	3
	T	11
	U	19
	V	23
	θ	27
4	P	4
	T	12
	θ	28
5	P	5
	T	13
	θ	29
6	P	6
	T	14
	θ	30

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