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FEHMN 1.0: Finite Element Heat and Mass Transfer Code

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Prepared by Kay Coen, Group EES-5

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George Zyvoloski
Zora Dash
Sharad Kelkar

Los Alamos
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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by

George Zyvoloski, Zora Dash, and Sharad Kelkar

ABSTRACT

A computer code is described which can simulate non-isothermal multiphase multicomponent flow in porous media. It is applicable to natural-state studies of geothermal systems and ground-water flow. The equations of heat and mass transfer for multiphase flow in porous and permeable media are solved using the finite element method. The permeability and porosity of the medium are allowed to depend on pressure and temperature. The code also has provisions for movable air and water phases and noncoupled tracers; that is, tracer solutions that do not affect the heat and mass transfer solutions. The tracers can be passive or reactive. The code can simulate two-dimensional, two-dimensional radial, or three-dimensional geometries. A summary of the equations in the model and the numerical solution procedure are provided in this report. A user's guide and sample problems are also included.

I. MODEL DESCRIPTION

A. Nature and Purpose

The FEHMN (Finite Element Heat and Mass Nuclear) code, described in this report, is a version of FEHM (Finite Element Heat and Mass, Zyvoloski et al., 1988) developed for the Yucca Mountain Site Characterization Project (YMP) and documented as required by NUREG-0856. This report satisfies the document requirements for model description and user's manual as presented in the LANL YMP Computer Software Control Quality Procedure (SQAP-3.7, R0). The verification and validation reports are produced as separate documents. The main use of FEHMN will be to assist in the understanding of flow fields in the saturated zone below the potential Yucca Mountain repository. This is referred to as the C-Wells project (YMP-LANL-SP-8.3.1.2.3.1.7). Also in regards to that project, the code will be used to design tracer tests (reactive and non-reactive) to characterize the flow field below Yucca Mountain. In addition, FEHMN will be used to study coupled processes (multicomponent and natural convection) in the unsaturated zone (YMP-LANL-SCP-8.3.1.3.7.1). We note here that the model requirements may be found in the above mentioned study plans.

Yucca Mountain is extremely complex both hydrologically and geologically. The computer codes that are used to model flow must be able to describe that complexity. For example, the flow at Yucca Mountain, in both the saturated and unsaturated zones is dominated by fracture and fault flow in many areas. With permeation to and from faults and fractures, the flow is inherently three-dimensional (3-D). Birdsell et al. (1990) recently presented calculations showing the importance of 3-D flow at Yucca Mountain. Coupled heat and mass transport occurs in both the unsaturated and saturated zones. In the far field unsaturated zone, Weeks (1987) has described natural convection that occurs through Yucca Mountain due to seasonal temperature changes. Heat and mass transfer are important in the saturated zone modeling of temperature logs and pressure tests.

The governing equations and solution techniques used in the FEHMN code are described below. In addition, a user's manual with example problems is provided. Future changes to the code and documentation will be made in accordance with quality assurance procedures being established for the Yucca Mountain Site Characterization Project.

B. Mathematical Formulation

1. Governing equations. Detailed derivations of the governing equations for two-phase flow including heat transfer have been presented by several investigators (Mercer and Faust, 1975, and Brownell et al., 1975, for example), and therefore only a brief development will be presented here. The notation used in this report is given in Table I.

Conservation of mass is expressed by the equation

$$\frac{\partial A_m}{\partial t} + \overline{\nabla} \cdot \overline{f}_m + q_m = 0 \quad , \tag{1}$$

where the mass per unit volume, A_m, is given by

$$A_m = \phi(S_v \rho_v + S_\ell \rho_\ell) \tag{2}$$

and the mass flux, $\overline{f}_m$, is given by

$$\overline{f}_m = \rho_v \overline{V}_v + \rho_\ell \overline{V}_\ell \quad . \tag{3}$$

Here ϕ is the porosity of the matrix, S_v and S_ℓ are saturations, ρ_v and ρ_ℓ are densities, and $\overline{V}_v$ and $\overline{V}_\ell$ are velocities with the subscripts v and ℓ indicating quantities for the vapor phase and the liquid phase, respectively. Source and sink terms (such as bores, reinjection wells, or groundwater recharge) are represented by the term q_m.

Conservation of fluid-rock energy is expressed by the equation

$$\frac{\partial A_e}{\partial t} + \overline{\nabla} \cdot \overline{f}_e + q_e = 0 \quad . \tag{4}$$

TABLE I. Notation

A	parameter used in nonlinear adsorption model (Freundlich, modified Freundlich)
$[A]$	solution matrix for system of nonlinear equations
A_c	accumulation term for tracer (M/L^3)
A_e	energy accumulation term ($M/^2L$)
A_m	mass accumulation term (M/L^3)
$[\widetilde{A}]$	approximation of matrix $[A]$
a	weighting factor for time discretization
a_1, a_2, a_3, a_4	coefficients used in reaction rate model
$\{b\}$	right hand side (forcing function) for system of linear equations
C_ℓ	tracer concentration in liquid
C_R	tracer concentration adsorbed on rock
C_v	tracer concentration in vapor
C_{max}	parameter used in nonlinear adsorption model (modified Freundlich)
$[\hat{C}]$	capacitance matrix
C_{ij}^{up}	upwind value of tracer concentration
c_g	parameter used in linear porosity model
c_{pa}	heat capacity of air L^2/θ^2T
c_r	parameter used in linear porosity model
cp_1, cp_2	parameters used in the capillary pressure models
cp_3, cp_4	parameters used in the capillary pressure models
D_c	dispersion coefficient for tracer (L^2/θ)
$[D_c]$	finite element coefficients for tracer dispersion term
$D_{e\ell}$	energy transmissibility term for liquid (L^2/θ)
$D_{e,v}$	energy transmissibility term for vapor (L^2/θ)
$D_{m\ell}$	mass transmissibility term for liquid (θ)
$D_{m,v}$	mass transmissibility term for vapor (θ)
D_e^{up}	upwind energy transmissibility term (L^2/θ)
D_m^{up}	upwind mass transmissibility term (θ)
$\{e\}$	unit vector
E	Youngs modulus (ML/θ^2)
F	function representation
$\|F\|$	L^2 norm of residuals
$[F_c]$	residual for tracer equation
F_e	flux vector for energy equation (M/θ^3)
F_m	flux vector for mass equation (M/L^2)
$\overline{F}(\overline{x})$	vector of equation residuals
$\{F_e\}$	residual for energy equations
$\{F_m\}$	residual for mass equation
$f(y)$	intermediate calculation in GMRES acceleration
g	acceleration of gravity (L/θ^2)
$[H]^m$	intermediate calculation in GMRES acceleration

TABLE I. Notation

h	generalized energy variable (T or L^2/θ^2)
h_a	enthalpy of air (L^2/θ^2)
h_m^{mel}	parameter in GMRES acceleration
h_v	mass fraction of air in the vapor phase
$h_{v,w}$	vapor enthalpy (L^2/θ^2)
h_ℓ	mass fraction of air in the liquid phase
$h_{\ell,w}$	liquid enthalpy (L^2/θ^2)
I_i	impedance at node i (θ/L^2)
$I_{e,i}$	heat flow impedance at node I ($M/L^3\theta T$)
$[K]$	finite element coefficient for heat conduction term
K_D	retardation coefficient (linear adsorption)
$K_{h,v,w}$	thermal conductivity ($ML/T\theta^3$)
k	intrinsic rock permeability (L^2)
L_f, L_0	length scales used in dual porosity problem
L_{f1}, L_{f2}	length scales used in dual porosity problem
$[\tilde{L}]$	approximate lower factorization of matrix
m	exponent used in Gangi stress model
$[N]$	finite element shape function
Q_m	source term for mass equation ($M/\theta L^3$)
q_c	source term for tracer ($M/\theta L^3$)
q_e	source term for energy equation ($M/L^3\theta$)
q_i	mass source term at node i ($M/\theta L^3$)
$q_{e,i}$	energy source term at node i ($M/L^3\theta$)
$\{q_e\}$	coefficient for energy source terms
$\{q_m\}$	coefficient for mass source terms
P_c	closure stress for use in Gangi stress model (ML)
P_o	initial pressure (ML/θ^2)
P_ℓ	liquid pressure ($M/L\theta^2$)
P_v	vapor pressure ($M/L\theta^2$)
P_{cap}	capillary pressure ($M/L\theta^2$)
P_{flow}	flowing pressure at node i ($M/L\theta^2$)
$[R_c]$	coefficients for tracer gravity term
R_ℓ	liquid relative permeability
$\{R_e\}$	gravity term coefficient for energy
$\{R_m\}$	gravity term coefficient for mass

Table I. Notation

R_v	vapor relative permeability
$\{r\}$	residual of linear system of equations
r, r_b	parameters used in nonlinear adsorption model (Langmuir)
r_{p1}, r_{p2}	parameters used in relative permeability models
r_{p3}, r_{p4}	parameters used in relative permeability models
S	normalized liquid saturation
S_ℓ	liquid saturation
$\hat{S}_\ell$	normalized liquid saturation
$S_{\ell r}$	residual liquid saturation
$S_{\ell s}$	maximum liquid saturation
S_v	vapor saturation
T	temperature (T)
T^*	absolute temperature (T)
$[T_e(P,h)]$	stiffness matrix for energy equation
$[T_c(C)]$	stiffness matrix for concentration equation
$[T_m(P,h)]$	stiffness matrix for mass equation
T_{flow}	flowing temperature at node i (T)
T_{ff}, T_{ff1}	transfer terms in dual porosity solution
T_{ff2}	transfer terms in dual porosity solution
t	time (θ)
u_ℓ	liquid internal energy (L^2/θ^2)
u_v	vapor internal energy (L^2/θ^2)
u_r	rock internal energy (L^2/θ^2)
V_f	volume fraction for fractures in a dual porosity problem
V_{f0}, V_{f1}	volume fractions used in a dual porosity problem
V_{f2}	volume fractions used in a dual porosity problem
V_ℓ	liquid velocity (L/θ)
V_v	vapor velocity (L/θ)
$[V]^m$	intermediate calculation in GMRES acceleration
$[\hat{V}]$	approximate upper factorization of matrix
$\{v\}$	intermediate calculation of GMRES acceleration
$\{w\}$	parameter in GMRES acceleration
$\{y\}$	intermediate calculations in GMRES acceleration
$\overline{x}^i$	vector of corrections at iteration i
α	coefficient of thermal expansion $(1/T)$
α_1, α_2	coefficients used in sorption models

Table I. Notation

ε	tolerance taken for solution scheme
λ	parameter used in defining the van Genutchen capillary pressure model
μ_a	air viscosity $(M/L\theta)$
μ_ℓ	liquid phase viscosity $(M/L\theta)$
$\mu_{\ell,w}$	liquid water viscosity $(M/L\theta)$
μ_v	vapor phase viscosity $(M/L\theta)$
$\mu_{v,w}$	steam viscosity $(M/L\theta)$
ϕ	porosity
ϕ_o	initial porosity
σ	fractional vapor flow parameter
σ	*in situ* stress (ML/θ^2)
$\left(\frac{\partial \overline{F}}{\partial \overline{x}^k}\right)$	Jacobian matrix for nonlinear system

* Units given in MLθT system of dimensions:
Mass [M], length [L], time [θ], temperature [T]

where the energy per unit volume, A_e, is given by

$$A_e = (1-\phi)\rho_r u_r + \phi(S_v \rho_v u_v + S_\ell \rho_\ell u_\ell) \tag{5}$$

and the energy flux, $\overline{f}_e$, is given by

$$\overline{f}_e = \rho_v h_v \overline{V}_v + \rho_\ell h_\ell \overline{V}_\ell - K\overline{\nabla} T \quad . \tag{6}$$

Here the subscript r refers to the rock matrix; u_r, u_v, and u_ℓ are specific internal energies; h_v and h_ℓ are specific enthalpies; K is an effective thermal conductivity; T is the temperature; and q_e is the energy contributed from sources and sinks.

To complete the governing equations it is assumed that Darcy's Law applies to the movement of each phase:

$$\overline{V}_v = -\frac{kR_v}{\mu_v}\ (\overline{\nabla} p_v - \rho_v \overline{g}) \tag{7}$$

and

$$\overline{V}_\ell = -\frac{kR_\ell}{\mu_\ell}\ (\overline{\nabla} p_\ell - \rho_\ell \overline{g}) \quad . \tag{8}$$

Here k is the permeability, R_v and R_ℓ are the relative permeabilities, μ_v and μ_ℓ are viscosities, p_ℓ and p_v the phase pressures, and g represents the acceleration due to gravity (the phase pressures are related by $p_v = p_\ell + p_{cap}$). For simplicity, the equations are shown for an isotropic medium, though this restriction does not exist in the computer code.

Using Darcy's Law the basic conservation equations (1) and (4) can be rewritten

$$-\overline{\nabla} \cdot (D_{m\ell}\overline{\nabla} p_\ell) - \overline{\nabla} \cdot (D_{m\ell}\overline{\nabla} p_v) + q_m + \frac{\partial}{\partial z} g(D_{m\ell}\rho_\ell + D_{mv}\rho_v) + \frac{\partial A_m}{\partial t} = 0 \quad (9)$$

and

$$-\overline{\nabla} \cdot (D_{e\ell}\overline{\nabla} p_\ell) - \overline{\nabla} \cdot (D_{ev}\overline{\nabla} p_v) + \overline{\nabla} \cdot (K\overline{\nabla} T) + q_e + \frac{\partial}{\partial z} g(D_{e\ell}\rho_\ell + D_{ev}\rho_v) + \frac{\partial A_e}{\partial t} = 0, \quad (10)$$

where z is oriented in the direction of gravity. Here the transmissibilities are given by

$$D_{ev} = h_v D_{mv}, \quad D_{e\ell} = h_\ell D_{m\ell} \quad (11)$$

and

$$D_{m\ell} = \frac{kR_\ell \rho_\ell}{\mu_\ell}, \quad D_{mv} = \frac{kR_v \rho_v}{\mu_v} \quad . \quad (12)$$

The source and sink terms in equations (1) and (4) arise from bores, and if the total mass withdrawal, q_m, for each bore is specified, then the energy withdrawal, q_e, is determined as follows:

$$q_e = q_v h_v + q_\ell h_\ell \quad (13)$$

where

$$q_v = \sigma q_m, \quad q_\ell = (1 - \sigma) q_m \quad (14)$$

and

$$\sigma = \frac{1}{\left(1 + \frac{\rho_\ell R_\ell \mu_v}{\rho_v R_v \mu_\ell}\right)} \quad . \quad (15)$$

The form of equation (15) shows how important the relative permeability ratio R_ℓ/R_v is in controlling the discharge composition. The relative permeability and capillary pressure functions are summarized in the next section, Constitutive Relationships.

In addition to the flow of heat and mass, FEHMN is also capable of simulating noncondensible gas flow (usually air) and passive tracer flow. The noncondensible gas conservation equation is

$$-\overline{\nabla}\cdot(C_\ell D_{m\ell}\overline{\nabla}p_\ell)-\overline{\nabla}\cdot(C_v D_{mv}\overline{\nabla}p_v)$$
$$+\frac{\partial}{\partial z}g(C_\ell D_{m\ell}\rho_\ell+C_v D_{mv}\rho_v)+\frac{\partial A_c}{\partial t}+q_c=0 \quad . \tag{16}$$

Here C is the concentration of the noncondensible gas and is expressed as a fraction of total mass. The term $\overline{f}_c$ is the mass flux, q_c is the source (or sink) strength, and A_c is the accumulation term:

$$\overline{f}_c = C_v\rho_v\overline{V}_v+\rho_\ell\overline{V}_\ell C_l \tag{17}$$
$$q_c = C_v q_v + C_\ell q_\ell \tag{18}$$
$$A_c = \phi(S_v\rho_v C_v + S_\ell\rho_\ell C_\ell) \tag{19}$$

The passive tracer equation is not directly coupled to the pressure field but merely uses the pressure field obtained by the heat and mass transfer solution:

$$-\overline{\nabla}\cdot(C_\ell D_{m\ell}\overline{\nabla}p_\ell)-\overline{\nabla}\cdot(C_v D_{mv}\overline{\nabla}p_v)+\overline{\nabla}\cdot(D_c\overline{\nabla}C_\ell)$$
$$+g\frac{\partial}{\partial z}(C_\ell D_{m\ell}\rho_\ell+C_v D_{mv}C_v)+\frac{\partial A_c}{\partial t}+q_c=0 \tag{20}$$

(where the terms are defined analogously to the condensible gas equation terms) the additional term $\overline{\nabla}\cdot(D_c\overline{\nabla}C_\ell)$ is the dispersion term. At present the code allows for up to 10 tracers.

2. Constitutive Relationships. In the equations described above the porosity, permeability, density, enthalpy, and viscosity can be strong functions of pressure and temperature. These functions make the code very nonlinear. In addition the relative permeabilities and capillary pressure can be strong functions of saturation.

The pressure and temperature dependent behavior of the density, enthalpy, and viscosity are represented by rational polynomials. Using a technique developed at the University of Auckland, New Zealand, accurate fits to the National Bureau of Standards (NBS) steam table data were obtained over the ranges:

$$0.001MPa \le P \le 110.MPa \tag{21}$$
$$0.001°C \le T \le 360°C$$

The maximum error was 0.3% for all the functions. The rational polynomial representation proved to be both accurate and fast. For details the reader is referred to Zyvoloski and Dash (1991). In addition a low pressure thermodynamics set is provided with the ranges $0.001MPa \leq P \leq 20MPa, 0.5°C \leq T \leq 360°C$. The maximum error for this set is also 0.3%.

The tracer module of FEHMN has provisions for reactive tracers. At present four adsorption models have been included. These are the linear, Langmuir (Satter et al., 1980), Freundlich, and modified Freundlich isotherm models. The discussion follows the description given by Robinson (1988). With adsorption the equations describing the conservation of species, Eq. (16) is modified by the addition of the term

$$\rho_r \frac{\partial C_R}{\partial t}$$

where ρ_r is the rock density and C_R represents the adsorption of species onto the reservoir rock and is given by

$$C_R = \frac{\alpha_1 C_\ell^\beta}{1 + \alpha_2 C_\ell^\beta} \quad . \tag{22}$$

The terms in Eq. (22) are given in Table II where K_D, A, β, C_{max}, r_b, and r are parameters associated with the sorption models. The adsorption term is included in the tracer solution by replacing the A_c term, Eq. (19), with the new term

$$A_c = \phi(S_v \rho_v C_v + S_\ell \rho_\ell C_\ell) + \rho_r C_R \quad . \tag{23}$$

Chemical reactions are modeled by modifying the source term, q_c in Eq. (18), with the addition of the term q_{cR} given below:

$$q_{cR} = \frac{a_1 C_\ell^{a2}}{a_3 + a_4 C_\ell} \tag{24}$$

TABLE II. Sorption Isotherm Models

Model	Expression	α_1	α_2	β
Linear	$C_R = K_D C_\ell$	K_D	0	1
Freundlich	$C_R = AC_\ell^\beta$	A	0	$0 < \beta < 1$
Modified Freundlich	$\frac{C_R}{C_{max} - C_R} = AC_\ell^\beta$	C_{max}	A	$0 < \beta < 1$
Langmuir	$C_R = \frac{r_b C_\ell}{1 + rC_\ell}$	r_b	r	1

where the quantities a_1, a_2, a_3, and a_4 are user inputted parameters. The general case given in Eq. (24) can sometimes be replaced by a simplier expression $q_{cR} = a_1(C_\ell - a_2)$. Both of the models are addressed in the input section.

Several well known relative permeability functions are available to the user. They are the simple linear functions, the Corey (1954) relationships, and the Sandia functions (van Genuchten, 1980).

The linear functions are given by

$$\begin{aligned}
R_\ell &= 0 &&, S_\ell \leq rp_1 \\
R_\ell &= (S_\ell - rp_1)/(rp_3 - rp_1) &&, rp_1 < S_\ell < rp_3 \\
R_\ell &= 1 &&, S_\ell \geq rp_3 \\
R_v &= 0 &&, S_v \leq rp_2 \\
R_v &= (S_v - rp_2)/\ (rp_4 - rp_2) &&, rp_2 < S_v < rp_4 \\
R_v &= 1 &&, S_v \geq rp_4
\end{aligned} \tag{25}$$

where rp_1, rp_2, rp_3 and rp_4 are user supplied quantities.

The Corey relative permeability functions are given by

$$\begin{aligned}
R_\ell &= \hat{S}_\ell^4 \\
R_v &= (1 - \hat{S}_\ell)^2(1 - \hat{S}_\ell^2)
\end{aligned} \tag{26}$$

where $\hat{S}_\ell = (S_\ell - rp_1 - rp_2)/(1 - rp_1 - rp_2)$ and where the input quantities rp_1 and rp_2 are the residual liquid and vapor saturations respectively.

The van Genuchten (van Genuchten, 1980) functions are described by the following formulae:

$$\begin{aligned} \hat{S} &= \frac{(S_\ell - rp_2)}{(rp_3 - rp_2)} \\ R_\ell &= \sqrt{\hat{S}}\left[1.0 - (1.0 - (\hat{S})^{1/\lambda})^\lambda\right]^2 \ , \hat{S}_\ell < rp_3 \\ &= 1.0 \qquad\qquad\qquad\qquad\qquad , \hat{S}_\ell \geq rp_3 \\ R_v &= 1.0 - R_\ell \end{aligned} \tag{27}$$

where $\lambda = rp_1$ and rp_1, rp_2 and rp_3 are parameters supplied by the user.

Composite relative permeability curves, as described by Klavetter and Peters (1986), are also available. See Section III B, macro-command *RLP* for an input description.

R_ℓ and R_v are restricted by the relationships

$$\begin{aligned} 0 \leq R_v \leq 1.0 \\ 0 \leq R_\ell \leq 1.0 \end{aligned} \tag{28}$$

and the relative permeability functions are truncated to the appropriate value if the above conditions are violated.

The capillary functions included with FEHMN are the linear function and the Sandia capillary pressure model. Our terminology follows that of Pruess (1987).

The linear capillary function model is given by the following equations

$$\begin{aligned} P_{cap} &= cp_1, && S_\ell \leq cp_2 \\ P_{cap} &= 0.0, && S_\ell \geq cp_3 \\ P_{cap} &= cp_1 \frac{cp_3 - S_\ell}{cp_3 - cp_1}, && cp_2 < S_\ell < cp_3 \end{aligned} \tag{29}$$

where cp_1, cp_2, and cp_3 are parameters supplied by the user. The restriction $cp_3 > cp_2$ is also necessary.

The van Genuchten functions (van Genuchten, 1980) are described by the following equations

$$\begin{aligned} \hat{S} &= \frac{S_\ell - S_{\ell r}}{S_{\ell s} - S_{\ell r}} \\ P_{cap} &= 0, \quad S_\ell \geq cp_5 \\ P_{cap1} &= P_o\left\{(\hat{S})^{-1/\lambda} - 1.0\right\}^{1.0-\lambda} \\ P_{cap} &= P_{max}, P_{cap1} \geq P_{max} \\ P_{cap} &= P_{cap1}, P_{cap1} < P_{max} \end{aligned} \tag{30}$$

where $\lambda = cp_1$, $P_o = 1.0/cp_3, P_{max} = cp_4$, $S_{\ell s} = cp_5$, $S_{\ell r} = cp_2$.

The capillary pressure curves approach an infinite value as S_ℓ approaches 0. This was observed by Nitao (1988) who suggested using Eq. (30) only to a value of one-half the maximum suction observed in the rock (P_{max}) and linearly extrapolating the capillary pressure to the maximum capillary pressure at $S_\ell = 0$. We have also employed this technique in FEHMN.

The van Genuchten relative permeability curves and capillary pressure functions are the primary ones used for Yucca Mountain calculations.

If the flow of air is also modeled, appropriate thermodynamic information for air must also be provided. The density of air is assumed to obey the ideal gas law, using atmospheric conditions as our reference state we have

$$\rho_a = 1.292864\left(\frac{273.0}{T+273.0}\right)\left(\frac{P}{0.101325}\right) \tag{31}$$

where ρ_a has the units kg/m^3, T is in $°C$, and P is in MPa. The mixture density is given by

$$\rho_v = \rho_{v,w} + \rho_a \tag{32}$$

where $\rho_{v,w}$ is the density of the water vapor. The density of the liquid phase is assumed to be unaffected by the amount of dissolved air it contains.

The enthalpy of air is a function of temperature only

$$\begin{aligned} C_{pa} &= 6122.0 - 11.76(T^*) + 0.0177(T^*)^2 \\ h_a &= C_{pa}(T \cdot 10^{-6}) \end{aligned} \tag{33}$$

where h_a is the enthalpy of air (MJ/kg), C_{pa} is the heat capacity of air (MJ/kg $°C$), and $T^* = T + 273$. The mixture enthalpy for the vapor phase is

$$h_v = h_{v,w}(1-\eta_v) + h_a\eta_v \tag{34}$$

where $h_{v,w}$ is the enthalpy of steam and η_v is the fraction by mass of air in the vapor phase. The enthalpy of the liquid phase is given by the enthalpy of the dissolved air, the heat of solution, and the enthalpy of the water. At present, we neglect the heat of solution and use the enthalpy of air described above:

$$h_\ell = h_{\ell,w}(1-\eta_\ell) + h_a\eta_\ell \tag{35}$$

where $h_{\ell,w}$ is the enthalpy of liquid water and η_ℓ is the mass fraction of a in the liquid phase.

Assuming ideal gas behavior, the mass fraction of air in the vapor phase may be expressed as

$$\eta_v = \frac{\rho_a}{\rho_v}$$

the mass fraction of air in the liquid phase is assumed to obey Henry's law or

$$\eta_e = \alpha P_a$$

where α is the Henry's law constant ($\alpha = 1.611 \times 10^{-4} P_a^{-1}$) for air and P_a is the partial pressure of air.

The viscosity of the vapor phase is assumed to be a linear combination of the air viscosity and the water viscosity

$$\mu_v = \mu_{v,w}(1 - \eta_v) + \mu_a \eta_v \tag{36}$$

where $\mu_{v,w}$ is the steam viscosity and is obtained from steam data. The viscosity of air is assumed constant

$$\mu_a = 1.82 \times 10^{-5} cp \quad . \tag{37}$$

The liquid phase viscosity is assumed to be independent of the amount of dissolved air and is obtained from steam table data:

$$\mu_\ell = \mu_{\ell,w} \quad . \tag{38}$$

Often it is necessary to accommodate changes in the rock porosity and permeability due to changes in effective stress caused by temperature and pore fluid pressure changes. A linear and nonlinear model are currently incorporated into the code for this purpose.

The linear pore pressure model for porosity is given by

$$\phi = \phi_o + (1 - \phi_o)(c_r - c_g)(P - P_o) \tag{39}$$

where ϕ is the porosity at pressure P, ϕ_o is the initial porosity at pressure P_o, c_r is the pore volume compressibility of the rock and c_g is the compressibility of the matrix grain material.

The nonlinear model for porosity (Gangi, 1978) currently used in the code is given by

$$\phi = \phi_o \left[1 - \left(\frac{P_c}{P_o} \right)^m \right] \tag{40}$$

and

$$P_c = \sigma - P - \alpha E \Delta T \tag{41}$$

where P_c is the closure stress, σ is the *in situ* stress (assumed isotropic), α is the coefficient of thermal expansion of the rock, E is Young's modulus, ΔT is the temperature change and P_o and m are parameters in the model.

For either case the effect of stress and temperature changes on permeability are modeled with

$$k = k_o \left(\frac{\phi}{\phi_o} \right)^3 \tag{42}$$

where k is the permeability at porosity ϕ.

C. Discretization of the Governing Equations

The time derivatives in the Eqs. (1-42) are discretized using the standard first order method given by

$$f(t^{n+1}) = f(t^n) + \Delta t \Big(a f'(t^{n+1}) + (1-a) f'(t^n) \Big) \tag{43}$$

where $f(t^{n+1})$ is the desired function at time t^{n+1}, $f(t^n)$ is the known value of f at time t^n, Δt is the time step, f' is the derivative of f with respect to time and a is a weighting factor. For $a = 1$, the scheme is fully implicit (backward Euler) and for $a = 0$, the scheme is fully explicit (forward Euler).

The space derivatives in the governing equations are discretized using the finite element formulation. The finite element equations are generated using the Galerkin formulations. For a detailed presentation of the finite element method the reader is referred to Zienkiewicz (1977). In this method the flow domain, Ω, is assumed to be divided into finite elements; and variables P, h and T, along with the accumulation terms A_m and A_e, are interpolated in each element:

$$P = [N]\{P\}, \;\; h = [N]\{h\}, \;\; T = [N]\{T\}, \;\; A_m = [N]\{A_m\}, \;\; \text{and} \;\; A_e = [N]\{A_e\}$$

where $[N]$ is the shape function. Here h is used to represent the generalized energy variable; T in single phase water states, S in 2-phase water states.

These approximations are introduced in Eqs. (9), (10), and (20), and the Galerkin formulation (described by Zienkiewicz and Parekh, 1970) is applied. The following equations are derived:

$$[T_m(P,h)]\{P\} + \hat{C}\frac{\partial A_m}{\partial t} + \{q_m\} - g\{R_m\} = \{F_m\} \tag{44}$$

and

$$[T_e(P,h)]\{P\} + [K]\{T\} + \hat{C}\frac{\partial A_e}{\partial t} + \{q_e\} - g\{R_e\} = \{F_e\} \tag{45}$$

where

$$T_{mij} = \int_\Omega \overline{\nabla} N_i \cdot D_m^{UP} \overline{\nabla} N_j dV \quad , \tag{46}$$

$$T_{eij} = \int_\Omega \overline{\nabla} N_i \cdot D_e^{UP} \overline{\nabla} N_j dV \quad , \tag{47}$$

$$K_{ij} = \int_\Omega \overline{\nabla} N_i \cdot \overline{\nabla} N_j dV \quad , \tag{48}$$

$$\hat{C}_{ij} = \int_{\Omega j} N_i N_j dV \quad , \tag{49}$$

$$R_{mi} = \int_{\Omega j} \frac{\partial N_i}{\partial y} N_j D_m^{UP} \rho_m dV \quad , \tag{50}$$

and

$$R_{ei} = \int_{\Omega j} \frac{\partial N_i}{\partial y} N_j D_e^{UP} \rho_e dV \quad . \tag{51}$$

Equations (50) and (51) need some comment. The term D_e^{UP} indicates an upstream-weighted transmissibility (Dalen, 1979). This technique has worked well in the low-order elements (3-node triangle, 4-node quadrilateral), where the schemes resemble difference techniques. The upstream weighting is determined by comparing the velocities at the nodes i and j. The shape function coefficients are generated in a unique way that requires the integrations in Eqs. (50) and (51) to be performed only once and the nonlinear coefficients to be separated from this integration. The reader is referred to Zyvoloski (1983) for more details.

The integration scheme used in this report is similar to that described by Young (1981). His implementation differs from common methods in that it uses Lobatto instead of Gauss integration. The net effect is that, while retaining the same order of integration accuracy (at least for linear and quadratic elements), there are considerably fewer nonzero terms in the resulting matrix equations. Figure 1 shows a comparison of the nodal connections for Lobatto and Gauss integration methods. It should be noted that these results hold on an orthogonal grid only. If a nonorthogonal grid were introduced, then additional

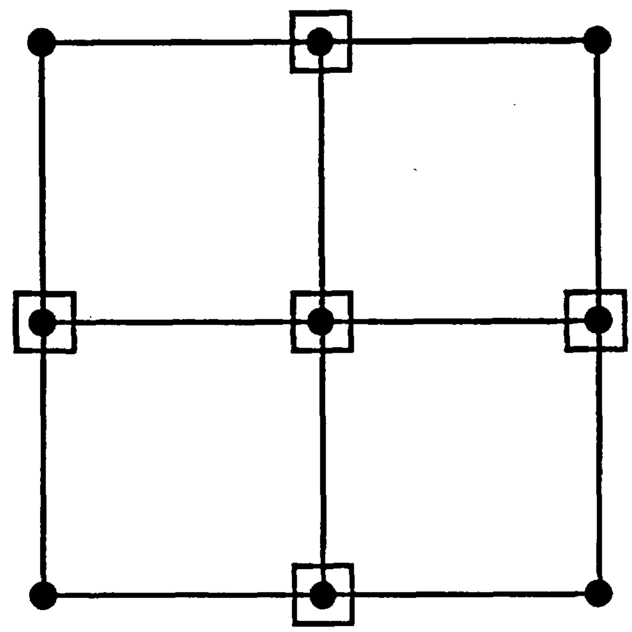

Fig. 1. Comparison of nodal connections for conventional and Lobatto integrations for an orthogonal grid.

nonzero terms would appear in the Lobatto quadrature method. Note also that the linear elements yield the standard 5- or 7-point difference scheme. The reader is referred to Young's paper for more details.

A similar approach is used to solve the transport equation. Following the discussion above the species concentration, C, and the species accumulation term, A_c, are interpolated in each element.

$$C = [N]^T\{C\}, \quad A_c = [N]^T\{A_c\}$$

Using these approximators and using a Galerkin approach, we obtain the following equation

$$[T_c(C)]\{P\} + [D_c]\{C\} + \hat{C}\frac{\partial A_c}{\partial t} + \{q_c\} + \{R_c\} = \{F_c\} \tag{52}$$

when

$$T_{cij} = \int_{\Omega} \overline{\nabla} N_i \cdot D_m C_{ij}^{UP} \overline{\nabla} N_j dv \tag{53}$$

$$D_{cij} = \int_{\Omega} \overline{\nabla} N_i \cdot D_c \overline{\nabla} N_j dv \tag{54}$$

$$R_{cij} = \int_{\Omega} \frac{\partial N_i}{\partial y} \cdot D_m C_{ij}^{UP} \overline{\nabla} N_j dv \tag{55}$$

where C_{ij} was defined previously and C_{ij}^{UP} is an upstream weighted species concentration. This approach is similar to the finite difference method for solving the transport equations.

D. Boundary Conditions

Two mass flow boundary conditions are allowed in FEHMN. They are no flow and specified variable values. The no flow conditions are automatically satisfied by the finite element mesh. Specified variable quantities are obtained in the following manner. A pressure dependent flow term is used:

$$q_i = I_i(P_{flow,i} - P_i) \tag{56}$$

where P_i is the pressure at node i, q_i is the flow rate, I_i is the impedance, and $P_{flow,i}$ is the specified flowing pressure at node i. By specifying a large I_i, we can force the pressure to be equal to $P_{flow,i}$. The energy (or temperature) specified at node i refers only to the incoming fluid value, if fluid flows out of the reservoir, stability dictates that the energy of the in-place fluid be used in the calculations. Species concentration is handled in a manner analogous to the energy variable. Only the incoming species concentration can be specified; if the flow is out of the reservoir the in-place species concentration is used.

In addition to the mass flow boundary conditions, heat flow boundary conditions are also provided. A specified heat flow can be input or a specified temperature obtained

$$q_{e,i} = I_{e,i}(T_{flow,i} - T_i)$$

where T_i is the nodal temperature, $T_{flow,i}$ is the specified flowing temperature at node i, $I_{e,i}$ is the impedance to heat flow at node i, and $q_{e,i}$ is the heat flow at node i. This heat flow is superimposed on any existing heat flow from the other boundary conditions or source terms.

E. Solution Methods

The application of the discretization methods to the governing partial differential equations yields a system of nonlinear algebraic equations. To solve these equations, the Newton-Raphson iterative procedure is used. This is an iterative procedure that makes use of the derivative information to obtain an updated solution from an initial guess. Let the set equations to be solved be given by

$$\overline{F}(\overline{x}) = 0 \tag{57}$$

where $\overline{x}$ is the vector of unknown values of the variables that satisfy the above equation. The procedure is started by making an initial guess at the solution, say $\overline{x}^\circ$. This is usually taken as the solution from the previous time step. Denoting the value of $\overline{x}$ at the kth iteration by $\overline{x}^k$, the updating procedure is given by

$$\overline{x}^{(k+1)} = \overline{x}^k - \overline{F}(x^k)\left(\frac{\partial \overline{F}}{\partial \overline{x}^k}\right)^{-1} \quad . \tag{58}$$

At each step, the residuals $\overline{F}(x^k)$ are compared with a prescribed error tolerance. The prescribed error tolerance, ϵ, is an input parameter and an ℓ^2 norm is used:

$$\|F\|_k = \left(\sum_i F_i^2\right)_k^{1/2} \quad .$$

Convergence is achieved when

$$\|F\|_k \leq \epsilon\|F\|_o \quad .$$

ϵ is usually in the range 10^{-4}-10^{-7}. Semiautomatic timestep control is designed based on the convergence of the Newton iterations. If the code is unable to find a solution $\overline{x}^k$ such that the residuals become less than the tolerance within a given number of iterations, the time step is reduced and the procedure repeated. On the other hand, if convergence is rapid, the timestep is increased by multiplying with a user supplied factor, thus allowing for large timesteps when possible.

The matrix equation to be solved at each Newton-Raphson iteration has the form

$$[A]\{x\} = \{b\} \quad , \tag{59}$$

where $[A]$ is the Jacobian matrix, $\{x\}$ is the solution vector, and $\{b\}$ is the residual. The $[A]$ matrix is sparse and banded. For computation, $\{x\}$ is replaced by $\{\delta x\} = \{x\}^{n+1} - \{x\}^n$, and $\{b\}$ is replaced by $\{r\} = \{b\} - [A]\{x\}^n$, where n is the iteration number. (Note that this is different from the overall Newton iteration.) Thus, only changes in $\{x\}$ are calculated.

Complete Gaussian elimination or factorization on Eq. (59) would result in fill-in of all the bands between the lowest subdiagonal and the highest superdiagonal bands. Incomplete factorization involves finding only approximate upper and lower triangular matrices $\tilde{L}$ and $\tilde{U}$, requiring very little fill-in. The computing effort for obtaining the incomplete factors is much less than for the complete factors. However, an iterative procedure is now required. The presentation of the theory below follows that of Saad and Schultz (1986). The matrix $[A]$ is partially factored into upper and lower triangular form

$$[\overline{A}] = [\tilde{L}][\tilde{U}] \ , \tag{60}$$

where $[\overline{A}] \neq [A]$ because, in general, $[\tilde{L}]$ and $[\tilde{U}]$ will contain only some of the steps of the elimination process. To incompletely factor a matrix, a prior knowledge of the fill-in pattern is required. A symbolic factorization is performed (just once) to establish where the fill-in occurs and to determine the order of each term. Figure 2 shows a matrix and its first level of fill (0's) resulting from factorization of the original matrix elements (x's). We could continue the process to get higher-order terms, but usually the lower-order terms are all that are necessary (Zyvoloski, 1986). The amount of factorization is limited by computer storage considerations. Once factored, the solution is easy to carry out as it consists of a forward and a backward substitution:

$$\{v\} = [\tilde{U}]^{-1}\left\{[\tilde{L}]^{-1}\{r\}\right\} \tag{61}$$

where $\{v\}$ is the approximate change in $\{x\}$. The following recursion scheme is used to refine the approximation:

$$\{v\}^{n+1} = [\overline{A}]^{-1}\{r\}^n = [\tilde{U}]^{-1}\left\{[\tilde{L}]^{-1}\{r\}^n\right\} \ , \tag{62}$$

$$\{x\}^{n+1} = \{x\}^n + \{v\}^{n+1} \ , \tag{63}$$

$$\{r\}^{n+1} = \{r\}^n - [\overline{A}]\{v\}^{n+1} \tag{64}$$

where n is the iteration index and $\{x\}^0 = 0$ since the original matrix equation is written in residual form [see paragraph after Eq. (59)]. The solution scheme, comprising Eqs. (61)-(64), may be accelerated by over-relaxation procedures, but it is better to use orthogonalization-minimization. If the Jacobian matrix were symmetric, conjugate gradient could be used. For nonsymmetric matrices, the GMRES (Generalized Minimal Residual Equation Solver) procedure (Saad and Schultz, 1986) is used.

For comparison purposes, the simple over-relaxation procedure is discussed first. In the recursion scheme [Eqs. (62)-(64)], Eq. (63) is replaced by $\{x\}^{n+1} = \{x\}^n + w\{v\}^{n+1}$, and Eq. (64) is replaced by $\{r\}^{n+1} = \{r\}^n - w[A]\{v\}^{n+1}$. Here w is the over-relaxation parameter and satisfies the relation $1 < w < 2$. After Eq. (64) is calculated, the procedure returns to Eq. (61) and continues until $\{r\}^{n+1}$ is reduced to some predetermined value. For many reservoir problems, convergence is extremely slow, and the ortho-minimization procedures provide a valuable alternative.

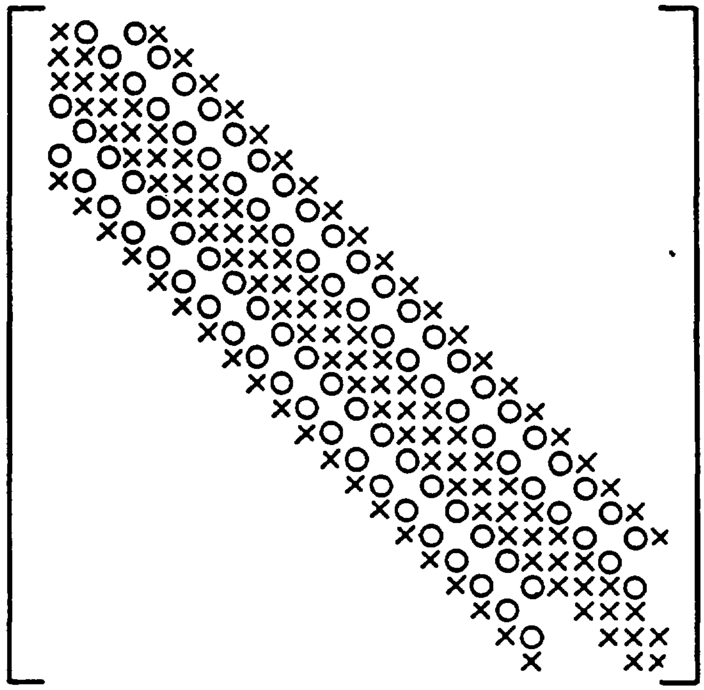

Fig. 2. Matrix band structures showing second-order fill-in.
x - original matrix positions.
o - fill-in with order 2 factorization.

The GMRES algorithm is

1. Set $\{r\}^\circ = \{b\}$ and set $\{v\}^1 = \{r\}^\circ/\|r^\circ\|$ where $\|r\|$ is the sum squared norm ($\|r\| = \{\sum_{i=1}^{n} r_i\}^{1/2}$) of $\{r\}$ and n is the number of unknowns. We also assume that $\{x\}^\circ = \{0\}$.
2. Perform orthogonalization calculation, $m = 1$, NORTH

$$\{w\}^{m+1} = [A]\{v\}^m - \sum_{i=1}^{m}([A]\{v\}^i, \{v\}^i)\{v\}^i \tag{65}$$

$$h_m^{m+1} = \|\{w\}^{m+1}\| \tag{66}$$

$$\{v\}^{m+1} = \{w\}^{m+1}/h_m^{m+1} \tag{67}$$

Where NORTH is the maximum number of orthogonalizations allowed.

3. Form approximate solution (n = NORTH)

$$\{x\}^m = \{x\}^\circ + [V]^m\{y\}^m \tag{68}$$

where $[V]^m$ is an n by m matrix which contains the $\{v\}^i$ (i = 1, m) and $\{y\}^m$ is an n dimensional vector which minimizes the function.

$$f(y) = \|B\{e\}^1 - [H]^m\{y\}\| \quad . \tag{69}$$

Here $B = \|r^\circ\|$, $\{e\}^1$ is the unit vector, and $[H]^m$ is a $k + 1$ (= n) by k matrix whose only nonzero entries are the h_i^{i+1} calculated in Eq. (66). This minimization is economically done using $Q-R$ factorization. (See Saad and Shultz, 1986, for details.)

4. Calculate $\|r_m\|$ where

$$\{r\}^m = \{b\} - [A]\{x\}^m \tag{70}$$

If $\|r_m\| \leq \epsilon$, some specified tolerance, then the process is complete. Otherwise we set $\{x\}^\circ = \{x\}^m$, $\{v\}^1 = \{r\}^m/\|r^m\|$ and proceed from Eq. (65) of the GMRES algorithm. There is an intimate relationship between the outer iteration (Newton-Raphson) and the inner iteration (solution of linear equations). If the outer iteration is far from convergence, we can solve the linear system of equations with a rather large tolerance. As the outer iterations converge we must likewise have a finer tolerance for the inner iteration. The method used here is one developed by Diaz, Jines, and Steihaug (1985). Regions of linear and quadratic convergence are defined, and multipliers for the square of the residuals and the residuals are specified. Comparing the magnitude of the terms determines the largest possible tolerance for the inner iteration.

A mathematical theory similar to that for conjugate gradient methods (for example, showing a reduction in condition number with each iteration) is not available. In basic terms the h_m^{m+1} in Eqs. (66) and (67) ensure that the $\{v\}^i$ are orthogonal and that the $\{y\}^m$ in Eqs. (68) and (69) are such that the square of the $\{r\}^{n+1}$ is minimized. For more details the reader is referred to Meijerink and Van der Vorst (1981), Behie and Forsythe (1984), and Behie and Vinsome (1982). To minimize the storage required, the procedure is restarted after every NORTH iteration. The more orthogonalizations before restarting, the faster the convergence, but this benefit must be weighed against the greater storage and longer running time required for the additional orthogonalizations.

F. Dual Porosity Formulation

Many problems are dominated by fracture flow. In these cases the fracture permeability controls the pressure communication in the reservoir even though local storage around the fracture may be dominated by the porous rock which communicates only with the closest fractures. Moench (1984) has studied several wells in the saturated zone beneath Yucca Mountain and found the results could be understood if dual porosity methods were used. Figure 3 depicts the dual porosity concept. The computational volume in the figure consists of a fracture which communicates with fractures in other computational cells, and matrix material which only communicates with the fracture in its computational cells. This behavior of the matrix material is both a physical limitation and a computational tool. The physical limitation results from the model's inability to allow the matrix materials in different cells to communicate directly. This yields only minor errors in saturated zone calculations, but could pose larger errors in the unsaturated zone where capillary pressures would force significant flow to occur in the matrix material. The computational advantages will be addressed at the end of this section.

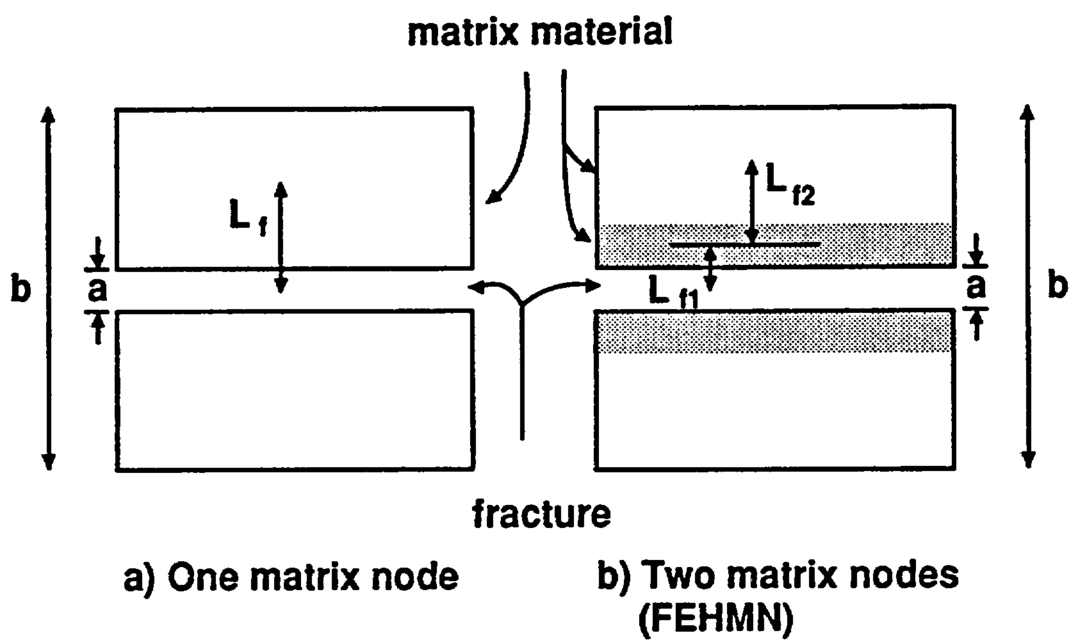

Fig. 3. Computational volume element showing dual porosity parameters.

Two parameters characterize a dual porosity reservoir. The first is the volume fraction, V_f, of the fractures in the computational cell. For the simple system shown in Fig. 3a this fraction is a/b. The second parameter is related to the fracture's ability to communicate with the local matrix material. In the literature this parameter takes a variety of forms. The simplest is a length scale, L_f. This quantifies the average distance the matrix material is from the fracture. This length scale is also shown in Fig. 3a. With just one node in the matrix material the transient behavior in the matrix material cannot be modeled. To improve this situation, two nodes are used in FEHMN to represent the matrix material. Conceptually, this is the same formulation as just described with only additional fracture volume needed (it is assumed the length scale of each matrix volume is proportional to the volume fraction). This is shown in Fig. 3b. More matrix nodes could be added, but data is rarely good enough to justify the use of even two matrix nodes. We note here that the simple slab model depicted in Fig. 3 is just one of several different geometric arrangements. Moench (1984) and Warren and Root (1963) list other reservoir types. All of them are similar in the assumption of a local one dimension connection of the matrix to the fracture.

Computationally, the volume fraction and length scale are used to create one dimensional versions of Eq. (9), Eq. (10), Eq. (16), and Eq. (20). The length scale is used to modify spacial difference terms and the volume factors are used to modify the accumulation terms [the $\hat{C}$ matrix in Eq. (44)]. The volume fractions for FEHMN are given by

V_f $= 1 - V_{f1} - V_{f2}$, volume fraction of fractures
V_{f1} - fraction of first matrix volume (input)
V_{f2} - fraction of second matrix volume (input)
the length scales are given by
L_f $= L_{f0}V_f$, length scale for the fracture volume
L_{f0} - length scale (input)
L_{f1} $= L_{f0}V_{f1}$ length scale of first matrix volume
L_{f2} - $L_{f0}V_{f2}$, length scale of second matrix volume

The geometric factor representing the spacial differencing of the one dimensional equation for flow between the fracture and the first matrix node [analogous to the geometric part of Eq. (46) and Eq. (47)] is given by

$$T_{ff1} = \frac{1.0}{L_{f1}}(L_{f1} + L_f) \quad . \tag{71}$$

The analogous term for the flow from the first matrix volume to the second matrix volume is given by

$$T_{f1f2} = \frac{1.0}{L_{f2}}(L_{f1} + L_{f2}) \quad . \tag{72}$$

The one dimensional nature of the equations provides a computationally efficient method to solve the algebraic equations arising from the dual porosity simulation. Equation (73) shows the matrix equation arising from a dual porosity simulation.

$$\begin{bmatrix} A_{00} & A_{01} & A_{02} \\ A_{10} & A_{11} & A_{12} \\ A_{20} & A_{21} & A_{22} \end{bmatrix} \begin{Bmatrix} P_0 \\ P_1 \\ P_2 \end{Bmatrix} = - \begin{Bmatrix} R_0 \\ R_1 \\ R_2 \end{Bmatrix} \tag{73}$$

Here the subscript 0 refers to the fracture, 1 refers to the first matrix volume, and 2 refers to the second matrix volume.

The P represents the unknown variable or variable pair. The one dimensional character of the matrix diffusion means that the second matrix node can only depend on the first matrix node. Therefore, the submatrix A_{20} is empty. The fact that matrix nodes cannot communicate with matrix nodes in other computational cells means that the submatrices A_{21} and A_{22} are diagonal. Therefore we may write

$$\{P_2\} = [A_{22}]^{-1}[-\{R_2\} - [A_{21}]\{P_1\}] \tag{74}$$

where the inversion is trivial because $[A_{22}]$ is diagonal. Substituting this expression into the equation for the first matrix node we have

$$[A_{10}]\{P_0\} + [A_{11}]\{P_1\} + [A_{12}][A_{22}]^{-1}\Big\{-\{R_2\} - [A_{21}]\{P_1\}\Big\} = -\{R_1\} \quad . \tag{75}$$

Rearranging, we have

$$[A_{10}]\{P_0\} + \Big[[A_{11}] - [A_{12}][A_{22}]^{-1}[A_{21}]\Big]\{P_1\} = -\{R_1\} + [A_{12}][A_{22}]^{-1}\{R_2\}$$

or

$$\{P_1\} = [\widetilde{A}_{11}]^{-1}[\{\widetilde{R}_1\} - [A_{10}]\{P_0\}] \tag{76}$$

where

$$[\widetilde{A}_{11}] = [A_{11}] - [A_{12}][A_{22}]^{-1}[A_{21}]$$

and

$$\{\widetilde{R}_1\} = -\{R_1\} + [A_{12}][A_{22}]^{-1}\{R_2\}$$

where the inversion and multiplications are trivial because of the diagonal nature of the matrices involved. Equation (76) may next be substituted into the equation for the fracture variables. Noting that $[A_{02}]$ is empty (the fracture can only communicate with the first matrix volume) we have

$$[A_{00}]\{P_0\} + [A_{01}][\widetilde{A}_{11}]^{-1}\Big\{\{\widetilde{R}_1\} - [A_{10}]\{P_0\}\Big\} = -\{R_0\} \quad . \tag{77}$$

Rearranging terms we have

$$\Big[[A_{00}] - [A_{01}][\widetilde{A}_{11}]^{-1}[A_{10}]\Big]\{P_0\} = -\{R_0\} + [A_{01}][\widetilde{A}_{11}]^{-1}\{\widetilde{R}_1\} \tag{78}$$

Equation (78) consists of an augmented fracture matrix of the same form as the original fracture matrix $[A_{00}]$. The operations carried out only add a few percent to the solution time required to solve a single porosity system. After the solution of Eq. (78) is obtained with the methods described in Section E, the solution in the fracture volume can be obtained by using Eq. (74) and Eq. (76).

II. CODE DESCRIPTION

In this section we present three important descriptions of FEHMN. First descriptions of all the subroutines are presented. Next the common block variables and calling parameters are described. Finally, the subroutine call tree structure for FEHMN is provided.

A. Subroutines

The main program of the code FEHM is GZ. This program calls subroutine DATA to initialize most of the common block variables and calls subroutine INPUT which initializes most non-array variables and directs the data input. GZ also performs one time startup calculations: scaling of some variables, directing the calculation of element coefficient arrays, and the setting up of equation solution schemes. The major time step loop is contained within GZ. In this loop the model equations are solved at each time step, solution parameters adjusted, and variables updated for the next time step. Plotting data is also output from this loop.

The following subroutines are called from GZ (excluding calls to intrinsic functions): ANONP, BNSWER, COEFFC, CONCEN, CONTR, CO2CTR, DATA, DATCHK, DISK, DUAL, ENTHP, INPUT, NEAR3, PEINT, PLOT, RADIUS, RARNG, RESETV, SETORD, SICE, SLVESU, STEADY, STORSX, STRESS, TIMCRL, TYMING, USER, VARCHK, VELOC, WELBOR, WRTOUT.

Table III contains a complete alphabetical listing of the FEHMN subroutines. A brief description of each routine is provided along with listings of which subroutines call the given routine and which subroutines it calls (intrinsic functions are excluded).

TABLE III. Subroutine Calls Within FEHMN

Name	Description	Calls	Called by
ANONP	Categorize elements. Call routines to generate finite element coefficients.	GENCOF	GZ
BNSWER	Call routines to assemble finite element equations and solve for the Newton-Raphson equations.	VARCHK, OUTBND, GENSL13, GENSL14, GENSL1	INPUT, THRMWC, THERMW
CAPPR	Calculate capillary pressure functions.		GZ, THRMWC
CNSWER	Call routine to generate tracer transport equations. Call tracer equation of state routines.	THERMC, GENCON	CSOLVE

TABLE III. Subroutine Calls Within FEHMN

Name	Description	Calls	Called by
COEFFC	Change coefficients of polynomial fits of the thermodynamic properties specified.		GZ
CONCEN	Organize calls required to run tracer transport model.	RDCON, CSOLVE, WRTCON, PLOTC, DISKC, CONTRC	GZ, WRTOUT, DISK, INPUT, CONTR
CONEQ1	Generate the equations of tracer transport.		GENCON
CONTR	Write out data for time history plots at particular nodes.	CONCEN, VELOC	GZ, TIMCRL
CONTRC	Write out tracer data for contour plots.		CONCEN
CO2CTR	Read input for noncondensible gas and initialize variables associated with the noncondensible gas.	PSAT	GZ, TIMCRL, WRTOUT, INPUT
CSOLVE	Organize tracer solution so smaller time steps can be used for the tracer solution than for the flow solution.	CNSWER, PLOTC1 THERMC	CONCEN
DATA	Initialize common block variables.		GZ
DATCHK	Initial value analysis and data check.		GZ
DISK	Read and/or write to files for restart purposes.	CONCEN, STRESS	GZ,TIMCRL
DISKC	Read and write restart files for tracer variables.		CONCEN
DUAL	Read dual porosity data. Initialize dual porosity variables.	VARCHK, DUALFA, DUALEX	GZ, TIMCRL, GENSL4, GENSL1, INPUT
DUALEX	Extract dual porosity solution from primary variable solution.		DUAL

TABLE III. Subroutine Calls Within FEHMN

DUALFA	Assemble and load dual porosity solution and modify primary variables solution to account for dual porosity effects.	VARCHK, GENEQ1, GENEQ3	DUAL
ENTHP	Calculate the temperature for a given input enthalpy.		GZ, STEADY
GENCOF	Call routines to generate finite element coefficients. Perform the numerical integration of the elements.	GNCF3, GNCF2	ANONP
GENCON	Call routines to generate tracer equations. Call solver to obtain Newton-Raphson equations for tracer variables.	CONEQ1, SOLVE, RD1DOF	CNSWER
GENDAT	Generate coordinates and element information in simple geometric problems.		INPUT, ZONE
GENEQC	Generate equations for Newton-Raphson corrections for the water and noncondensible gas flow.		GENSL4
GENEQ1	Generate equations for Newton-Raphson corrections for water/vapor flow with no noncondensible gas.		DUALFA, GENSL1
GENEQ3	Generate equations for Newton-Raphson corrections for heat conduction only (i.e., permeability).		DUALFA, GERSL4, GENSL1, GENSL3
GENSL1	Call routines to generate the Newton-Raphson equations for water only problems. Call equation solver subroutine.	GENEQ1, GENEQ3, DUAL, NORMAL, SOLVE2, RD2DOF	BNSWER
GENSL3	Call routines to generate the Newton-Raphson equations for heat conductions only. Call equation solver routine.	GENEQ3, SOLVE, RD1DOF	BNSWER
GENSL4	Calls routines to generate equations for water/noncondensible gas problems and calls equation solver.	GENEQC, GENEQ3, DUAL, NORMAL, SOLVE3, RD3DOF	BNSWER

TABLE III. Subroutine Calls Within FEHMN

Name	Description	Calls	Called by
GEOIN	Reads element and coordinate information from MARC preprocessor.	INPUT,ZONE	
GNCF2	Generate 2-D finite element coefficients.	SHAP2R	GENCOF
GNCF3	Generate 3-D finite element coefficients.	SHAP3R, SHAP3P	GENCOF
INPUT	Initialize variables, read input, write out some input information.		CAPPR,CONC CO2CTR,DUA GENDAT,GEC IOFILE,PORO RLPERM, SIC STHER,STRES USER,WELBO ZONE
IOFILE	Open up initial pressure distribution when gravity is present (enabled).		INPUT
LUDBKSB	Performs forward and rock substitution for *N* degree of freedom matrix elements.	SOLVEN	
LUDCOMP	Performs Gauss elemination on *N* degree of freedom matrix elements.	SOLVEN	
NEAR3	Finds nearest node to a set of coordinates.	GZ	
NELMFL	Load nodal connection array.		GENCOF
NOPCNR	Identify form of incomplete LU decomposition matrix for the Newton-Raphson solution matrix with reordering of the node numbering.		SLVESU
NOPCNV	Identify form of LU decomposition matrix for the Newton-Raphson solution matrix with no recording of the node numbers.		SLVESU
NORMAL	Normalize Newton-Raphson equations and calculates sum-squared sum of residuals.		GNSL4, GENS

TABLE III. Subroutine Calls Within FEHMN

Name	Description	Calls	Called by
OUTBND	Test the dependent variables to determine if they are within the bounds set by the thermodynamics properties.		BNSWER
PEINT	Set up initial temperature gradients where gradient information is user specified.		GZ
PLOT	Write out data for time history plots at particular nodes.		GZ, TIMCRL
PLOTC1	Write out tracer data for time history plots. Print out at flow time steps.		CONCEN RDCON
POROSI	Read in data for pressure dependent porosity and permeability models. Calculate porosity and permeability functions.	ROCK	INPUT, WRTOUT, THERMW
PSAT	Calculate the saturation pressure of water for a given temperature.		VARCHK, CO2CTR, THRMWC
RADIUS	Modify finite element coefficients to obtain a radial model.		GZ
RARNG	Rearrange 3-D coordinates to obtain 2-D problems when enabled.		GZ
RDCON	Read in tracer data. Initialize tracer variables.	THERMC PLOTC1	CONCEN
RD1DOF	Solves the equations generated for heat conduction by a reduced degree of freedom method.	SOLVE	GENSL3, GENCON
RD2DOF	Solve the equations generated for the water only problems by the reduced degree of freedom method.	SOLVE	GENSL1
RD3DOF	Solve the equations generated for water/noncondensible gas problems by the reduced degree of freedom method.	SOLVE2, SOLVE	GENSL4

TABLE III. Subroutine Calls Within FEHMN

Name	Description	Calls	Called by
RESETV	Reset the dependent variables to the last time step value. Used when iteration limits are exceeded and a particular time step is restarted.		GZ
RLPERM	Calculate relative permeability functions.		GZ, THRMWC, THERMW
SFN2R	Interpolation routine used by ZONE (2-D).		ZONE
SFN3R	Interpolation routine used by ZONE (3-D).		ZONE
SHAP2R	Evaluate 2-D finite element shape functions at quadrature points.		GNCF2
SHAP3P	Evaluate 3-D prism elements at quadrature points.		GNCF3
SHAP3R	Evaluate 3-D finite elements shape functions at quadrature points.		GNCF3
SICE	Reads in data for simulation with ice present.	STHER	GZ,WRTOUT INPUT
SLVESU	Set up equation solver by identifying fill-in positions in the Newton-Raphson matrix.	NOPCNV, NOPCNR, STORAG	GZ
SOLVE	Solve the one degree of freedom linear system of equation.		RD3DOF, RD2DOF, GENSL3, RD1DOF, GENCON
SOLVEN	Solve the N degree of freedom linear system of equations.	LUBKSB LUDCMP	
SOLVE2	Solve the two degree of freedom linear system of equations.		RD3DOF, GENSL1

TABLE III. Subroutine Calls Within FEHMN

Name	Description	Calls	Called by
SOLVE3	Solve the three degree of freedom linear system of equations.		GNSTR3, GENSL4, RD3DOF
STEADY	Set up initial pressure distribution when gravity is present (enabled).	BNSWER, ENTHP	GZ
STORAG	Write out storage requirements of matrices and arrays associated with the solution of linear equations (Newton-Raphson equations).		SLVESU
STORSX	Manage the storage or retrieval of element coefficients from auxiliary file.	GZ	
THERMC	Evaluate tracer equation of state information.		RDCON, CNSWER
THERMW	Evaluate the thermodynamic properties (density, enthalpy, and viscosity) as a function of pressure and temperature (or saturation).	CAPPR, POROSI RLPERM VFCAL	VARCHK, SOLVE
THRMWC	Evaluate the thermodynamic properties (density, enthalpy, and viscosity) as a function of pressure, temperature and partial pressure of noncondensible gas for water/noncondensible gas problems.	RLPERM CAPPR, PSAT, VFCAL	VARCHK
TIMCRL	Control time step information and stopping criteria.	DUAL, DISK, CO2CTR, PLOT, CONTR	GZ
TYMING	Calculate CPU time for a particular computer run.	SYSTEM CLOCK*	GZ
USER	A user programmed subroutine that provides for changing common block variably every time step. Disabled for YMP work.		GZ,INPUT

*Call is made to the system clock of the computer on which it is run.

TABLE III. Subroutine Calls Within FEHMN

Name	Description	Calls	Called by
USERC	User defined subroutine for changing common variables associated with tracer transport. Disabled for YMP project.		CONCEN
VARCHK	Decide, based on current pressure, temperature and saturation values current phase state (fully saturated, partially saturated). Call routine THERMW or THRMWC to update thermodynamic properties of density, enthalpy, and viscosity. Add the Newton-Ralphson corrections to the dependent variables.	THRMWC, THERMW, PSAT	GZ, BNSWER, DUAL, DUALFA
VELOC	Calculate velocities in coordinate directions.		GZ, CONTR
VFCAL	Change porosity and permeability as functions of pressure (when enabled).		THRMWC, THERMW
WRTCON	Write output for tracer at specified intervals.		CONCEN
WRTOUT	Print output information at a user specified interval.	POROSI, CO2CTR, CONCEN, SICE,	GZ
ZONE	Divide the input problem space by allowing the user to define zones geometrically and then labeling the nodes as to which zone they belong to. These zones are then used to assign properties to the nodes.	GENDAT, SFN3R, SFN2R, GEOIN	INPUT

B. Common Block and Parameter Statements

The common block and parameter statements are contained in INCLUDE files. The INCLUDE files needed to compile FEHMN are COMAI, COMBI, COMCI, COMDI, COMEI, COMFI, COMGI, COMHI, COMII, COMPRI, and DAVIDI. The INCLUDE file COMDTI contain the parameter statements and will be described first. If a variable is entered, the input MACRO statement is indicated parenthetically.

INCLUDE file COMDTI (parameter statements)

Only parameters that are different from those found in COMPRI are described.

N0	- maximum number of nodes allowed
N2	- 2 * N0, storage parameter
N3	- 3 * N0, storage parameter
N4	- array storage parameter for noncondensible gas solution
N5	- array storage parameter for dual porosity solution
N6	- array storage for ice solution
N7	- array storage for tracer solution
N8	- array storage for variable porosity solution
NR	- maximum space allowed for each finite element coefficient array
NBD	- 180 * N0 maximum array space for incomplete LU decomposition matrix
LDN	- maximum array space needed for Jacobian array matrix
NELMD	- maximum array space for element connectivity array and (later) the nodal connectivity array
NNOP	- maximum array space for LU decomposition connectivity array
NN	- maximum number of connected elements
NQ	- maximum array space for each finite element coefficient array associated with the stress solution
NE1	- array size of common block /FEBB/, NELMD + NNOP + 4N0
NE2	- array size of common /FEB/, N0 + 9NR + 6NQ
NE3	- array size of common block /FBS/, 3N0 + 336
NE5	- array size of common block / FCC/, 39N0 + 5N7
NE6	- array size of common block / FDD/, 36N0
NE7	- array size of common block / FDD1/, 14N7 + 870
NE8	- array size of common block / FFD2/, 7N8 + 4
NE9	- array size of common block / FDDI/, 5N0 + 1
NE10	- array size of common block / FHH/, 14N0
NE11	- array size of common block / CO2/, 32N4 + 1
NE12	- array size of common block / FGG/, 9NN + 2N3
NE13	- array size of common block / DUALP/, 23N5
NE14	- array size of common block /FICE/2*N6 +1
NE15	- array size of common block /ICE/N6

INCLUDE File COMAI

common/FAA/

IAB	- iteration counter in stress routines
IAC	- counter for print-out interval
IAD	- current iteration number in flow solution
IACCMX	- maximum iterations allowed for time step increase (tracer solution)
IAMM	- maximum iterations allowed for time step increase (heat and mass solution)
IAMX	- iteration count after which the time step will be halved
ICAPP	- indicates capillary pressure model
ICE	- parameter which indicates if the ICE solution is enabled
ICEN	- parameter which indicates if the tracer solutions enabled
ICF	- parameter indicating status of tracer solution
ICS	- parameter indicating status of tracer solution
ICGTS	- parameter controlling the time of solution parameter changes
ICHNG	- number of thermodynamic region changes
ICNL	- indicates problem dimension
ICO2	- indicates if noncondensible gas solution is enabled (CO2I)
ICONTR	- parameter used in contour plot management
IDOF	- number of degrees of freedom per node for the current problem
IDUALP	- parameter which indicates if the dual porosity solution is enabled (DUAL)
IFINSH	- indicates if the finishing criteria for the simulation is achieved
IHF	- parameter indicating status of flow solution (TRAC)
IHS	- parameter indicating status of flow solution (TRAC)
III	- print-out interval, number of time steps (TIME)
IFLAG	- flag used in input subroutine
IINP	- unit number input file
ILT	- parameter used in time step control
INTG	- indicates integration type used
IPOROS	- indicates if deformation model is enabled (PPOR)
IPQZ	- the number of nodes used for the contour plot output
IPSAT	- parameter regulating call to subroutine PSAT (EOS)
IOUT	- unit number for output file
IREAD	- unit number for restart file (to read)
IREORD	- parameter to reorder system of linear equations
IRPD	- indicates relative permeability model
ISTRS	- parameter indicating if the stress solution is enabled
ISAVE	- unit number for restart file (to write)
ITER	- number of iterations of last call to SOLVE(N) subroutine
ITERT	- intermediate iteration counter
ITOTAL	- total iteration count
ITSAT	- parameter specifying the setting of saturation temperature
IYEAR	- current year in simulation

IVFCAL	- indicates if VFCAL subroutine will be called
IW	- number of storage locations needed to store geometric input types
IWELB	- indicates if wellbore solution is enabled
L	- current time step number
LDA	- parameter which specifies if the geometric coefficients are saved (CTRL)
M	- total number of nodes used for output information (NODE)
MLZ	- out of bounds node
MAXIT	- maximum number of iterations allowed before time step is halved (CTRL)
MINK	- number of active variables
MONTH	- current month in simulation
N	- total number of nodes
NBND	- maximum number of nonzeros per row in the incidence matrix
NCNTR	- contour plot interval (CONT)
NDEM	- coordinate direction perpendicular to the contour plane
NI	- number of integration points per element
NICG	- parameter used in time step control
NEI	- total number of elements in the problem (ELEM)
NEQ	- number of nodes, not including dual porosity nodes (CORD)
NEIGH	- maximum number of neighbors occur in tracer solution
NEMX	- number of unique (geometrically) elements
NORTH	- maximum number of orthogonalizations allowing in (CTRL)
NS	- number of nodes per element (ELEM)
NSAVE	- indicates if a restart file will be created in the current problem
NSNK	- number of source or sink terms
NSTEP	- maximum number of time steps

/FAAR/

AIAA	- time step multiplication factor (CTRL)
AN0	- initial tracer concentration (TRAC)
AM0	- initial mass in problem
AMASS	- current mass in problem
AMP	- initial energy in system problem
ASTEAM	- current steam mass in problem
ASTM0	- initial stem mass in problem
AENER	- current energy in problem
AW	- time step weighting parameter for heat and mass solution (CTRL)
AWC	- time step weighting parameter (TRAC)
AWT	- value of implicitness factor
AY	- time step weighting parameter for tracer (TRAC)
AYC	- time step weighting parameter for tracer
CONTIM	- interval (days) for contour plot output
DAY	- current time step size in days
DAYCF	- time at which tracer solution stops (TRAC)
DAYCMM	- minimum time step size for tracer solution
DAYCMX	- maximum time step size for tracer solution

DAYCS	- time at which tracer solution starts (TRAC)
DAYHF	- time at which flow solution stops (TRAC)
DAYHS	- time at which flow solution starts (TRAC)
DAYMAX	- maximum time step allowed (CTRL)
DAYMIN	- minimum time step allowed (CTRL)
DAYNEW	- parameter used in time step control
DAYS	- current simulation time
DAYSCN	- next time for contour plot
DAYSI	- simulation time at last time step
DAYSP	- time at next time step
DEN	- intermediate value of mass accumulation term
DENE	- intermediate value of energy accumulation term
DEPCNG	- depth at which temperature gradient changes
DIFE	- energy balance error
DIFM	- mass balance error
DITND	- next time step change time
DNWGT	- upwind weighting parameter
DNWGTA	- upwind weighting parameter in tracer solution
DTOT	- current time step size in seconds
DTOTC	- tracer time step size in seconds
DTOTDM	- last time step size in seconds
EPC	- specified solution tolerance for tracer solution
EPE	- tolerance for Newton-Raphson iteration
EPS	- tolerance for linear equation solver
F0	- initial time step residual
FDUM	- current sum squared of residuals
GRAD2	- parameter in description of temperature gradient
GRADNT	- parameter used in description of temperature gradient
GRAV	- value of gravity
G1	- iteration accuracy control parameter (ITER)
G2	- iteration accuracy control parameter (ITER)
G3	- iteration accuracy control parameter (ITER)
OVERF	- over relaxation factor for SOR equations (ITER)
PEIN	- initial pressure of problem (INIT)
POW	- power output for a given time step
QT	- total outflow for time step
QTE	- total energy outflow for time step
QTOT	- total outflow for problem
QTOTE	- total energy outflow for problem
QTOTEI	- intermediate energy flow total
QTOTI	- intermediate flow total
QUAD	- parameter used in temperature gradient
RNMAX	- maximum run time allowed
SECMA	- maximum time step size in seconds

STR	- multiplier for Newton-Raphson corrections
STRD	- multiplier for Newton-Raphson corrections
SV	- vapor saturation of a node
SW	- liquid saturation of a node
TEOUTF	- parameter used in calculation of energy output
TIMS	- ending simulation time (TIME)
TIN	- parameter used in temperature gradient
TIN0	- initial problem temperature (INIT)
TIN1	- parameter used in temperature gradient
TMCH	- machine tolerance (ITER)
TOUTFL	- parameter used in calculation of flow output
UPWGT	- upwind weighting parameter
UPWGTA	- upwind weighting factor for tracer solution (TRAC)
UPWGTB	- upwind weighting factor for tracer solution
VLMAX	- maximum liquid phase velocity
VTOT	- total volume in problem
VVMAX	- maximum vapor phase velocity

common/FAAC/

SSSOL	- indicates if initial steady state solution is needed
VEQNO	- contains version number of FEHMN code used

common/FAAC1/

IDATE	- contains the date (mm/dd/yr)

INCLUDE file COMBI

common/FBB/

NELM(NELMD)	- initially information about nodes in each element, later nodal connectivity information
NOP(NNOP)	- matrix sparsity structure for LU decomposition
NAR(N0)	- array containing gauss elimination order for each node
ISTRW(N0)	- starting positions in sx(nr,9) array of finite element coefficients for each node
KA(N0)	- contains boundary type information for each node
NELMDG(N0)	- contains position of (i,i) element in connectivity array

common/FBC/

SX1(N0)	-	contains volume associated with each node
SX(NR,9)	-	contains finite element geometric coefficients necessary for heat and mass transfer simulation
SXS(NQ,6)	-	contains more finite element geometric coefficients (ie., those necessary for the stress module)

common/FBS/

CORD(N0,3)	-	contains the coordinates of each node
XD(8),YD(8),ZD(8)	-	global coordinates of the nodes in a finite element
SI(8),ETA(8),EXCI(8)	-	local coordinates in a finite element of the numerical integration points
XT(8),YT(8),ZT(8)	-	parameters needed in element calculations
W(8,8)	-	finite element shape functions
WX(8,8)	-	derivative of shape functions with respect to x
WY(8,8)	-	derivative of shape functions with respect to y
WZ(8,8)	-	derivative of shape functions with respect to z
DR(8)	-	contains weights for integration points (bricks, rectangles)
DP(6)	-	contains weights for integration points (prisms, triangles)
WR(8,8)	-	finite element shape functions (rectangles)
WXR(8,8)	-	derivative of shape functions with respect to x (rectangles)
WYR(8,8)	-	derivative of shape functions with respect to y (rectangles)
WZR(8,8)	-	derivative of shape functions with respect to z (rectangles)
WP(8,8)	-	finite element shape functions (prisms)
WXP(8,8)	-	derivative of shape functions with respect to x (prisms)
WYP(8,8)	-	derivative of shape functions with respect to y (prisms)
WZP(8,8)	-	derivative of shape functions with respect to z (prisms)

INCLUDE File COMCI

common/FCC/

DANL(N7)	-	derivative of liquid phase concentration with respect to total concentration
DANV(N7)	-	derivative of vapor phase concentration with respect to total concentration
AKC(N7)	-	tracer accumulation term derivative with respect to total concentration
DRC(N7)	-	tracer source term derivative with respect to total concentration
DEEF(N0)	-	derivative of energy accumulation with respect to energy variable
DEPF(N0)	-	derivative of energy accumulation term with respect to pressure

DMPF(N0) - derivative of mass accumulation term with respect to pressure
DMEF(N0) - derivative of mass accumulation term with respect to energy variable
DQ(N0) - derivative of mass source term with respect to pressure
DQH(N0) - derivative of energy source term with respect to pressure
DEQH(N0) - derivative of energy source term with respect to energy variable
DTPAE(N0) - derivative of temperature with respect to energy variable
DTPA(N0) - derivative of temperature with respect to pressure
DEVEF(N0) - derivative of enthalpy with respect to energy variable
DEVF(N0) - derivative of enthalpy with respect to pressure
DRVPF(N0) - derivative of vapor relative permeability with respect to pressure
DRVEF(N0) - derivative of vapor relative permeability with respect to energy variable
DGLE(N0) - derivative of liquid mass gravity term with respect to energy variable
DGLP(N0) - derivative of liquid mass gravity term with respect to pressure
DELEF(N0) - derivative of liquid enthalpy with respect to energy variable
DELF(N0) - derivative of liquid enthalpy with respect to pressure
DRLPF(N0) - derivative of liquid relative permeability with respect to pressure
DRLEF(N0) - derivative of liquid relative permeability with respect to energy variable
DILE(N0) - derivative of liquid transmissibility with respect to energy variable
DILP(N0) - derivative of liquid transmissibility with respect to pressure
ENLF(N0) - liquid enthalpy
ENVF(N0) - vapor enthalpy
DSTM(N0) - steam mass
DENI(N0) - mass accumulation term
DENEI(N0) - energy accumulation term
DIL(N0) - liquid transmissibility
DIV(N0) - vapor transmissibility
ROLF(N0) - liquid density
ROVF(N0) - vapor density
RLF(N0) - liquid phase relative permeability
RVF(N0) - vapor phase relative permeability
DENCI(N7) - tracer accumulation term
GL(N0) - liquid phase gravity term
GV(N0) - vapor phase gravity term
DIVE(N0) - derivative of vapor transmissibility with respect to energy variable
DIVP(N0) - derivative of vapor transmissibility with respect to pressure
DGVP(N0) - derivative of vapor mass gravity term with respect to pressure
DGVE(N0) - derivative of vapor mass gravity term with respect to energy variable
DPCEF(N0) - derivative of capillary pressure with respect to the energy variable

INCLUDE file COMDI

common/FDD/

THX(N0) - thermal conductivity x-direction

THY(N0) - thermal conductivity y-direction
THZ(N0) - thermal conductivity z-direction
VOLUME(N0) - volume associated at each node
SK(N0) - source strength of each node
ESK(N0) - inlet enthalpy associated with a source
QFLUX(N0) - heat flux at each node
QFLXM(N0) - heat flux impedance at each node
PNX(N3) - permeability in the x-direction, liquid velocity in the x-direction, vapor velocity in the x-direction
PNY(N3) - permeability in the y-direction, liquid velocity in the y-direction, vapor velocity in the y-direction
PNZ(N3) - permeability in the z-direction, liquid velocity in the z-direction, vapor velocity in the z-direction
PS(N0) - porosity at each node
EFLOW(N0) - energy flow at each source node
PHI(N0) - pressure at each node
PHO(N0) - last time step pressure at each node
T(N0) - temperature at each node
TO(N0) - last time step pressure at each node
VF(N0) - volume factor at each node
PFLOW(N0) - flowing pressure at each source node
DENEH(N0) - last time step energy accumulation term at each node
QH(N0) - energy source term at each node
S(N0) - liquid saturation at each node
SO(N0) - last time step saturation at each node
WELLIM(N0) - well impedance at each source node
DENH(N0) - last time step mass accumulation term at each node
DENJ(N0) - last time step mass accumulation time derivative at each node
DENEJ(N0) - last time step energy accumulation time derivative at each node
DENR(N0) - rock density at each node
CPR(N0) - rock specific heat at each node
PCP(N0) - capillary pressure at each node

common/FDDI/

NSKW(N0) - contains nodes for print-out

common/FDD1/

AN(N7) - total tracer concentration at each node
ANL(N7) - liquid tracer concentration at each node
ANV(N7) - vapor tracer concentration at each node
CNSK(N7) - tracer concentration source term at each node

T1SK(N7)	- time when the tracer source term is activated at each node
T2SK(N7)	- time when the tracer source term is terminated at each node
RC(N7)	- tracer source term at each node
DENCH(N7)	- last time step tracer accumulation term at each node
DENCJ(N7)	- last time step tracer accumulation derivative term at each node
ANLO(N7)	- last time step total tracer concentration at each node
FC(N7)	- tracer equation residual at each node
TCX(N7)	- tracer diffusion term in the x-direction
TCY(N7)	- tracer diffusion term in the y-direction
TCZ(N7)	- tracer diffusion term in the z-direction
CM(10)	- total tracer mass for each specie
CM0(10)	- initial total tracer mass for each specie
QCIN(10)	- total injected tracer mass for each specie
QOUT(10)	- total produced tracer mass for each specie
A1ADF(10)	- alpha1 parameter for each specie(nonlinear adsorbtion)
A2ADF(10)	- alpha2 parameter for each specie (nonlinear adsorbtion)
BETADF(10)	- beta parameter for each specie (nonlinear adsorbtion)
A1R	- parameterin reaction rate model
A2R	- parameterin reaction rate model
A3R	- parameterin reaction rate model
A4R	- parameterin reaction rate model
RP1F(25)	- parameter in relative permeability model
RP2F(25)	- parameter in relative permeability model
RP3F(25)	- parameter in relative permeability model
RP4F(25)	- parameter in relative permeability model
RP5F(25)	- parameter in relative permeability model
RP6F(25)	- parameter in relative permeability model
RP7F(25)	- parameter in relative permeability model
RP8F(25)	- parameter in relative permeability model
RP9F(25)	- parameter in relative permeability model
RP10F(25)	- parameter in relative permeability model
RP11F(25)	- parameter in relative permeability model
RP12F(25)	- parameter in relative permeability model
RP13F(25)	- parameter in relative permeability model
RP14F(25)	- parameter in relative permeability model
RP15F(25)	- parameter in relative permeability model
RP16F(25)	- parameter in relative permeability model
RP17F(25)	- parameter in relative permeability model
CP1F(10)	- parameter in capillary pressure model
CP2F(10)	- parameter in capillary pressure model
CP3F(10)	- parameter in capillary pressure model
DIT(300)	- array containing time step changes

common/FDD1I/

NSPECI	- number of species for tracer solution
NSP	- current specie number
NPN	- parameter used in storing tracer data
NPT(10)	- storage parameter used in tracer solution
IADD(10)	- iteration count for tracer solution
IADDT(10)	- iteration count used for linear equation solver in tracer solution
IADSF(10)	- adsorption model used in tracer solution
ICAPT(10)	- capillary pressure model
IRLPT(10)	- relative permeability model
ICNS(10)	- liquid or gas phase tracer model
ICRATE	- reaction rate model
ITC(100)	- array containing information used in time step changes

common/FDD2/

PHINI(N8)	- initial pressure at each node
PSINI(N8)	- initial porosity at each node
DPORP(N8)	- derivative of porosity with respect to pressure at each node
DPORT(N8)	- derivative of porosity with respect to temperature at each node
TINI(N8)	- initial temperature at each node
SIGINI	- parameter used in rock deformation model
PHYDRO	- parameter used in rock deformation model
THEXP	- parameter used in rock deformation model
YOUNG	- parameter used in rock deformation model
AMGANG(N8)	- parameter used in gangi model at each node
PGANGI(N8)	- parameter used in gangi model at each node

common/FICE/

SII(N6)	- ice saturation at each node
SIO(N6)	- last time step value of ice saturation
TMELT	- freezing temperature of water

common/IICE/

ICES(N6) - state of ice at each node

IIEOS(N0) - thermodynamics set at each node
IEOS(N0) - phase state of fluid at each node
IEOSC - phase change parameter
IPORF(N0) - deformation model at each node
IRLP(N0) - relative permeability model at each node
ICAP(N0) - capillary pressure model at each node

INCLUDE file COMEI

common/FEE/

A(LDN) - array containing the Jacobian matrix

common/FFF/

B(NBD) - array containing the incomplete LU decomposition of the Jacobian matrix

common/FHH/

IRB(N0) - array containing the reordered node numbers
IIRB(N0) - inverse of irb
NOPT(N0) - array indicating active variables
NPVT(N0) - pivot information for the LU decomposition matrix
IG(N0) - variable order LU decomposition information
PIV(N0,9) - the pivot elements of the LU decomposition

INCLUDE file COMFI

DMC(N4) - derivative of mass accumulation term with respect to gas at each node
DEC(N4) - derivative of energy accumulation term with respect to gas at each node
DCP(N4) - derivative of gas accumulation term with respect to pressure at each node
DCE(N4) - derivative of gas accumulation term with respect to energy at each node
DQC(N4) - derivative of mass source term with respect to gas
DEQC(N4) - derivative of energy source term with respect to gas
DCQC(N4) - derivative of gas source term with respect to gas

DENPCI(N4) - gas accumulation term at each node
DENPCH(N4) - last time step value of the mass accumulation term at each node
DIVC(N4) - derivative of vapor transmissibility with respect to gas
DGVC(N4) - derivative of vapor gravity term with respect to gas
DCVCF(N4) - derivative of gas concentration with respect to gas
DCVEF(N4) - derivative of gas concentration with respect to energy
DCVF(N4) - derivative of gas concentration with respect to pressure
DEVCF(N4) - derivative of energy with respect to gas
CNVF(N4) - concentration of gas in the vapor phase
DILC(N4) - derivative of liquid transmissibility with respect to gas
DGLC(N4) - derivative of liquid gravity term with respect to gas
ESKC(N4) - source term for gas equation
DCLCF(N4) - derivative of liquid concentration with respect to gas
DCLEF(N4) - derivative of liquid concentration with respect to energy
DCLF(N4) - derivative of liquid concentration with respect to pressure
DELCF(N4) - derivative of liquid energy with respect to gas
CNLF(N4) - gas concentration in the liquid phase
QC(N4) - source term for the gas equation
DCC(N4) - derivative of gas accumulation term with respect to gas
DTPAC(N4) - derivative of temperature with respect to gas
DENPCJ(N4) - last time step accumulation term of gas equation
DCQH(N4) - derivative of gas source term with respect to energy
PCI(N4) - gas pressure
PCIO(N4) - last time step gas pressure
DIFC - noncondensible gas mass balance error

INCLUDE file COMGI

common/FGG/

DFMP(NN) - derivative of mass accumulation term with respect to pressure for neighbor nodes
DFME(NN) - derivative of mass accumulation term with respect to energy for neighbor nodes
DFEP(NN) - derivative of energy accumulation term with respect to pressure for neighbor nodes
DFEE(NN) - derivative of energy accumulation term with respect to energy for neighbor nodes
DFMPC(NN) - derivative of mass accumulation term with respect to gas for neighbor nodes
DFEPC(NN) - derivative of energy accumulation term with respect to gas for neighbor nodes
DFPCP(NN) - derivative of gas accumulation term with respect to pressure for neighbor nodes
DFPCE(NN) - derivative of gas accumulation term with respect to energy for

neighbor nodes

DFPCPC(NN) - derivative of gas accumulation term with respect to gas for neighbor nodes

BP(N3) - array of Newton-Raphson residuals, after solution, an array of Newton-Raphson corrections

BPC(N3) - array of Newton-Raphson residuals for gas, after solution, an array of Newton-Raphson corrections

INCLUDE file COMHI

common/DUALP/

VOLF1(N5) - volume fraction at each node for the first matrix layer
VOLF2(N5) - volume fraction at each node for the second matrix layer
APUV1(N5) - area per unit volume for the first matrix layer
WB11(N5) - array needed to store intermediate dual porosity results
WB12(N5) - array needed to store intermediate dual porosity results
WB21(N5) - array needed to store intermediate dual porosity results
WB22(N5) - array needed to store intermediate dual porosity results
TB11(N5) - array needed to store intermediate dual porosity results
TB12(N5) - array needed to store intermediate dual porosity results
TB21(N5) - array needed to store intermediate dual porosity results
TB22(N5) - array needed to store intermediate dual porosity results
A21MPF(N5) - array needed to store intermediate dual porosity results

A21MEF(N5) - array needed to store intermediate dual porosity results

A21EPF(N5) - array needed to store intermediate dual porosity results
A21EEF(N5) - array needed to store intermediate dual porosity results
A32MPF(N5) - array needed to store intermediate dual porosity results

A32MEF(N5) - array needed to store intermediate dual porosity results

A32EPF(N5) - array needed to store intermediate dual porosity results
A32EEF(N5) - array needed to store intermediate dual porosity results
RB2MF(N5) - array needed to store intermediate dual porosity results
RB2EF(N5) - array needed to store intermediate dual porosity results
RB3MF(N5) - array needed to store intermediate dual porosity results
RB3EF(N5) - array needed to store intermediate dual porosity results

INCLUDE file COMII

common/COEFF/

CEL(20,2) - polynomial coefficients for liquid water enthalpy equations
CRL(20,2) - polynomial coefficients for liquid water density equations
CEV(20,2) - polynomial coefficients for vapor water enthalpy equations

CRV(20,2) - polynomial coefficients for vapor water density equations
CVL(20,2) - polynomial coefficients for liquid water viscosity equations
CVV(20,2) - polynomial coefficients for vapor water viscosity equations
TSA0 - polynomial coefficient for saturation temperature equation
TSPA1 - polynomial coefficient for saturation temperature equation
TSPA2 - polynomial coefficient for saturation temperature equation
TSPA3 - polynomial coefficient for saturation temperature equation
TSPA4 - polynomial coefficient for saturation temperature equation
TSB0 - polynomial coefficient for saturation temperature equation
TSPB1 - polynomial coefficient for saturation temperature equation
TSPB2 - polynomial coefficient for saturation temperature equation
TSPB3 - polynomial coefficient for saturation temperature equation
TSPB4 - polynomial coefficient for saturation temperature equation
PSA0 - polynomial coefficient for saturation pressure equation
PSTA1 - polynomial coefficient for saturation pressure equation
PSTA2 - polynomial coefficient for saturation pressure equation
PSTA3 - polynomial coefficient for saturation pressure equation
PSTA4 - polynomial coefficient for saturation pressure equation
PSB0 - polynomial coefficient for saturation pressure equation
PSTB1 - polynomial coefficient for saturation pressure equation
PSTB2 - polynomial coefficient for saturation pressure equation
PSTB3 - polynomial coefficient for saturation pressure equation
PSTB4 - polynomial coefficient for saturation pressure equation

common/COEFF1/

PMAX(3) - maximum pressure allowed for each coefficient set
PMIN(3) - minimum pressure allowed for each coefficient set
TMAX(3) - maximum temperature allowed for each coefficient set
TMIN(3) - minimum temperature allowed for each coefficient set

common/COEFF2/

EW1 - coefficient used in simplifying thermodynamics relations
EW2 - coefficient used in simplifying thermodynamics relations
EW3 - coefficient used in simplifying thermodynamics relations
EW4 - coefficient used in simplifying thermodynamics relations
EW5 - coefficient used in simplifying thermodynamics relations
EW6 - coefficient used in simplifying thermodynamics relations
EW7 - coefficient used in simplifying thermodynamics relations
EW8 - coefficient used in simplifying thermodynamics relations
EW9 - coefficient used in simplifying thermodynamics relations
EW10 - coefficient used in simplifying thermodynamics relations
EW11 - coefficient used in simplifying thermodynamics relations

EV1	- coefficient used in simplifying thermodynamics relations
EV2	- coefficient used in simplifying thermodynamics relations
EV3	- coefficient used in simplifying thermodynamics relations
EV4	- coefficient used in simplifying thermodynamics relations
EV5	- coefficient used in simplifying thermodynamics relations
EV6	- coefficient used in simplifying thermodynamics relations
EV7	- coefficient used in simplifying thermodynamics relations
EV8	- coefficient used in simplifying thermodynamics relations
EV9	- coefficient used in simplifying thermodynamics relations
EV10	- coefficient used in simplifying thermodynamics relations
EV11	- coefficient used in simplifying thermodynamics relations

INCLUDE file DAVIDI

common/DAVID1/

IRDOF	- reduced degree of freedom model used
ISLORD	- parameter used in the reduced degree of freedom model
IBACK	- LU factorization save parameter
ICOUPL	- number of SOR iterations
ITEST	- parameter used in the reduced degree of freedom model

common/DAVID2/

NMAT(9)	- array used in the reduced degree of freedom method
NRHS(3)	- array used in the reduced degree of freedom method
NMAT32(4)	- array used in the reduced degree of freedom method

C. Subroutine Structure for FEHMN

Figure 4 presents the general subroutine call tree structure for the code FEHMN. Due to its complexity, the entire structure could not fit within a page, hence it is broken into several branches. As an example of the tree's use we trace the call structure from GZ (the main program), which calls INPUT (0003), which calls CONCEN(0021), which calls CSOLVE (0026), which calls CNSWER (0028) which calls THERMC (0028). At subroutine THERMC, the tree is directed to line 0024 where the calls from THERMC have been previously explained. We see that THERMC calls DABS. This was only one path of many possible; all paths may be traversed in a way analogous to above.

```
0001 GZ-------+--TYMING-----*CLOCK
0002          +--DATA
0003          +--INPUT----+--IOFILE
0004          !           +-*IABS
0005          !           +-*MAXO
0006          !           +--STHER
0007          !           +--GEOIN
0008          !           +--USER
0009          !           +--ZONE-----+--GEOIN
0010          !           !           +-*IABS
0011          !           !           +--GENDAT
0012          !           !           +--SFN3R
0013          !           !           +-*SQRT
0014          !           !           +-*ABS
0015          !           !           +--SFN2R
0016          !           +--POROSI---+-*IABS
0017          !           !           +-*MAXO
0018          !           !           +--ROCK-------*MAXO
0019          !           +-*DABS
0020          !           +--GENDAT
0021          !           +--CONCEN---+--RDCON----+-*DMIN1
0022          !           !           !           +-*MAXO
0023          !           !           !           +-*IABS
0024          !           !           !           +--THERMC-----*DABS
0025          !           !           !           +--PLOTC1
0026          !           !           +--CSOLVE---+-*DMIN1
0027          !           !           !           +-*DABS
0028          !           !           !           +--CNSVER---+--THERMC----> 0024
0029          !           !           !           !           +--GENCON---+--CONEQ1
0030          !           !           !           !                       +-*DSQRT
0031          !           !           !           !                       +-*DMAX1
0032          !           !           !           !                       +-*DMIN1
0033          !           !           !           !                       +--SOLVE----+-*DSQRT
0034          !           !           !           !                       !           +-*DMAX1
0035          !           !           !           !                       !           +-*DABS
0036          !           !           !           !                       +--RD1DOF---+-*DSQRT
0037          !           !           !           !                                   +--SOLVE-----> 0033
0038          !           !           !           +--THERMC----> 0024
0039          !           !           !           +--PLOTC1
0040          !           !           +--WRTCON-----*DABS
0041          !           !           +--DISKC
0042          !           !           +--CONTRC
0043          !           +--STRESS
0044          !           +--CO2CTR---+-*MAXO
0045          !           !           +-*IABS
0046          !           !           +--PSAT-------*DABS
0047          !           !           +-*DABS
0048          !           +--DUAL-----+--VARCHK---+-*MAXO
0049          !           !           !           +--PSAT------> 0046
0050          !           !           !           +-*DABS
0051          !           !           !           +--THRMWC---+--RLPERM---+-*IABS
0052          !           !           !           !           !           +-*MAXO
0053          !           !           !           !           !           +-*DSQRT
0054          !           !           !           !           +--CAPPR----+-*IABS
0055          !           !           !           !           !           +-*MAXO
0056          !           !           !           !           +--PSAT------> 0046
0057          !           !           !           !           +--VFCAL----+-*DLOG
0058          !           !           !           !                       +-*DEXP
0059          !           !           !           +--THERMW---+--RLPERM----> 0051
0060          !           !           !                       +--POROSI----> 0016
0061          !           !           !                       +--CAPPR-----> 0054
0062          !           !           !                       +--VFCAL-----> 0057
0063          !           !           +-*DMAX1
0064          !           !           +--DUALFA---+--VARCHK----> 0048
0065          !           !           !           +--GENEQ1
0066          !           !           !           +--GENEQ3
```

Fig. 4. Structure for subroutine calls for FEHMN.

```
0067            !           !           !           +-@ALI
0068            !           !           !           +-@ALN
0069            !           !           +--DUALEX-----@ALN
0070            !           +--CAPPR-----> 0054
0071            !           +--RLPERM----> 0051
0072            !           +--SICE-----+-*IABS
0073            !           !           +-*MAXO
0074            !           !           +--STNER
0075            !           +--VELBOR
0076            +-*MAXO
0077            +--NEAR3------*DSQRT
0078            +--CONTR----+--VELOC----+-*DSQRT
0079            !           !           +-*DMAX1
0080            !           !           +-*DABS
0081            !           +--CONCEN----> 0021
0082            +--ANONP----+-*DSQRT
0083            !           +-@TP
0084            !           +-@AL
0085            !           +-*DABS
0086            !           +-@VP
0087            !           +-*IABS
0088            !           +-*MAXO
0089            !           +--GENCOF---+--GNCF3----+--SHAP3R-----*DSQRT
0090            !                       !           +--SHAP3P
0091            !                       +--GNCF2-------SHAP2R-----*DSQRT
0092            +--STORSX
0093            +-*DABS
0094            +--DISK-----+--CONCEN----> 0021
0095            !           +--STRESS
0096            +--PEINT----+-*DABS
0097            !           +-*DMAX1
0098            +--RARNG
0099            +--RADIUS
0100            +--SLVESU---+--NOPCNV---+-*MAXO
0101            !           !           +-*MINO
0102            !           +--NOPCNR---+-*MAXO
0103            !           !           +-*MINO
0104            !           +--STORAG-----*MINO
0105            +--SETORD
0106            +--DUAL------> 0048
0107            +--CO2CTR----> 0044
0108            +--COEFFC
0109            +--SICE------> 0072
0110            +--VARCHK----> 0048
0111            +--STEADY---+-*DABS
0112            !           +--ENTHP
0113            !           +--BNSVER---+--VARCHK----> 0048
0114            !                       +--OUTBND
0115            !                       +--GENSL3---+--GENEQ3
0116            !                       !           +-*DSQRT
0117            !                       !           +-*DMAX1
0118            !                       !           +-*DMIN1
0119            !                       !           +--SOLVE-----> 0033
0120            !                       !           +--RD1DOF----> 0036
0121            !                       +--GENSL4---+--GENEQC
0122            !                       !           +--GENEQ3
0123            !                       !           +--DUAL------> 0048
0124            !                       !           +--NORMAL---+-@ALI
0125            !                       !           !           +-@ALN
0126            !                       !           !           +-@ALI3
0127            !                       !           !           +-@ALN3
0128            !                       !           +-*DSQRT
0129            !                       !           +-*DMAX1
0130            !                       !           +-*DMIN1
0131            !                       !           +--SOLVE3---+-*DSQRT
0132            !                       !           !           +-@ALI
```

Fig. 4. (Continued)

```
0133            !                       !           !           +-BALN
0134            !                       !           !           +-*DMAX1
0135            !                       !           !           +-*DABS
0136            !                       !           +--RD3DOF---+--SOLVE2---+-*DSQRT
0137            !                       !                       !           +-BALI
0138            !                       !                       !           +-BALN
0139            !                       !                       !           +-*DMAX1
0140            !                       !                       !           +-*DABS
0141            !                       !                       +--SOLVE-----> 0033
0142            !                       +--GENSL1---+--GENEQ1
0143            !                                   +--GENEQ3
0144            !                                   +--DUAL------> 0048
0145            !                                   +--NORMAL----> 0124
0146            !                                   +-*DSQRT
0147            !                                   +-*DMAX1
0148            !                                   +-*DMIN1
0149            !                                   +--SOLVE2----> 0136
0150            !                                   +--RD2DOF---+--SOLVE-----> 0033
0151            !                                               +-*DSQRT
0152            +--CONCEN----> 0021
0153            +--PLOT
0154            +--DATCHK---+-*DMIN1
0155            !           +-*DMAX1
0156            +--TIMCRL---+--DUAL------> 0048
0157            !           +--DISK------> 0094
0158            !           +--CO2CTR----> 0044
0159            !           +--PLOT
0160            !           +--CONTR-----> 0078
0161            !           +-*ABS
0162            +--USER
0163            +--WELBOR
0164            +--ENTHP
0165            +--BNSWER----> 0113
0166            +--RESETV
0167            +--STRESS
0168            +--VELOC-----> 0078
0169            +-*DMAX1
0170            +--WRTOUT---+-*MAXO
0171            !           +-*DFLOAT
0172            !           +--POROSI----> 0016
0173            !           +--CO2CTR----> 0044
0174            !           +--CONCEN----> 0021
0175            !           +--STRESS
0176            !           +--SICE------> 0072
0177            +-*MOD
```

Fig. 4. (Continued)

III. USER'S MANUAL

This section provides the instructions necessary for using the code FEHMN. Section A describes an automatic mesh generation code, GENMSH, that can be used to generate the finite element mesh input required by FEHMN. Section B describes in detail the input macro-commands for FEHMN. A graphics postprocessor is described in Section C and several example problems are given in Section D.

A. Automatic Mesh Generation

The code GENMSH, which is designed to be used in conjunction with the finite element code FEHMN, operates by dividing a user-defined solution space into a prescribed number of finite elements. The solution space may be either two or three dimensional. In order to simplify geometric considerations, the solution space is broken up into a number of "blocks." Each block is then further divided into "elements." A given block uses the same "type" of element throughout, although the elements need not be of the same size. Different blocks may use different types of elements. The choice of elements available in two dimensions for output to FEHMN are 4-noded quadrilaterals and 3-noded triangles. In three dimensions, the choice is 8-noded quadrilateral polyhedrons or 3-noded triangular prisms, shown schematically in Fig. 5.

The solution space, and each block, is defined by giving the corner and/or midpoint nodes. This amounts to specifying 4 or 8 nodes per block in 2-D problems and 8 or 20 nodes per block in 3-D problems as shown in Fig. 6. The same block definition is needed for both quadrilateral and triangular elements. After discretizing the solution space and the blocks, it is necessary to specify the desired division of each block into elements. This is done by specifying the relative weights of each subdivision in each direction for each block. The reader is referred to *An Introduction to Finite Element Computations* by Hinton and Owen (pp. 328-346) for the details of the procedure and the algorithm. Note that material properties are specified at each node in FEHMN, unlike conventional finite element procedure.

A detailed description of the input to the code follows. The input must be placed in a file called MDAT. Examples of the MDAT file are given in Section D. The output is found on a file called GEOM.DAT. The output consists of a list of nodal coordinates and elements in a suitable format for the code FEHMN. Free format is used for the input. In addition, a zone definition of the input blocks is provided in file ZONE. The files GEOM.DAT and

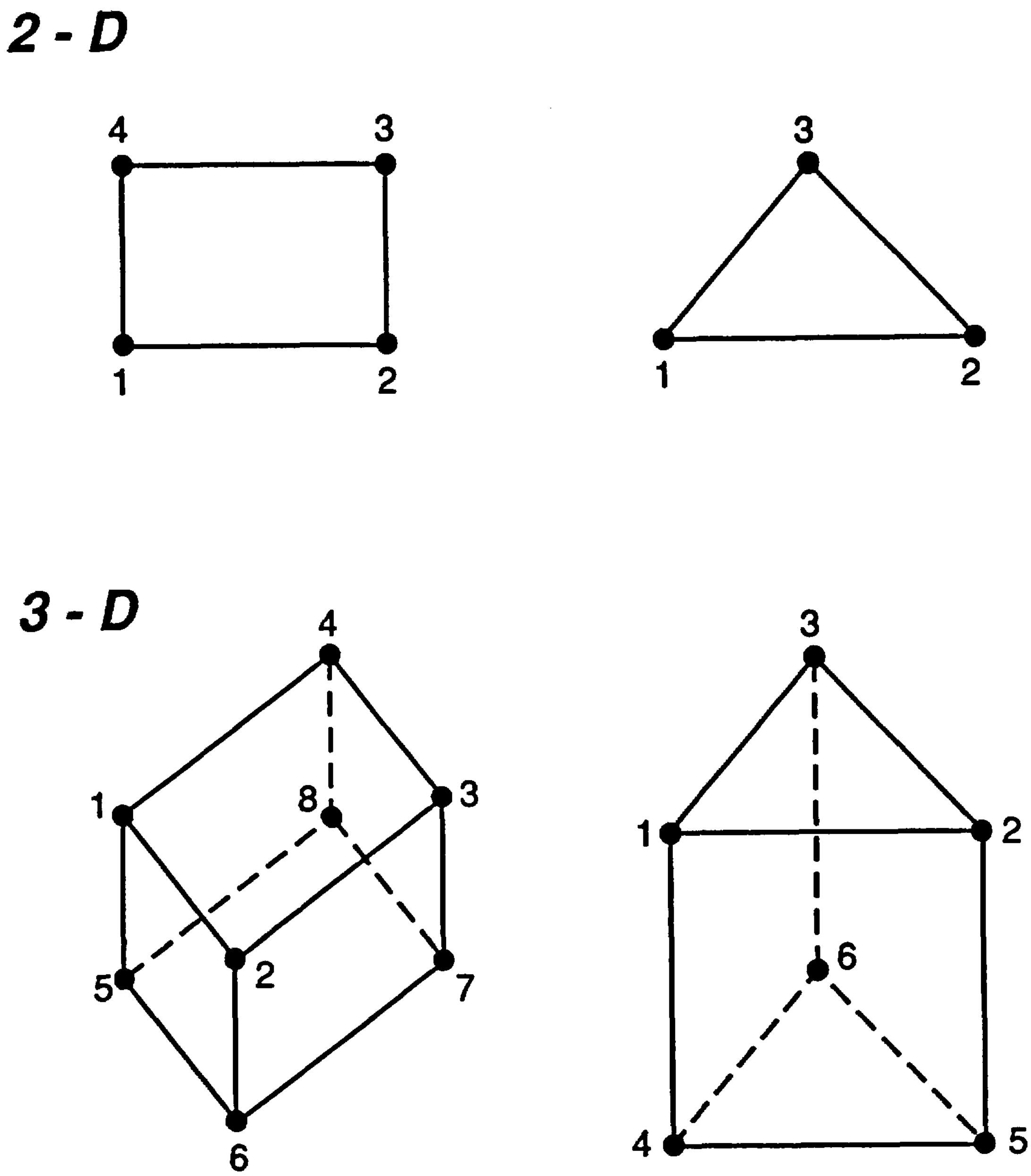

Fig. 5. Elements available with FEHMN in 2-D and 3-D problems showing numbering convention.

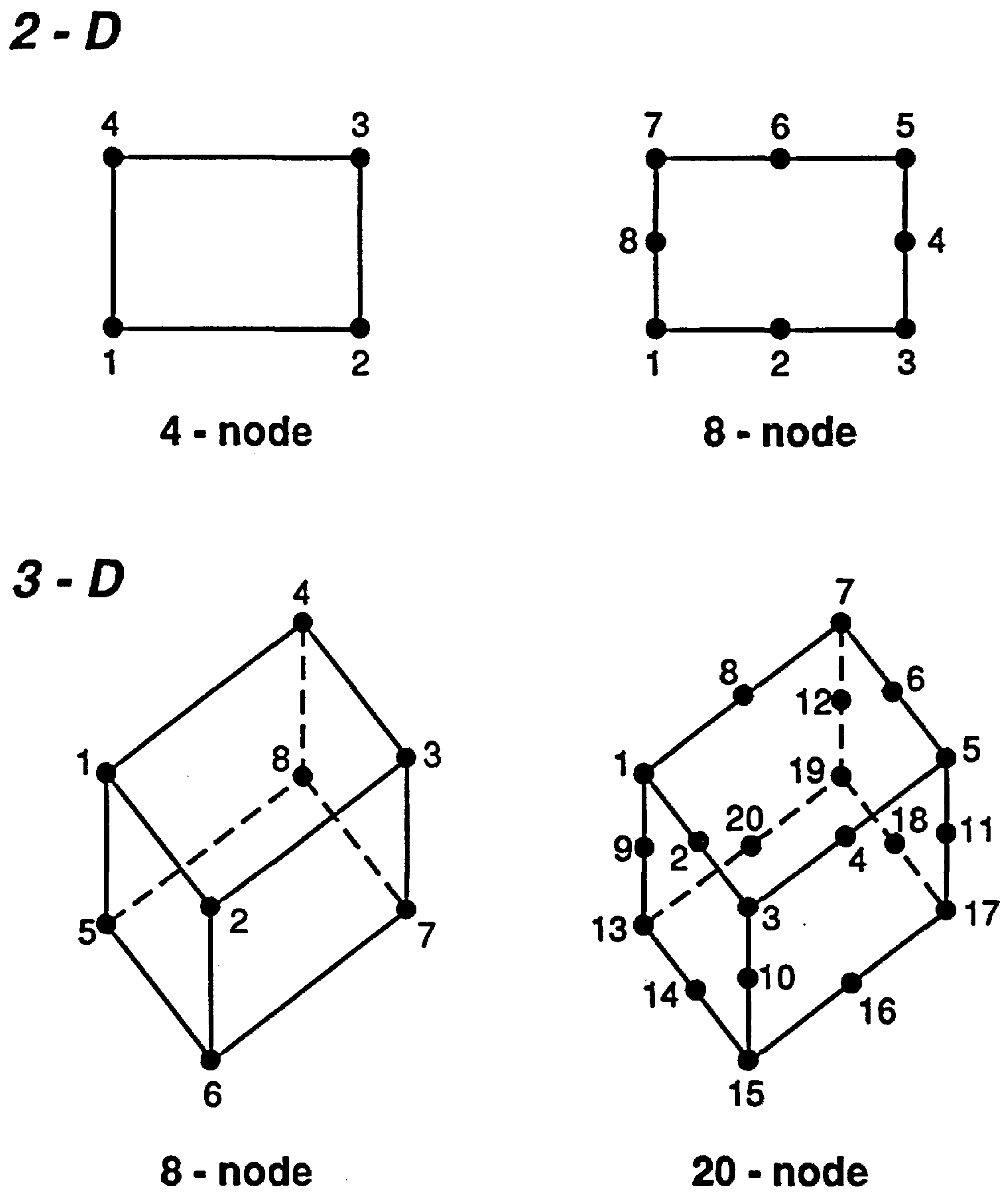

Fig. 6. Nodal ordering for defining 2-D and 3-D domain blocks for input to GENMSH.

ZONE may be used directly in the input file for FEHMN as they already include the appropriate macro command headings.

Group 1

Title, up to 80 characters long

Group 2

NPOIN, NELEM, LNODE, IT, NDIME, KF, NRN

NPOIN - total number of points used to define the solution space

NELEM - number of blocks used to define the solution domain

LNODE - number of nodes per block used to define the solution domain

IT - element triangulation parameter, if IT=0, then no element splitting occurs, if IT$\neq$ 0, then triangle elements are generated in 2-D and prism elements are generated in 3-D.

NDIMB - dimension of problem (2 or 3)

KF - determines the vertical axis direction in 2-D. If KF $<$ 0 then the y-axis is positive downward. If KF $\geq$0, the y-axis is positive upward in 3-D, the z-axis is always positive upward. See note on plotting below.

NRN - renumber parameter. If NRN $\neq$ 0 the code will renumber to minimize the band width. If NRN = 0 then no renumbering will occur.

Group 3 (NUMEL, Block Times)

NUMEL, (LNODS(NUMEL,INOD), INODE = 1, LNODE)

NUMEL - Block number

LNODS (NUMEL, INOD) - LNODE nodes defining the block NUMEL

Group 4

CORDX (I), I = 1, NPOIN

CORDX (I) - x-coordinates of points used to define the solution space

Group 5

CORDY (I), I = 1, NPOIN

CORDY (I) - y-coordinates of points used to define the solution space

Group 6 (only if NDIME = 3)

CORDZ (I), I = 1, NPOIN

CORDZ (I) - z-coordinates of points used to define the solution space

NOTE: Groups 7-10 are repeated for each block.

Group 7

KBLOC, NDIVX, NDIVY, NDIVZ

KBLOC - block number

NDIVX - number of divisions in x-direction

NDIVY - number of divisions in y-direction

NDIVZ - number of divisions in z-direction (only if NDIME = 3).

NOTE: The number of nodes in a direction = number of divisions + 1.

Group 8

WEITX (I), I = 1, NDIVX

WEITX (I) - weighting of the Ith division in the x-direction in block KBLOC

Group 9

WEITY (I), I = 1, NDIVY

WEITY (I) - weighting of the Ith division in the y-direction in block KBLOC

Group 10

WEITZ (I), I = 1, NDIVZ (only if NDIME = 3)

WEITZ (I) - weighting of the Ith division in the z-direction in block KBLOC

Group 11 (only if NDIME = 3)

XV, YV, ZV

XV - x-coordinate of viewing point for 3-D plot

YV - y-coordinate of viewing point for 3-D plot

ZV - z-coordinate of viewing point for 3-D plot

NOTE: XV = 300, YV = 300, ZV = 50 gives a good viewing angle for many problems.

Group 12 (only if NDIME = 3)

XMIN, XMAX, YMIN, YMAX, ZMIN, ZMAX

XMIN - minimum x-cordinate for plot of mesh

XMAX - maximum x-coordinate for plot of mesh
If XMIN = XMAX then the limits will be determined from the generated mesh

YMIN - minimum y-cordinate for plot of mesh

YMAX - maximum y-coordinate for plot of mesh
If YMIN = YMAX then the limits will be determined from the generated mesh

ZMIN - minimum z-cordinate for plot of mesh

ZMAX - maximum z-coordinate for plot of mesh
If ZMIN = ZMAX then the limits will be determined from the generated mesh

Group 13 (optional)

NREF, XR, YR, ZR, IRFN

NREF - reference node for refinement
XR - x-coordinate of reference node
YR - y-coordinate of reference node
ZR - z-coordinate of reference node
IRFN - refinement level for reference node

If NREF < 0 then the node closest to the reference coordinates is used as the reference node. If IRFN < 0 then the node closest to the reference coordinates is used as the reference node **and** the coordinates set to the reference coordinates.

The refinement level is ABS (IRFN). If the refinement level is 1 then the elements surrounding the reference node are subdivided once and new elements created. A refinement level of 2 means this is done twice, and so on.

Note on plotting. If KF $\neq 0$ in Group 2 a plot of the mesh is provided, and if $ABS(KF) > 1$ node numbers are printed on the plot.

B. Macro Command Input For FEHMN

The finite element heat and mass transfer code (FEHMN) contains a macro control structure for data input that offers added flexibility to the input process. Blocks of data can be entered in any order, and any blocks unnecessary to a particular problem can be disregarded. All entries are free format, which adds flexibility, but requires that values be entered for all input variables (no assumed null values). As an aid to the user, the capabilities of FEHMN are summarized in Table IV with reference to the macro commands. Values of parameters are entered either by node number or a geometric description (macro command **ZONE**). The user is encouraged to read the macro **ZONE** description.

TABLE IV. Capabilities of FEHMN with Macro Command References

I.	Mass, energy balances in porous media A. Variable rock properties (**ROCK**) B. Variable permeability (**PERM**) C. Variable thermal conductivity (**COND**) D. Variable fracture properties, dual porosity (**DUAL**)
II.	Multiple components available A. Air water mixture available, fully coupled to heat and mass transfer (**NCON**) B. Up to 10 passive tracers available (**TRAC**) C. Several different capillary pressure models (**CAP**) D. Several different relative permeability models (**RLP**)
III.	Equation of state flexibility inherent in code (**EOS**)
IV.	Psuedo-stress models available A. Linear porosity deformation (**PPOR**) B. Gangi stress model (**PPOR**)
V.	Numerics A. Finite element with multiple element capabilities (**ELEM**) B. Short form input methods available (**COOR, ELEM**) C. Flexible properties assignment (**ZONE**) D. Flexible solution methods 1. Upwinding, implicit solution available (**CTRL**) 2. Iteration control adaptive strategy (**ITER**)
VI.	Flexible time step and stability control (**TIME**)

TABLE V. FEHMN Files

TAPEn1($1 \leq$ n1 ≤ 10)	input file (user supplied)
TAPEn2($11 \leq$ n2 ≤ 20)	output file (code generated)
TAPEn3($21 \leq$ n3 ≤ 30)	initial value tape (read a restart, user supplied)
TAPEn4($31 \leq$ n4 ≤ 40)	final value tape (write a restart, code generated)
FE.HIS	time history of variables (code generated)
FE.CON	contour plot data (code generated)
FE.MIS	contains program information of the code crashes (code generated)
FE.TRC	tracer time history data (code generated)
STOR.FE	storage of finite element coefficients (user supplied or code generated)
FE.CHK	contains input analysis

Although most input data are contained in the input deck, some information must first be entered from the **terminal**. Most of the information required before the input deck can be read pertains to input and output files and is prompted for from within the program. Figure 7 shows the output for a typical FEHMN run on a CRAY computer. All files are of the form TAPEn, where *n* is the tape (unit) number. Table V contains a description of FEHMN files. The terminal input follows:

(free format) INPT, IOUT, IREAD, ISAVE, IDC

INPT - unit number of the input file

IOUT - unit number of the file to which nodal information (pressures, enthalpies, etc.) is printed

IREAD - unit number of file on which initial values of pressure and enthalpy are found. (If IREAD = 0, initial values are generated from input data. See macro control statement **PRES**)

ISAVE - unit number of file on which final time nodal information is printed for restart purposes (if ISAVE = 0, no restart file is created).

IDC - user subroutine parameter
if IDC = 0 the code makes no USER subroutine calls
if IDC $\neq$ 0 the code calls subroutine USER (user defined) at each time step. The form is CALL USER (IDC).

In Fig. 8, the user entered data is after the "?". Here INPT = 1, IOUT = 11, IREAD = 0, ISAVE = 0, and IDC = 0. The remainder of the data is read from unit INPT (which was defined above).

The macro command structure makes use of a set of control statements recognized by the input module of the program. When a macro control statement is encountered in the input deck, a certain set of data is expected and read from the input deck. In this way, the input is divided into separate, unordered blocks of data. The input deck is therefore a collection of macro control statements, each followed by its associated data block, as the example input files (Section D) show. Note that, although the input is free format, macro control statements must appear in the first four columns of a line. Table VI lists the macro control statements with brief descriptions of the data associated with each. The macro control statements may be in any order, although the data associated with each macro control statement must follow with the prescribed format. Some statements are necessary and others are optional, as indicated in Table VI.

A detailed list of the macro control statements and the input variables associated with each is given in Table VII. In Section D example input files are given.

```
xfehmz / 6 1.2

version  fehm.4.0   ,george zyvoloski(505 6671581)


**** program files must obey the following conventions ****

          input files: tape1-10
          output files: tape11-20
          read files(if they exist): tape21-30
          write files(if they exist): tape31-40

**** note ****

     history plot file is fe.his
     contour plot file is fe.con
     tracer plot file is fe.trc
     input check file is fe.chk
     fe.mis is used for error recovery

**** and ****

     tape59(terminal) is available for any use

input tape,output file,rd tape,wt tape,user call/step
? 1 11 0 0 0
 input title : node
 input title : rlp
 input title : sol
 input title : init
 input title : rock
 input title : cond
 input title : perm
 input title : flow
 input title : time
 input title : ctrl
 input title : coor
 input title : elem
 input title : stop
 stop
xfehmz   ctss time      41.483   seconds
cpu=     18.305 i/o=     2.519 mem=     20.660
```

Fig. 7. Terminal output for a FEHMN run on a CRAY computer.

TABLE VI. Macro Control Statements for FEHMN

Control Statement	Description
CAP	capillary pressure data, optional.
COOR	node coordinate data, **required.**
COND	thermal conductivity data, **required.**
CONT	contour plot data, optional.
CTRL	program control parameters, **required.**
DUAL	input for dual porosity solution, optional.
ELEM	element node data, **required.**
EOS	equation of state data, optional.
FLOW	flow data, optional.
HFLX	heat flux data, optional.
INIT*	initial value data, optional.
ITER	iteration parameters, optional.
NGAS	noncondensible gas (air) data, optional.
NODE	node numbers for output and time histories, **required.**
PERM	permeability and velocity data, **required.**
PPOR	pressure and temperature dependent porosity and permeability, optional.
PRES	initial pressure and enthalpy data, optional.
RLP	relative permeability data, optional (**required** for 2-phase problem).
ROCK	rock density, specific heat, and porosity data, **required.**
SOL	solution specifications, **required.**
STEA	steady state solution generated for initial variable field, optional.
STOP	signals the end of input, **required.**
TEXT	text input, optional.
TIME	time step and time of simulation data, **required.**
TRAC	tracer data, optional.
ZONE	geometric definition of grid for input definition, optional.

*One or both INIT and PRES macros are necessary.

The user is encouraged to look at the file FE.CHK. This file contains information on where the maximum and minimum input parameters occur and suggestions on decreasing the storage requirements for the run; it also summarizes initial mass and energy values.

Many input parameters such as porosity or permeability vary throughout the grid and need to be assigned different values on different nodes. This is accomplished in two ways. The first is a nodal loop-type definition:

JA,JB,JC,PROP1,PROP2, ...

where

JA	- first node to be assigned with the properties PROP1, PROP2 ...
JB	- last node to be assigned with the properties PROP1, PROP2 ...
JC	- loop increment for assigning properties PROP1, PROP2, ...
Prop1,Prop2	- properties to be assigned to the nodes.

In the input blocks to follow one or more properties are manually entered in the above structure. When a value of 0 is entered for any JA, that input block is terminated and the code proceeds to the next group or control statement.

The nodal definition above is useful in simple geometries where the node numbers are easily found. The boundary nodes, in this case come at regular node intervals and the increment counter JC can be adjusted so the boundary conditions are easily entered.

In more complicated geometries, such as 3-D grids, the node numbers are often difficult to determine. Here a geometric description is preferred. To enable the geometric description the control statement **ZONE** (p. 74) is used in the input file before the other property macro statements occur. The input macro **ZONE** requires the specification of the coordinates of 4-node parallelograms for 2-D problems and the 8-node polyhedrons in 3-D. In one usage of the control statement **ZONE** all the nodes are placed in geometric zones and assigned an identifying number. This number is then addressed in the property input macro commands by specifying a JA < 0 in the definition of the loop parameters given above. For example if JA = -1, the properties defined on the input line would be assigned to the nodes defined as belonging to geometric Group 1. The control statement **ZONE** may be called more than once to redefined geometric groupings.

TABLE VII. Input Description for FEHMN

Control Statement CAP (optional)

Capillary pressure model [see Eq. (29)]

Group 1- ICAP(i), cp1(i), cp2(i), cp3(i),

ICAP(i) - Relative permeability model type

ICAP(i) = 1, linear capillary pressure

cp1(i) - maximum capillary pressure

cp2(i) - maximum liquid saturation for capillary pressure calculation

cp3(i) - not used

Note: Only ICAP(I) = 1 is allowed. The parameter *i* is incremented each time a Group 1 line is read. Group 2 lines will refer to this parameter. Group 1 is ended when a line with ICAP(i) = 0 is encountered.

Group 2- JA, JB,JC, ICAPT

JA, JB, JC - defined on page 60

ICAPT - reference counter for model defined in Group 1

It is recommended that macro **CAP** be preceded by macro RLP because capillary pressures are defined in macro RLP if van Genuchten models are employed. Care should be taken to ensure that capillary pressures are not defined twice.

Control statement COOR (required)

Group 1 - N

N - number of nodes in the grid

Group 2 - MB, CORD1, CORD2, CORD3

MB - node number. If MB < 0 then the difference between the absolute value of MB and the previously read absolute value of MB is used to generate intermediate values by interpolation.

CORD1 - x-coordinate (m) of node MB

CORD2 - y-coordinate (m) of node MB

CORD3 - z-coordinate (m) of node MB

NOTE: To end the control section a line with MB = 0 is entered.

Control statement COND (required)

Assign thermal conductivities of the rock [see Section I-B, Eq. (6)]

Group 1 - JA, JB, JC, THXD, THYD, THZD

JA, JB, JC - defined on page 60

THXD - thermal conductivity (W/mK) in the x-direction

THYD - thermal conductivity (W/mK) in the y-direction

THZD - thermal conductivity (W/mK) in the z-direction

Control statement CONT (optional)

Group 1 - NCNTR, CONTIM

NCNTR - time step interval for contour plots

CONTIM - time (days) interval for contour plots

NOTE: the contour data will be output whenever either of the above criteria is satisfied

Control statement CTRL (required)

Assign various control parameters needed for equation solvers and matrix solver routines (see Section I-D)

Group 1 - MAXIT, EPM, NORTH [see Eqs. (55)-(68)]

MAXIT - maximum number of iterations allowed in either the overall Newton cycle or the inner cycle to solve for the corrections at each iteration [see Eqs. (55)-(57) and Eqs. (63)-(68)]

EPM - tolerance for Newton cycle (nonlinear equation tolerance)

NORTH - number of orthogonalizations in the linear equation solver [see Eqs. (63)-(65)]

Group 2 - JA, JB, JC, IGAUS [see Eqs. (58)-(62)]

JA, JB, JC - defined on page 60

IGAUS - the order of partial Gauss elimination

Group 3 - AS, GRAV, UPWGT

AS - implicitness factor [see Eq. (40)]
if AS $\leq$ 1, a standard pure implicit formulation will be used
if AS $\geq$ 1, a second-order implicit method will be used

GRAV - direction of gravity 1 = x-direction, 2 = y-direction, 3 = z-direction. If GRAV > 3, GRAV is set equal to 3. If GRAV = 0, then no gravity is used. If GRAV $\neq$ 0 then a value of gravity of 9.8 m/s^2 is used in the code.

UPWGT - value of upstream weighting (0.5 $\leq$ UPWGT $\leq$ 1.0) [see Sec. I-C, and the paragraph following Eq. (49)]
If UPWGT < 0.5 UPWGT is set to 0.5
If UPWGT > 1.0 UPWGT is set to 1.0

Group 4 - IAMM, AIAA, DAYMIN, DAYMAX

IAMM - maximum number of iterations for which the code will multiply the time step size

AIAA - time step multiplier (see Sec. I-D)

DAYMIN - minimum time step size (days)

DAYMAX - maximum time step size (days)

Group 5 - ICNL, LDA

ICNL - parameter that specifies the geometry

if ICNL = 0	three-dimensional
if ICNL = 1	X - Y slice
if ICNL = 2	X - Z slice
if ICNL = 3	Y - Z slice

if ICNL = 4 X - Y radial slice
if ICNL = 5 X - Z radial slice
if ICNL = 6 Y - Z radial slice

LDA - parameter that specifies the external storage of geometric coefficients
LDA = +1, element coefficients are read in from file STOR.FE and no coefficients are calculated in the code (note: STOR.FE must be in local file space)
LDA = 0, element coefficients are calculated in the code and not saved
LDA = -1, element coefficients are calculated in the code and saved on file STOR.FE

Control statement DUAL (optional, see Section F)

Group 1 - JA, JB, JC, VOLFD1

JA, JB, JC - defined on page 60
VOLFD1 - volume fraction for first matrix node

Group 2 - JA, JB, JC, VOLFD2

JA, JB, JC - defined on page 60
VOLFD2 - volume fraction for second matrix node

Group 3 - JA, JB, JC, APUVD

JA, JB, JC - defined on page 60
APUVD - area per unit volume (length scale) for the matrix nodes

The quantities VOLFD1 and VOLFD2 are volume fractions and related to the total volume by

$$\text{VOLFD1} + \text{VOLFD2} + \text{VOLFF} = 1.0$$

where VOLFF is the volume fraction of the fractures. The above relation must be satisified at all nodes.

Control statement ELEM (required)

Group 1 - NS, NEI,

NS - number of nodes per element
NEI - number of elements

Group 2 - MB, NELM (1), NELM (2)... NELM (NS)

MB - node number. If MB < 0 then the difference between the absolute value of MB and the previous absolute value of MB is used to generate intermediate values by interpolation in the code.

NELM (1) - first node of element MB
NELM (2) - second node of element MB
NELM (NS) - last node of element MB

NOTE: To end the control section a line with MB = 0 is entered.

Control Statement EOS (optional)

Equation of state, see pages 8-9)

Group 1 - IIEOSD, IPSAT, ITSAT

IIEOSD - equation of state reference number. IIEOSD = 1 or 2 refer to high and low pressure data sets respectively in FEHMN. For these values the input in Group 2 and Group 3 will be ignored after it is entered.

IPSAT - parameter to set vapor pressure to zero. If IPSAT $\neq$ 0 the vapor pressure is set to zero, otherwise the vapor pressure is calculated in the code.

ITSAT - parameter to adjust the saturation temperature. If ITSAT < 0, the saturation temperature is set to -1000°C. If ITSAT > 0, the saturation temperature is set to 1000°C.

Group 2 - EWI, EW2, EW3, EW4, EW5, EW6, EW7, EW8, EW9, EW10, EW11

EW1 - liquid reference pressure
EW2 - liquid reference temperature
EW3 - liquid reference density
EW4 - derivative of liquid density with respect to pressure at reference conditions
EW5 - derivative of liquid density with respect to temperature at reference conditions
EW6 - liquid reference enthalpy
EW7 - derivative of liquid enthalpy with respect to pressure at reference conditions
EW8 - derivative of liquid enthalpy with respect to temperature at reference conditions
EW9 - liquid reference viscosity
EW10 - derivative of liquid viscosity with respect to pressure at reference conditions

EW11 - derivative of liquid viscosity with respect to temperature at reference conditions

Group 3 - EVI, EV2, EV3, EV4, EV5, EV6, EV7, EV8, EV9, EV10, EV11

EV1 - vapor reference pressure

EV2 - vapor reference temperature

EV3 - vapor reference density

EV4 - derivative of vapor density with respect to pressure at reference conditions

EV5 - derivative of vapor density with respect to temperature at reference conditions

EV6 - vapor reference enthalpy

EV7 - derivative of vapor enthalpy with respect to pressure at reference conditions

EV8 - derivative of vapor enthalpy with respect to temperature at reference conditions

EV9 - vapor reference viscosity

EV10 - derivative of vapor viscosity with respect to pressure at reference conditions

EV11 - derivative of vapor viscosity with respect to temperature at reference conditions

Control statement FLOW (optional)
[see Eq. (54)]

Group 1 - JA, JB, JC, SKD, EFLOW, AIPED

JA, JB, JC - defined on page 60

SKD - heat and mass source strength (kg/s), heat only (MJ/s). Negative value indicates injection into the rock mass.

EFLOW - enthalpy (MJ/kg) of fluid injected. If the fluid is flowing from the reservoir, then the in-place enthalpy is used. If EFLOW < 0, then ABS(EFLOW) is interpreted as a temperature and the enthalpy calculated accordingly. In heat only problems with EFLOW < 0, the node is in contact with a large heat pipe that supplies heat to the node through an impedance AIPED so as to maintain its temperature near ABS (EFLOW). Large values (approximately 1000) of AIPED are recommended.

AIPED - impedance parameter. If AIPED is nonzero, the code interprets SKD as a flowing wellbore pressure (MPa) with an impedance

ABS(AIPED). If AIPED < 0, flow is only allowed out of the well. For heat only, AIPED is the thermal resistance. If AIPED = 0, SKD is flow rate.

NOTE: If the porosity of the node is zero, then there is only a temperature solution, and the code forms a source proportional to the enthalpy difference E-EFLOW, where E is the in-place enthalpy and EFLOW is a specified enthalpy. The source term is given by

Q= AIPED (E-EFLOW).

Control Statement HFLX (optional)

Group 1 - JA, JB, JC, FLUX, QFLXM

JA, JB, JC - defined on page 60

QFLUX - If QFLXM = 0, then AFLUX is the heat flux (MW) if QFLXM ≠ 0, then QFLUX is a temperature and the heat flux is calculated according to the formula: $Q_H = QFLXM(TL-QFLUX)$

QFLXM - multiplier for heat flux equation given in QFLUX description $(MW/°C)$

Control Statement INIT (optional)

Set initial pressure and temperature at all nodes

Group 1 - PEIN, TIN, TIN1, GRAD1, DEPTH, TIN2, GRAD2, QUAD

PEIN - initial value of pressure (MPa). If initial values are read from IREAD (see terminal input), then this value is ignored. If gravity is present, this is the value of the pressure at node 1, and the other nodal pressures are adjusted by considering the hydraulic head.

TIN - initial value of temperature (°C). If TIN ≤ 0, then the initial temperatures are calculated using the pressure and temperature gradient.

NOTE: The initial temperatures are set according to the following formulas only if TIN ≤ 0. Otherwise, the initial temperatures are determined from PEIN and TIN.

0 ≤ Z ≤ DEPTH	T = TIN1 + GRAD1 x Z
Z > DEPTH	$T = TIN2 + GRAD2 \times Z + QUAD \times Z^2$

TIN1 - defined in formulas above (°C)

GRAD1 - defined in formulas above (°C/m)

DEPTH - defined in formulas above (m)

TIN2 - defined in formulas above (°C)

GRAD2 - defined in formulas above (°C/m)

QUAD - defined in formulas above (°C/m²)

Control statement ITER (optional, see defaults below)
NOTE: If the user is not familiar with the linear equation solver routines in FEHMN please leave out control statement **ITER** and associated lines (see Section I-D).

Group 1 - G1, G2, G3, TMCH, OVER

- G1 - multiplier for the linear convergence region of the Newton-Raphson iteration
- G2 - multiplier for the quadratic convergence region of the Newton-Raphson iteration
- G3 - tolerance for the adaptive implicit method (multiplying factor for Newton-Raphson tolerance)
- TMCH - machine tolerance. If satisfied by the residual norm, the Newton iteration is complete
- OVERF - over relaxation factor for passive nodes in adaptive implicit method

Group 2 - IRDOF, ISLORD, IBACK, ICOUPL, RNMAX

- IRDOF - enables the reduced degree of freedom method
- ISLORD - reordering parameter. The ordering can be understood by labeling the mass equation as 1, the heat equation as 2, and the CO_2 equation (if it exists) as 3. The value of ISLORD and the corresponding equation order is given below.

ISLORD	Mass, Heat	Mass, Heat, CO_2
0	1, 2	1, 2, 3
1	2, 1	1, 3, 2
2		2, 1, 3
3		2, 3, 1
4		3, 1, 2
5		3, 2, 1

the ordering has an effect on the speed of convergence of several solution algorithms, but will not affect most users

- IBACK - back substitution parameter
- ICOUPL - number of SOR iteration used in reduced degree of freedom methods
- RNMAX - maximum running time for problem before the solution is stopped

If control statement **ITER** is not present the following default values are used G1 = 0.001,

G2 = 0.0001, G3 = 0.0001, TMCH = 10^{-8}, OVERF = 0.0, IRDOF = 0.

Control statement NGAS (optional)

Noncondensable gas transport

Group 1 - ICO2D

ICO2D - solution descriptor for noncondensible gas transport

ICO2D - 0 data from control group NGAS is read but not used

ICO2D - 1, 2, reduced degree of freedom solver technology is used

ICO2D - 3, full 3 degrees of freedom solution water/noncondensible gas solution

Group 2 - JA, JB, JC, PC02

JA, JB, JC - defined as in control statement **ROCK**

PC02 - initial partial pressure of non-condensible gas. If PCO2 < 0 then ABS (PCO2) is interpreted as a temperature and the partial pressure of the noncondensible gas is calculated according to the formula: $PCO2 = P_T - P_{SAT}(T)$ where P_T is the total pressure and $P_{SAT}(T)$ is the water saturation pressure and is a function of temperature only.

Group 3 - JA,
JB,
JC,
CPNK

JA, JB, JC - defined on page 60

CPNK - injection concentration of noncondensible gas for injection mode (SK(i) < 0). If it is a production node (SK(i) > 0) then the in place concentration is used.

Note: For compatability with older versions the user may substitute "CO2I" for "NGAS" in the input file.

Control statement NODE (required)

Specify the node numbers for which detailed printed output is desired. The plotting post-processor FEHPLTR will also use these nodes.

Group 1 - M

M - number of nodes for which information will be printed on IOUT (see terminal input). If M < 0, pressure and temperature will be written for all nodes.

Group 2 - MN (1), MN (2) ... MN (M)

MN - node numbers for which information will be printed on IOUT, M nodes (see Group 1). If NN(I) < 0, then coordinates are used to define the print-out node. The coordinate sets (x, y, z) for each NM(I) < 0 are added after Group 2. For 2-D problems put z = 0.

Control statement PERM (required)

Assign absolute permeabilities of the rock [see section I-B, Eq. (7)-(8)]

Group 1 - JA, JB, JC, PNXD, PNYD, PNZD

JA, JB, JC - defined on page 60

PNXD - permeability in the x-direction (m^2)
PNYD - permeability in the y-direction (m^2)
PNZD - permeability in the z-direction (m^2)

Control Statement PPOR (Optional, default is IPOROS=0)

For variable porosity/permeability problems, define model type (see Section I-B)

Group 1 - IPOROS, R1, R2, R3

IPOROS - Porosity/permeability type [see Eqs. (39)-(42)]
= 0 constant porosity
= 1 simple linear model
= 2 Gangi stress model

R1,R2,R3 - parameters used in the various models

Group 2 - JA, JB, JC, R4, R5

JA,JB,JC - defined on page 60
R4 - variable parameter used in porosity/permeability models
R5 - variable parameter used in porosity/permeability models

	Model	
Parameter	Linear (Eq. 39)	Gangi(Eq. 40-41)
R1	C_r	$\propto$
R2	C_g	E
R3	not used	σ
R4	not used	m(exponent)
R5	not used	P_o

For the linear model P_o is PEIN in macro INIT. ϕ_o is PSD in macro ROCK and k_o is from macro PERM for both models.

Control statement PRES (optional)

Assign nonuniform initial pressure and temperature values

Group 1 - JA, JB, JC, PHRD, TIND, IEOSD

JA, JB, JC - defined on page 60

PHRD - initial pressure (MPa)

TIND - initial temperature (If IEOSD = 1 or 3) or initial saturation (if IEOSD = 2)

IEOSD - thermodynamic region parameter if IEOSD = 1, then in compressed liquid region, if IEOSD = 2, the saturation region, if IEOSD = 3, the superheated region.

NOTE: The initial values defined in control statement **PRES** supersede all others.

Control statement RLP (optional)

Relative permeability models [see Eqs. (25)-(27)]

Group 1 - IRLP(i), RP1, RP2, RP3, RP4

IRLP - Relative permeability model type

IRLP(i) = 1 linear type

RP1 - irreducible liquid saturation

RP2 - irreducible vapor saturation

RP3 - maximum liquid saturation

RP4 - maximum vapor saturation

IRLP(i) = 2 Corey type

RP1 - irreducible liquid saturation

RP2 - irreducible vapor saturation

RP3 - not used

RP4 - not used

IRLP(i) = 3 van Genuchten (note different input)

NOTE: With a van Genutchen formulation (IRLP=3, IRLP=4), both the relative permeability and capillary information are input. Therefore there is no capillary pressure input and information should not be input in the capillary pressure section (macro **CAP**) for those nodes.

RP1, RP2, RP3, RP4, RP5, RP6

RP1 - residual liquid saturation

RP2 - maximum liquid saturation

RP3 - α, parameter for model

RP4 - β parameter for model

RP5 - maximum capillary pressure

RP6 - fractional difference in pressure at maximum and cutoff saturation

IRLP(i) = 4 combined van Genutchen model. All the values for IRLP = 3 are read in plus the following RP7, RP8, RP9, RP10, RP11, RP12, RP13, RP14, RP15

RP7 - residual liquid saturation for fracture

RP8 - maximum liquid saturation for fracture

RP9 - α, for fractures

RP10 - β, for fractures

RP11 - maximum capillary pressure for fracture

RP12 - fractional difference in pressure at maximum and cutoff saturation

RP13 - fracture intrinsic permeability (m^2)

RP14 - matrix intrinsic permeability (m^2)

RP15 - fracture porosity

Group 1 is ended when a line with IRLP(i) = 0 is encountered.

Group 2 - JA, JB, JC, I

JA, JB, JC - defined on page 60

I - number referring to the sequence of models read in Group1

NOTE: The parameter i is incremented each time a Group 1 line is read. Group 2 lines will refer to this parameter.

Control statement ROCK (required)

Assign rock density, specific heat and porosity [see Section I-B, Eqs. (1)-(10)]

Group 1 - JA, JB, JC, DENRD, CPRD, PSD

JA,JB,JC - defined on page 60

DENRD - rock density (kg/m^3)

CPRD - rock specific heat (MJ/kg/°C). If CPRD > 1 the code will assume the units are J/kg/°C and multiply by 10^{-6}

PSD - porosity

Control Statement SOL (required)

Group 1 - NTT, INTG

NTT - parameter that defines the type of solution required
if NTT $\geq$ 0 heat and mass transfer solution
if NTT < 0 heat transfer solution

INTG - parameter that defines element integration type (refer to Section I-B)
if INTG $\leq$ 0 Lobatto quadrature is used, recommended for heat and mass problems without stress.

if INTG > 0 Gauss quadrature is used, recommended for problems requiring a stress solution.

Control Statement STEA

No input is associated with this macro statement. This statement enables a 1-D solution in the y-direction (2-D) or z-direction (3-D) when gravity is present to generate an initial steady state solution.

Control Statement STOP (required)

NOTE: No input is associated with this control statement. It signals the end of input, and as such it always appears as the last line of an input deck.

Control Statement TEXT

Following the control statement, text is input until a blank line is inserted to signal the end of the control statement. This text is printed on the output file.

Control statement TIME (required)

Group 1 - DAY, TIMS, NSTEP, II, YEAR, MONTH

- DAY - initial time step size (days)
- TIMS - simulation maximum time (days)
- NSTEP - maximum number of time steps allowed
- II - print-out interval for nodal information (pressure, enthalpy etc.), as set up under control statement node.
- YEAR - year that simulation starts
- MONTH - month that simulation starts

Group 2 - DIT1, DIT2, DIT3, ITC

- DIT1 - time (days) for time step change
- DIT2 - new time step size (days). If DIT2 < 0 then ABS (DIT2) is the new time step multiplier
- DIT3 - implicitness factor for new time step (use ≤ 1.0 backward Euler, > 1.0 for second-order implicit scheme).
- ITC - new print-out interval

NOTE: The code proceeds to the next control statement when a line is encountered with DIT1 = 0. A contour plot will be drawn at each DIT1. A restart file will be written at each DIT1.

Control statement TRAC (optional)
[see Eqs. (16)-(19) and (22)-(24) and Table II]

Group 1 - ANO, AWC, EPC, UPWGTA

- ANO - initial tracer concentration
- AWC - Implicitness factor for tracers. AWC > 1.0 gives 2nd order solution; AWC ≤ 1.0 gives 1st order solution
- EPC - equation tolerance for tracer solution
- UPWGTA - upstream weighting term for the tracer solution
  If UPWGT < 0.5 UPWGTA is set to 0.5
  If UPWGTA > 1.0 UPWGTA is set to 1.0

Group 2 - DAYCS, DAYCF, DAYHF, DAYHS

- DAYCS - time which the tracer solution is enabled
- DAYCF - time which the tracer solution is disabled
- DAYHF - time which the heat and mass transfer solution is disabled
- DAYHS - time which the heat and mass transfer solution is enabled

Group 3 - IACCMX, DAYCM, DAYCMM, DAYCMX

- IACCMS - maximum number of iterations allowed in tracer solution if time step multiplier is enabled
- DAYCM - time step multiplier for tracer solution
- DAYCMM - minimum time step for tracer solution
- DAYCMX - maximum time step for tracer solution

Group 4 - NSPECIES

- NSPECIES - number of different tracers

NOTE: TRAC groups 5, 6, 7, and 8 are entered as a unit for each different tracer.

Group 5 - ICNS, IADSF, AIADSF, A2ADSF, BETAD

- ICNS - phase designation. IF ICNS ≤ 0 a gas phase tracer is used. If ICNS > 0, then a liquid phase tracer is used.
- IADSF - designates tracer type [see Eq. (23)-(24) and Table II]
  = 0, refers to the conservative tracer
  = 1, refers to the linear model
  = 2, refers to the Freundlich model
  = 3, refers to the modified Freundlich model
  = 4, refers to the Langmuir model
- A1ADSF - α_1 parameter
- A2ADSF - α_2 parameter
- BETAD - β parameter

Group 6 - ICRATE, A1R, A2R, A3R, A4R

ICRATE - designates reaction model type see Eq. (24).
A1R - parameter in rate model
A2R - parameter in rate model
A3R - parameter in rate model
A4R - parameter in rate model

ICRATE = 1 refers to the simple model (p. 9) and ICRATE $\geq$ 2 refers to the more complicated model (p. 9).

Group 7 - JA, JB, JC, TCXD, TCYD, TCZD

JA,JB,JC - defined on page 60
TCXD - dispersivity coefficient in the x-direction (m^2/s)
TCYD - dispersivity coefficient in the y-direction (m^2/s)
TCZD - dispersivity coefficient in the z-direction (m^2/s)

Group 8 - JA, JB, JC, ANQO

JA,JB,JC - defined on page 60
ANQO - initial concentration of tracer, which will supersede the value given by ANO in Group 1. Note that if initial values of pressure and enthalpy are read from a file, then the code will also read initial values for the tracer from the file.

Group 9 - JA, JB, JC, CNSK, T1SK, T2SK

JA,JB,JC - defined on page 60
CNSK - injection concentration of injection node. If it is a production node, then the in-place concentration is used
T1SK - time (days) when tracer injection begins
T2SK - time (days) when tracer injection ends

NOTE: Injection nodes must be specified in control statement flow.

Control statement ZONE (Optional, default is input by nodes)

Group 1- IZONE

IZONE - identification number for geometric input

Group 2- X1, X2, X3, X4, Y1, Y2, Y3, Y4 (for 2-D problems)

X1-X4 - X coordinates for zone IZONE
Y1-X4 - Y coordinates for zone IZONE
X1-X8, Y1-Y8, Z1-Z8 (for 3-D problems)
X1-X8 - X coordinates for zone IZONE
Y1-Y8 - Y coordinates for zone IZONE
Z1-Z8 - Z coordinates for zone IZONE

NOTE: If the first four characters in Group 2 are 'LIST' then the code reads a list of x, y, z-coordinates, one set perline until a blank line is encountered. The nodes corresponding to these coordinates make up the zone. The geometric zone description is implemented by defining geometric regions. The coordinates given in Group 2 are defined in Fig. 5. All properties defined by node (JA, JB, JC) may be defined by **ZONE**. In the previous macro descriptions if JA < 0, then the zone IZONE = ABS (JA) is referenced. The macro **ZONE** must precede the usage of a **ZONE** reference. **ZONE** can be called more than once.

C. Graphics Postprocessing

Two graphics postprocessing codes are described in this section. They are written using the DISSPLA graphics package. Except for the plot area specification only the primitive line drawing commands are used. Therefore the routines should be easily convertible to other systems. A capability for time history plots for variables (FEHPLTR) and contour plotting (FECPLTR) are provided. Though these codes have not been verified, users may use them at their convenience.

1. **FEHPLTR** is a postprocessor program for FEHMN. It uses output information from FEHMN in the file FE.HIS. The program organizes information found in the file FE.HIS for plotting time histories of the variables temperature, pressure, enthalpy, flow rate, concentration, and capillary pressure. The user input is found in file **HIS.INS**.

Group 1 - HEADER - 80 character title

Group 2 - NNODE - number of input nodes. This must correspond to the number of print-out nodes specified in the input file for FEHMN.

Group 3 - ITYPE, IPLOT (I), II=1, NNODE

ITYPE - variable designator
= 1, enthalpy plot
= 2, flow rate plot
= 3, temperature plot
= 4, pressure plot
= 5, capillary pressure plot
= 6, concentration plot

IPLOT(I) - designates if the Ith node is to be plotted on the current plot.
IPLOT(I) $\neq 0$ then the Ith node will be plotted.
IPLOT(I) $= 0$ then the Ith node will not be plotted.

Group 4- A - parameter to scale the plot variable according to the formula $P* = A(P\text{-}B)$

B - parameter to scale the plot variable according to the formula given in the last description

C - parameter to scale the time variable according to the formula $t* = C(T - D)$

D - parameter to scale the time variable according to the formula given in this last description

Note: If 0,0,0,0 is entered, no action is taken (i.e., P = p)

Group 5 - XLEN, YLEN

XLEN - physical plot horizontal dimension in inches

YLEN - physical plot vertical dimension in inches

Group 6 - AXIS

AXIS - plot type

AXIS < 0 time axis is a log axis and the variable axis is linear

AXIS = 0, both axes are linear

AXIS > 0, both axes are log scales

Group 7 - DAYMIN, DAYMAX, DAYTIC, NTIC

DAYMIN - minimum limit for time axis

DAYMAX - maximum limit for time axis

DAYTIC - increment for time axis

NTIC - tic marks per increment for the time axis

Group 8 - VMIN, VMAX, VTIC, NIY

VMIN - minimum limit for variable axis

VMAX - maximum limit for variable axis

VTIC - increment value for variable axis

NIY - tic marks per interval for the variable axis

Group 9 - TITLE

TITLE - 30 character (max) heading for top of plot

Group 10 - TITLX

TITLX - 30 character (max) heading for time axis

Group 11 - TITLY

TITLY - 30 character (max) heading for the variable axis

Group 12 is entered only if ITYPE = 6 is chosen and a concentration plot is generated. Since several (up to 10) concentration profiles can be plotted, the species number to be plotted must be specified. Group 12 provides this information.

Group 12 - [ISPT (II) II=1, NSPECI]

ISPT(II) - plot designator for the IIth specie
$\neq 0$ then that specie is plotted
$= 0$ then that specie is not plotted

NOTE: the variable NSPECI is obtained by the code from the file FE.HIS. Groups 3-12 may be repeated for additional plots.

2. **FECPLTR.** The computer code **FECPLTR** is the postprocessor code for FEHMN which makes contour plots. Its input file is the unformatted file FE.CON generated by FEHMN. The plot instruction commands are given in the file CON.INS. The input lines are described below and are in free format except where noted.

Group 1 - ICHOS

ICHOS - dimensionality parameter
= 2, 2 dimensional contour plots are generated
$\neq$ 2, 3-dimensional contour plot information is provided

NOTE: the form of the input that follows is not implemented as yet for the value of ICHOS = 3.

Group 2 - HEADER

Header - title (80 characters maximum)

Group 3 - NCI, IGRID

NCI - contour label interval NCI = 0, no labels are drawn on contours, contours are given different line types (dash, solid, etc.) and identified on the side of the plot NCI $\neq$ 0, the contours are labeled on the contour line

IGRID - grid parameter
= 0, no grid drawn with contours
$\neq$ 0, grid is drawn with contours

Group 4- AX, BX, AY, BY

AX - minimum x coordinate for problem (m)

BX - maximum x coordinate for problem (m)

AY - minimum y coordinate for problem (m)
BY - maximum y coordinate for problem (m)

Group 5- VLENM, VRMAX
VLENM - length of maximum vector (in grid dimensions)
VRMAX - size of maximum vector (m/s)

Group 6- XWIN, YWIN
XWIN - physical size of the x direction of plot window (in)
YWIN - physical size of the y direction of plot window (in)

Group 7- IVLP, CNTRT, CNTRP, CNTRC, SCALE
IVLP - plot phase parameter IVLP < 0, vapor phase only plots will be drawn. IVLP > 0, liquid phase only plots will be drawn
CNTRT - contour interval for temperature (liquid region) or saturation (vapor region)
CNTRP - phase pressure contour interval
CNTRC - phase contour interval for species transport
SCALE - scaling parameter for velocity vectors. No vectors will be plotted for vectors of magnitude less than VRMAX * SCALE (see Group 5).

Note: If CNTRT, CNTRP, CNTRC are < 0, then the contour values are provided in a user supplied list. (Group 8 is used.) If they are > 0 then Group 8 is not used.

Group 8 - NV, (CVAL(I), I = 1, NV)

NV - number of contour values
CVAL(I) - contour value (can be temperature, saturation pressure, or concentration

If multiple contour plots are desired, the user may provide additional data sets for each plot (i.e., Groups 1-7). Alternatively, the user may specify the same parameter set for each plot by not providing additional sets in the data file CON.INS. This way all the plot sets output by FEHMN and in FE.CON will be plotted.

D. Example Input Files And Output Files

This section contains three example problem runs with FEHMN. Input files and output files are provided. Other examples may be found in the FEHMN software verification report (Zyvoloski and Dash, 1991).

1. Heat Conduction. This 3-D problem demonstrates the code performance on a purely conductive problem. It is useful in showing the numerical accuracy of the finite elements and providing the user with an example of 3-D input. While we give only the 4 x 4 x 4 mesh input and output, accuracy results are presented for the 4 x 4 x 4, 8 x 8 x 8, and 12 x 12 x 12 meshes. Table VIII shows the parameters used in the computer runs. Figure 8 depicts the problem geometry (due to symmetry only a quarter of the cube is depicted). Basically the cube is initially at 200°C and a boundary condition of 100°C is applied on all sides. Table IX gives the coordinate positions for the various error sampling points as well as defining the runs. As can be seen from Table X even the crudest grid produced errors of less than 9%. Other grids produced much better results. For the 4 x 4 x 4 grid, the input to the preprocessor GENMSH is shown in Fig. 9. The plot produced by GENMSH is given in Fig. 10. The input file for FEHMN is provided in Fig. 11. It is worth noting here that the part of the file from the macro command **COOR** to the end was produced by GENMSH (file GEOM.DAT) and appended to the other macro commands with a text editor. Figure 12 gives the output for the 4 x 4 x 4 run. The user

TABLE VIII. Input Parameters for the 3-D Heat Conduction Problem

Parameter	Symbol	Value
Rock thermal diffusivity	$^*\kappa$	
Rock thermal conductivity	κ_r	2.7 W/m K
Rock density	ρ_r	2700 kg/m^3
Rock specific heat	C_r	1000 J/kgK
Width	a	0.5 m
Length	b	0.5 m
Depth	c	0.5 m
Initial temperature	T_0	200°C
Surface temperature for all $x, y, z = 0.5$ m	T_s	100°C

$^*\kappa = \frac{\kappa_r}{\rho_r C_r}$

TABLE IX. Sample Problems for 3-D Heat Conduction

Problem	3-D Mesh Elements
1	4 x 4 x 4 brick
2	8 x 8 x 8 brick
3	12 x 12 x 12 brick
4	8 x 8 x 8 prism
5	8 x 8 x 8 mixed brick and prism
Comparison coordinate positions	x = 0.000 y = 0.000 z = 0.000
	x = 0.000 y = 0.125 z = 0.250
	x = 0.125 y = 0.250 z = 0.375
	x = 0.375 y = 0.375 z = 0.375

TABLE X. Comparison of Analytical and Model Results for 3-D Heat Conduction

	Maximum Error (%)				
Coordinate position	1	2	3	4	5
x = 0.000 y = 0.000 z = 0.000	2.139	0.710	0.427	0.718	0.570
x = 0.000 y = 0.125 z = 0.250	1.784	0.572	0.339	0.560	0.572
x = 0.125 y = 0.250 z = 0.375	3.546	1.382	0.862	1.372	1.382
x = 0.375 y = 0.375 z = 0.375	8.517	3.544	2.301	3.379	3.544

instruction file for the postprocessor FEHPLTR is shown in Fig. 13. The plot produced by FEHPLTR is given in Fig. 14.

2. Toronyi Two-Phase Example. This problem is a model of a two-phase, highly permeable geothermal reservoir originally proposed by Toronyi and Farouq Ali (1977) and solved by a number of authors (Mercer and Faust 1975, Thomas and Pierson 1978). The model reservoir is shown in Fig. 15. The input for the problem is presented in Table XI. As with Thomas and Pierson, time steps of 10 days with an initial time step of 8.3 days were used. The final state corresponds to 19% of the original water mass removed. Figure 15 also shows the results obtained in this study using quadrilateral elements compared with the results obtained by Thomas and Pierson. Good agreement is evident. This is somewhat surprising considering the elements have a length/width ratio of 10. The input for the GENMSH preprocessor is shown in Fig. 16. The input file is given in Fig. 17. The part of the input file from the macro **COOR** was generated by GENMSH and inserted in the input file using a text editor. Output for the first computer run is shown in Fig. 18.

TABLE XI. Parameters for Toronyi Example

Parameter	Symbol	Value
Reservoir permeabilty	k	9.869×10^{-13} m^2
Reservoir porosity	ϕ	0.05
Rock thermal conductivity	κ_r	1.73 W/m · K
Rock density	ρ_r	2500 kg/m^3
Rock specific heat	C_r	1000 J/kg · K
Aquifer length	—	1828 m
Aquifer width	—	182.8 m
Initial water saturation	s^0_{ij}	0.2
Aquifer discharge	q_m	0.05 kg/m · s
Initial Pressure	P^0_{ij}	4.4816 MPa

3. DOE Code Comparison Project, Problem 5, Case A. This problem involves multiphase flow in a 2-D horizontal reservoir. The problem is characterized by a moving two-phase region, i.e., the fluid produced at the production well is replaced by cold water recharge over one of the outer boundaries. The problem parameters are given in Table XII and the geometry and boundary conditions are shown in Fig. 19. Of particular note is the variable initial temperature field and the prescribed pressure and temperature boundary. This problem shows that two-phase coding as well as the phase change algorithm are working properly, since numerical difficulties can occur as nodes go from two-phase fluid to compressed water.

There is no analytical solution for this problem, but six researchers produced results for the DOE code comparison project (Molloy, 1980). The reader is referred to this reference for a more detailed discussion of this problem and the code comparison. Results from this problem are compared to those from the other codes, obtained from Molloy (1980) as a check on FEHMN. The results for the outlet temperature, shown in Fig. 20, are in excellent agreement with the other codes. The results for the outlet pressure, Fig. 21, and pressure at an observation well 125 m distant, Fig. 22 are also in good agreement with the other codes.

The input for the preprocessor GENMSH is given in Fig. 23. The input to FEHMN is given in Fig. 24. The printout for the computer is provided in Fig. 25. The part of the input file from the macro COOR was generated by GENMSH. A contour plot of temperature was also generated for this problem. The user generated input file CON.INS is shown in Fig. 26. The contour plot is given in Fig. 27.

TABLE XII. Input Parameters for the DOE Code Comparison Project, Problem 5, Case A

Parameter	Symbol	Value
Reservoir permeabilty	k	2.5×10^{-14} m^2
Reservoir porosity	ϕ	0.35
Rock thermal conductivity	κ_r	1 W/m · K
Rock density	ρ_r	2500 kg/m^3
Rock specific heat	C_r	1000 J/kg · °C
Reservoir length	x	300 m
Reservoir thickness	y	200 m
Liquid residual saturation	s_{lr}	0.3
Gas residual saturation	s_{gr}	0.1
Reservoir discharge	q_m	0.05 kg/m · s)
Initial Pressure	P_o	3.6 MPa

Production well coordinates: x = 62.5 m, y = 62.5 m
Observation well coordinates: x = 162.5 m, y = 137.5 m
Initial temperature distribution:

$$T(x,y,0) = \begin{pmatrix} 240 \\ 240 - 160 \left[\frac{r-100}{200}\right]^2 + 80\left[\frac{r-100}{200}\right]^4 \\ 160 \end{pmatrix} {}^\circ C \quad \begin{matrix} r \leq 100\ m \\ 100 < r < 300\ m \\ r \geq 300\ m \end{matrix}$$

where $r = \sqrt{x^2 + y^2}$

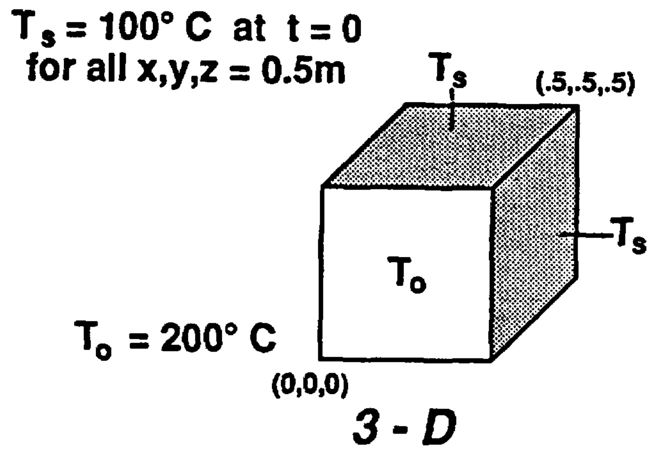

Fig. 8. Schematic diagram of the 3-D heat conduction problem.

```
3D Model of a Cube  (4x4x4 cubes)
20 1 20 0 3 1 0
1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
0.00 0.25 0.50 0.50 0.50 0.25 0.00 0.00
0.00 0.50 0.50 0.00
0.00 0.25 0.50 0.50 0.50 0.25 0.00 0.00
0.00 0.00 0.00 0.25 0.50 0.50 0.50 0.25
0.00 0.00 0.50 0.50
0.00 0.00 0.00 0.25 0.50 0.50 0.50 0.25
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.25 0.25 0.25 0.25
0.50 0.50 0.50 0.50 0.50 0.50 0.50 0.50
1 4 4 4
1 1 1 1
1 1 1 1
1 1 1 1
300. 300. 50.0
0 0 0 0 0 0.
```

Fig. 9. Input for preprocessor GENMSH for 3-D heat conduction example.

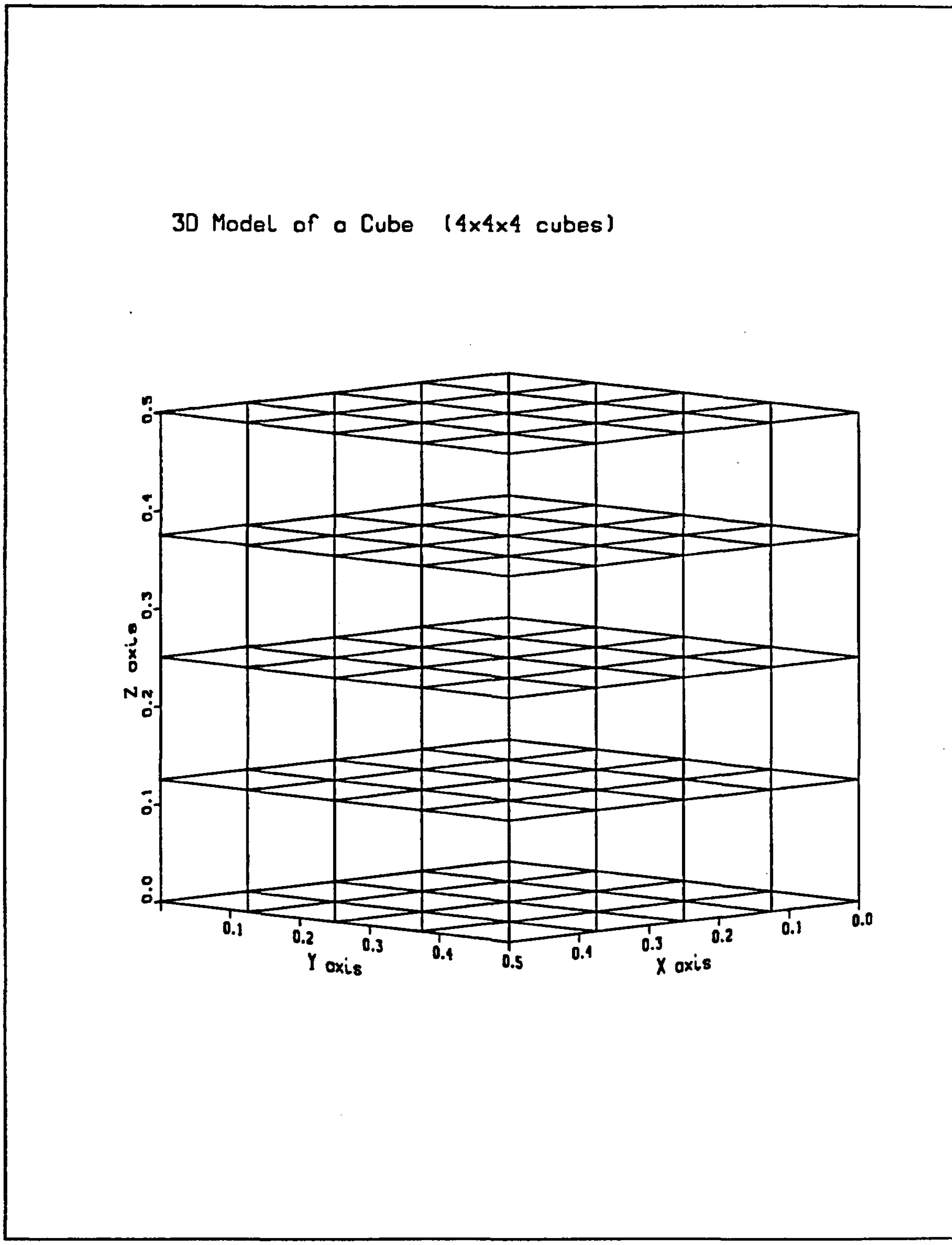

Fig. 10. Grid for 4 x 4 x 4 heat conduction problem.

```
***** 3-D Heat Conduction Model (4X4X4 cubes) *****
node
  8
  001  056  087  094
  005  025  002  125
rlp
2 0. 0. 0. 0.
0
1 125 1 1
0 0 0 0
sol
  -1    -1
init
  10.    0.    200.   0.    0.   200.    0.    0.
rock
     1  125    1    2700.      1000.      0.       1.0
     0    0    0    0.         0.         0.       0.
cond
     1  125    1    2.7e-00    2.7e-00    2.7e-00
     0    0    0    0.         0.         0.
perm
     1  125    1    1.e-30     1.e-30     1.e-30  0.  0.  0.
     0    0    0    0.         0.         0.      0.  0.  0.
flow
   101  125    1      10.00    -100.00  1.e03
     5  125   25      10.00    -100.00  1.e03
    10  125   25      10.00    -100.00  1.e03
    15  125   25      10.00    -100.00  1.e03
    20  125   25      10.00    -100.00  1.e03
    25  125   25      10.00    -100.00  1.e03
    21  125   25      10.00    -100.00  1.e03
    22  125   25      10.00    -100.00  1.e03
    23  125   25      10.00    -100.00  1.e03
    24  125   25      10.00    -100.00  1.e03
     0    0    0       0.         0.     0.
time
  0.005   3.00   1000    1000 1989   04
  0.   0.   0.   0
ctrl
  40   1.e-04   08
    1  125    1    1
    0    0    0    0
  1.0   0.0   1.0
  10   1.0   0.00005 0.005
  0   0
coor
  125
           1        0.00000        0.00000        0.00000
           2        0.12500        0.00000        0.00000
           3        0.25000        0.00000        0.00000
           4        0.37500        0.00000        0.00000
           5        0.50000        0.00000        0.00000
           6        0.00000        0.12500        0.00000
           7        0.12500        0.12500        0.00000
           8        0.25000        0.12500        0.00000
           9        0.37500        0.12500        0.00000
          10        0.50000        0.12500        0.00000
          11        0.00000        0.25000        0.00000
          12        0.12500        0.25000        0.00000
          13        0.25000        0.25000        0.00000
```

Fig. 11. Input file for FEHMN for 3-D heat conduction example.

14	0.37500	0.25000	0.00000
15	0.50000	0.25000	0.00000
16	0.00000	0.37500	0.00000
17	0.12500	0.37500	0.00000
18	0.25000	0.37500	0.00000
19	0.37500	0.37500	0.00000
20	0.50000	0.37500	0.00000
21	0.00000	0.50000	0.00000
22	0.12500	0.50000	0.00000
23	0.25000	0.50000	0.00000
24	0.37500	0.50000	0.00000
25	0.50000	0.50000	0.00000
26	0.00000	0.00000	0.12500
27	0.12500	0.00000	0.12500
28	0.25000	0.00000	0.12500
29	0.37500	0.00000	0.12500
30	0.50000	0.00000	0.12500
31	0.00000	0.12500	0.12500
32	0.12500	0.12500	0.12500
33	0.25000	0.12500	0.12500
34	0.37500	0.12500	0.12500
35	0.50000	0.12500	0.12500
36	0.00000	0.25000	0.12500
37	0.12500	0.25000	0.12500
38	0.25000	0.25000	0.12500
39	0.37500	0.25000	0.12500
40	0.50000	0.25000	0.12500
41	0.00000	0.37500	0.12500
42	0.12500	0.37500	0.12500
43	0.25000	0.37500	0.12500
44	0.37500	0.37500	0.12500
45	0.50000	0.37500	0.12500
46	0.00000	0.50000	0.12500
47	0.12500	0.50000	0.12500
48	0.25000	0.50000	0.12500
49	0.37500	0.50000	0.12500
50	0.50000	0.50000	0.12500
51	0.00000	0.00000	0.25000
52	0.12500	0.00000	0.25000
53	0.25000	0.00000	0.25000
54	0.37500	0.00000	0.25000
55	0.50000	0.00000	0.25000
56	0.00000	0.12500	0.25000
57	0.12500	0.12500	0.25000
58	0.25000	0.12500	0.25000
59	0.37500	0.12500	0.25000
60	0.50000	0.12500	0.25000
61	0.00000	0.25000	0.25000
62	0.12500	0.25000	0.25000
63	0.25000	0.25000	0.25000
64	0.37500	0.25000	0.25000
65	0.50000	0.25000	0.25000
66	0.00000	0.37500	0.25000
67	0.12500	0.37500	0.25000
68	0.25000	0.37500	0.25000
69	0.37500	0.37500	0.25000
70	0.50000	0.37500	0.25000
71	0.00000	0.50000	0.25000
72	0.12500	0.50000	0.25000
73	0.25000	0.50000	0.25000

Fig. 11. (Continued)

```
     74      0.37500      0.50000      0.25000
     75      0.50000      0.50000      0.25000
     76      0.00000      0.00000      0.37500
     77      0.12500      0.00000      0.37500
     78      0.25000      0.00000      0.37500
     79      0.37500      0.00000      0.37500
     80      0.50000      0.00000      0.37500
     81      0.00000      0.12500      0.37500
     82      0.12500      0.12500      0.37500
     83      0.25000      0.12500      0.37500
     84      0.37500      0.12500      0.37500
     85      0.50000      0.12500      0.37500
     86      0.00000      0.25000      0.37500
     87      0.12500      0.25000      0.37500
     88      0.25000      0.25000      0.37500
     89      0.37500      0.25000      0.37500
     90      0.50000      0.25000      0.37500
     91      0.00000      0.37500      0.37500
     92      0.12500      0.37500      0.37500
     93      0.25000      0.37500      0.37500
     94      0.37500      0.37500      0.37500
     95      0.50000      0.37500      0.37500
     96      0.00000      0.50000      0.37500
     97      0.12500      0.50000      0.37500
     98      0.25000      0.50000      0.37500
     99      0.37500      0.50000      0.37500
    100      0.50000      0.50000      0.37500
    101      0.00000      0.00000      0.50000
    102      0.12500      0.00000      0.50000
    103      0.25000      0.00000      0.50000
    104      0.37500      0.00000      0.50000
    105      0.50000      0.00000      0.50000
    106      0.00000      0.12500      0.50000
    107      0.12500      0.12500      0.50000
    108      0.25000      0.12500      0.50000
    109      0.37500      0.12500      0.50000
    110      0.50000      0.12500      0.50000
    111      0.00000      0.25000      0.50000
    112      0.12500      0.25000      0.50000
    113      0.25000      0.25000      0.50000
    114      0.37500      0.25000      0.50000
    115      0.50000      0.25000      0.50000
    116      0.00000      0.37500      0.50000
    117      0.12500      0.37500      0.50000
    118      0.25000      0.37500      0.50000
    119      0.37500      0.37500      0.50000
    120      0.50000      0.37500      0.50000
    121      0.00000      0.50000      0.50000
    122      0.12500      0.50000      0.50000
    123      0.25000      0.50000      0.50000
    124      0.37500      0.50000      0.50000
    125      0.50000      0.50000      0.50000
      0      0.00000      0.00000      0.00000
elem
  8,   64,   0
     1     1     2     7     6    26    27    32    31
     2     2     3     8     7    27    28    33    32
     3     3     4     9     8    28    29    34    33
     4     4     5    10     9    29    30    35    34
     5     6     7    12    11    31    32    37    36
```

Fig. 11. Continued

```
     6     7     8    13    12    32    33    38    37
     7     8     9    14    13    33    34    39    38
     8     9    10    15    14    34    35    40    39
     9    11    12    17    16    36    37    42    41
    10    12    13    18    17    37    38    43    42
    11    13    14    19    18    38    39    44    43
    12    14    15    20    19    39    40    45    44
    13    16    17    22    21    41    42    47    46
    14    17    18    23    22    42    43    48    47
    15    18    19    24    23    43    44    49    48
    16    19    20    25    24    44    45    50    49
    17    26    27    32    31    51    52    57    56
    18    27    28    33    32    52    53    58    57
    19    28    29    34    33    53    54    59    58
    20    29    30    35    34    54    55    60    59
    21    31    32    37    36    56    57    62    61
    22    32    33    38    37    57    58    63    62
    23    33    34    39    38    58    59    64    63
    24    34    35    40    39    59    60    65    64
    25    36    37    42    41    61    62    67    66
    26    37    38    43    42    62    63    68    67
    27    38    39    44    43    63    64    69    68
    28    39    40    45    44    64    65    70    69
    29    41    42    47    46    66    67    72    71
    30    42    43    48    47    67    68    73    72
    31    43    44    49    48    68    69    74    73
    32    44    45    50    49    69    70    75    74
    33    51    52    57    56    76    77    82    81
    34    52    53    58    57    77    78    83    82
    35    53    54    59    58    78    79    84    83
    36    54    55    60    59    79    80    85    84
    37    56    57    62    61    81    82    87    86
    38    57    58    63    62    82    83    88    87
    39    58    59    64    63    83    84    89    88
    40    59    60    65    64    84    85    90    89
    41    61    62    67    66    86    87    92    91
    42    62    63    68    67    87    88    93    92
    43    63    64    69    68    88    89    94    93
    44    64    65    70    69    89    90    95    94
    45    66    67    72    71    91    92    97    96
    46    67    68    73    72    92    93    98    97
    47    68    69    74    73    93    94    99    98
    48    69    70    75    74    94    95   100    99
    49    76    77    82    81   101   102   107   106
    50    77    78    83    82   102   103   108   107
    51    78    79    84    83   103   104   109   108
    52    79    80    85    84   104   105   110   109
    53    81    82    87    86   106   107   112   111
    54    82    83    88    87   107   108   113   112
    55    83    84    89    88   108   109   114   113
    56    84    85    90    89   109   110   115   114
    57    86    87    92    91   111   112   117   116
    58    87    88    93    92   112   113   118   117
    59    88    89    94    93   113   114   119   118
    60    89    90    95    94   114   115   120   119
    61    91    92    97    96   116   117   122   121
    62    92    93    98    97   117   118   123   122
    63    93    94    99    98   118   119   124   123
    64    94    95   100    99   119   120   125   124
     0     0     0     0     0     0     0     0     0
stop
```

Fig. 11. Continued

```
fehm.4.0      12/10/90

***** 3-D Heat Conduction Model (4X4X4 cubes) *****

output file,wt tape,rd tp,user call parameter
    11   44    0    0


  storage for geometric coefficients 726,   in common(nr) 48000
  pressures and temperatures set by gradients
  storage needed for ncon 851,  available 80000
  storage needed for nop 851,  available 100000
  storage needed for a matrix 725,  available 300000
  storage needed for b matrix 725,  available 720000
  storage needed for gmres 1125,  available 187200

 time for reading input,forming coefficients  7.49

  **** analysis of input data on file fe.chk ****


time step        1

        1       2.0      125.0

years       0.137e-04 days   0.5000000e-02 ts size    5.000e-03
 cpu sec for step    0.3677e-01 total time    0.7310e-01
  node      p(mpa)      e(mj)   l sat    temp(c)   well dis dis ent     r eq1   r eq2
     1      10.000       0.00   0.000    200.000  0.000e+00    0.000  0.3e-12  0.3e-03
    56      10.000       0.00   0.000    199.929  0.000e+00    0.000  0.4e-07  0.7e-01
    87      10.000       0.00   0.000    197.313  0.000e+00    0.000  0.2e-06  0.3e+01
    94      10.000       0.00   0.000    192.518  0.000e+00    0.000 -0.6e-07  0.7e+01
     5      10.000       0.00   0.000    100.000  0.000e+00    0.000 -0.2e-09  0.1e+03
    25      10.000       0.00   0.000    100.000  0.000e+00    0.000 -0.2e-09  0.1e+03
     2      10.000       0.00   0.000    199.998  0.000e+00    0.000  0.8e-09  0.2e-02
   125      10.000       0.00   0.000    100.000  0.000e+00    0.000 -0.2e-09  0.1e+03

res mass0.000000      kg vap mass0.000000      kq energy-55.8459      mj

net discharge     0.00000      kg net energy discharge     0.00000      mj
conservation errors:mass     0.00000       energy     0.00000

this time step discharges : ,mass,enthalpy,power
      0.000e+00 kg      0.000e+00 mj       0.000e+00 mw

cumulative discharges : ,mass,enthalpy,avg power
      0.000e+00 kg      0.000e+00 mj       0.000e+00 mw
  number of region changes this time step 0
```

Fig. 12. Computer output for the 3-D heat conduction example.

```
time step       601

        1       0.0      125.0

years       0.821e-02 days   0.3000050e+01 ts size    5.000e-05
 cpu sec for step   0.3268e-01 total time    0.3021e+02
  node       p(mpa)       e(mj)   l sat    temp(c)   well dis dis ent     r eq1   r eq2
     1       10.000       0.00   0.000    100.107  0.000e+00   0.000 -0.5e-11  0.1e-04
    56       10.000       0.00   0.000    100.070  0.000e+00   0.000  0.2e-12  0.9e-05
    87       10.000       0.00   0.000    100.027  0.000e+00   0.000 -0.7e-12  0.3e-05
    94       10.000       0.00   0.000    100.006  0.000e+00   0.000 -0.3e-12  0.8e-06
     5       10.000       0.00   0.000    100.000  0.000e+00   0.000 -0.4e-12 -0.4e-12
    25       10.000       0.00   0.000    100.000  0.000e+00   0.000 -0.8e-25 -0.2e-26
     2       10.000       0.00   0.000    100.099  0.000e+00   0.000  0.5e-14  0.1e-04
   125       10.000       0.00   0.000    100.000  0.000e+00   0.000  0.0e+00  0.1e-38

res mass0.000000      kg vap mass0.000000      kq energy-33.7589      mj

net discharge    0.00000      kg net energy discharge    0.00000      mj
conservation errors:mass    0.00000      energy    0.00000

this time step discharges : ,mass,enthalpy,power
      0.000e+00 kg       0.000e+00 mj        0.000e+00 mw

cumulative discharges : ,mass,enthalpy,avg power
      0.000e+00 kg       0.000e+00 mj        0.000e+00 mw
  number of region changes this time step 0

simulation ended: days  3.000e+00 timesteps   601
                    contour plt:fe.con , history plt:fe.his
  total newton-raphson iterations= 601
```

Fig. 12. Continued

```
temp plot
08
3 1 1 1 1 1 1 1 1
0 0 0 0
6.5 6.5
0
0 3. .5 2
0 200.0 20.0 2
temperature vs time in cube
days
temperature(deg c)
```

Fig. 13. Instruction file (HIS.INS) for postprocessor FEHPLTR for the heat conduction problem.

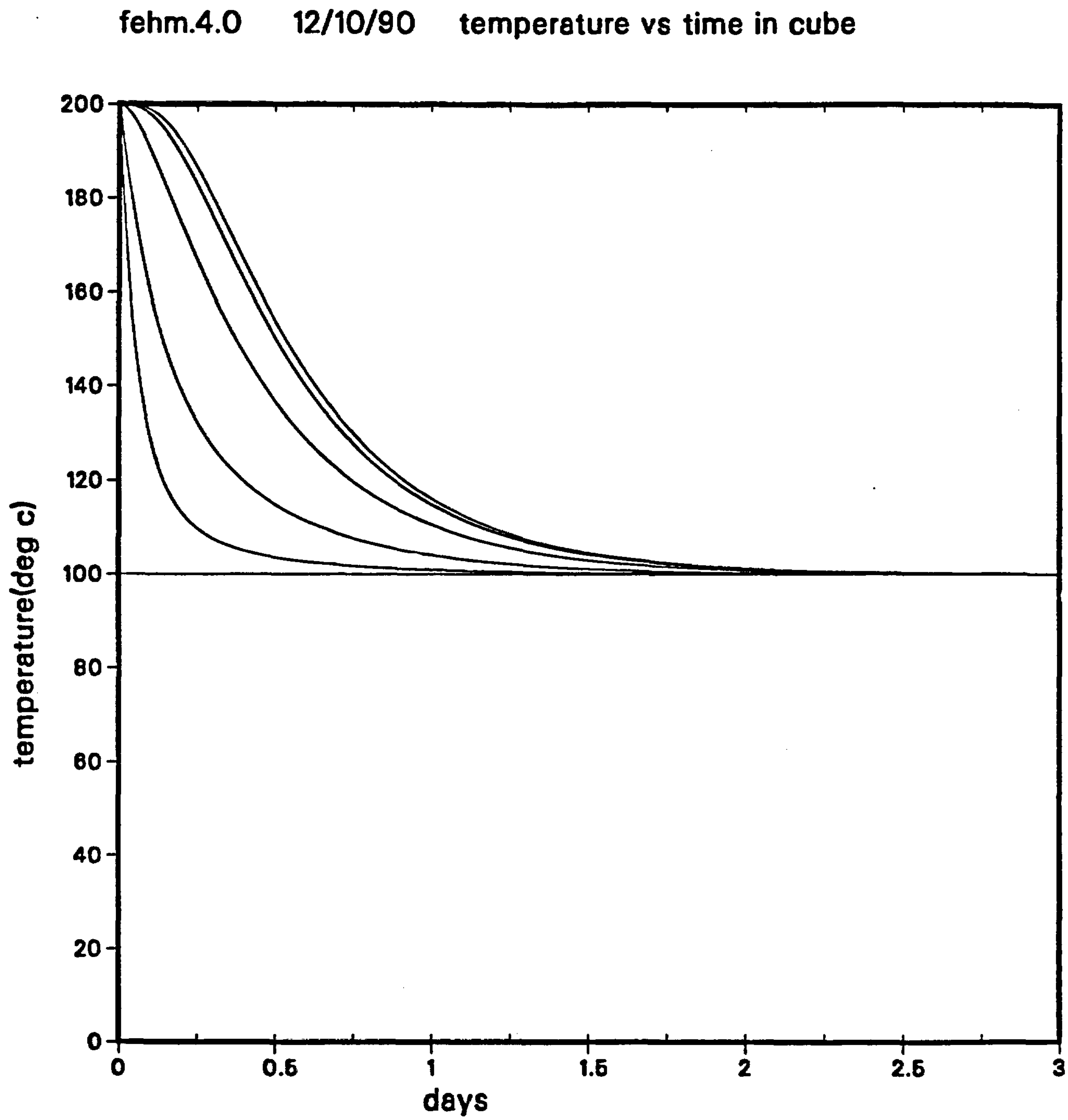

Fig. 14. History plot for the heat conduction problem.

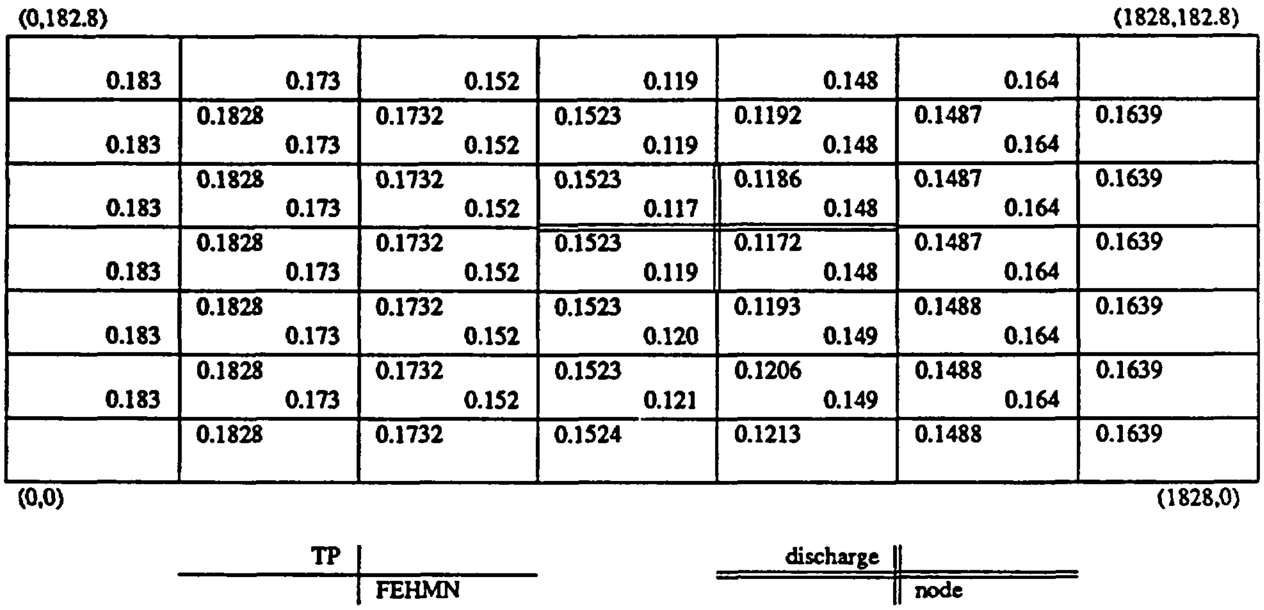

Fig. 15. Solution domain and results for the Toronyi example.

```
2D Model of a Rectangle
4 1 4 0 2 1 0
1 1 2 3 4
0. 1828. 1828. 0.
0. 0.   182.8 182.8
1 07 07 1
.5 1 1 1 1 1 .5
.5 1 1 1 1 1 .5
```

Fig. 16. Input for GENMSH for the Toronyi example.

```
**** toronyi example ****
node
   36
10 11 12 13 14 15
18 19 20 21 22 23
26 27 28 29 30 31
34 35 36 37 38 39
42 43 44 45 46 47
50 51 52 53 54 55
sol
   1   -1
init
      4.3000     000.       250. 0. 0. 250. 0. 0.
rlp
2 0.05 0.05 1.0 1.0
0
1 64 1 1
0 0 0 0 0
pres
1 64 1 4.3000 .2 2
0 0 0 0. 0. 0
rock
    1  64    1     2563.     1010.    0.0500    1.0000
  0  0  0  0. 0.  0.  0.
cond
    1  64   01  1.73e-00  1.73e-00   0.0e-00
  0  0  0  0.  0.  0.
perm
    1  64    1   9.869e-13 9.869e-13  0.e-00 0. 0. 0.
0 0 0 0. 0. 0. 0. 0. 0.
flow
  029  029    1  0.082011 -025.  0.
 0 0 0 0. 0. 0
time
    8.3 78.3 0009   10 1985   07
8.3 10. 1.0 10
0. 0. 0. 0
ctrl
   40     1.e-8    08
    1  64    1    1
 0 0 0 0
      1.0  0.0  0.75
   40       1.00 0.0001      010.00
1  0
coor
  64
         1       0.00000      182.80000        0.00000
         2     152.33333      182.80000        0.00000
         3     457.00000      182.80000        0.00000
         4     761.66667      182.80000        0.00000
         5    1066.33333      182.80000        0.00000
         6    1371.00000      182.80000        0.00000
         7    1675.66667      182.80000        0.00000
         8    1828.00000      182.80000        0.00000
         9       0.00000      167.56667        0.00000
        10     152.33333      167.56667        0.00000
        11     457.00000      167.56667        0.00000
        12     761.66667      167.56667        0.00000
        13    1066.33333      167.56667        0.00000
        14    1371.00000      167.56667        0.00000
        15    1675.66667      167.56667        0.00000
        16    1828.00000      167.56667        0.00000
        17       0.00000      137.10000        0.00000
        18     152.33333      137.10000        0.00000
        19     457.00000      137.10000        0.00000
        20     761.66667      137.10000        0.00000
        21    1066.33333      137.10000        0.00000
        22    1371.00000      137.10000        0.00000
        23    1675.66667      137.10000        0.00000
        24    1828.00000      137.10000        0.00000
        25       0.00000      106.63333        0.00000
```

Fig. 17. Input file for FEHMN for Toronyi example.

```
        26        152.33333        106.63333          0.00000
        27        457.00000        106.63333          0.00000
        28        761.66667        106.63333          0.00000
        29       1066.33333        106.63333          0.00000
        30       1371.00000        106.63333          0.00000
        31       1675.66667        106.63333          0.00000
        32       1828.00000        106.63333          0.00000
        33          0.00000         76.16667          0.00000
        34        152.33333         76.16667          0.00000
        35        457.00000         76.16667          0.00000
        36        761.66667         76.16667          0.00000
        37       1066.33333         76.16667          0.00000
        38       1371.00000         76.16667          0.00000
        39       1675.66667         76.16667          0.00000
        40       1828.00000         76.16667          0.00000
        41          0.00000         45.70000          0.00000
        42        152.33333         45.70000          0.00000
        43        457.00000         45.70000          0.00000
        44        761.66667         45.70000          0.00000
        45       1066.33333         45.70000          0.00000
        46       1371.00000         45.70000          0.00000
        47       1675.66667         45.70000          0.00000
        48       1828.00000         45.70000          0.00000
        49          0.00000         15.23333          0.00000
        50        152.33333         15.23333          0.00000
        51        457.00000         15.23333          0.00000
        52        761.66667         15.23333          0.00000
        53       1066.33333         15.23333          0.00000
        54       1371.00000         15.23333          0.00000
        55       1675.66667         15.23333          0.00000
        56       1828.00000         15.23333          0.00000
        57          0.00000          0.00000          0.00000
        58        152.33333          0.00000          0.00000
        59        457.00000          0.00000          0.00000
        60        761.66667          0.00000          0.00000
        61       1066.33333          0.00000          0.00000
        62       1371.00000          0.00000          0.00000
        63       1675.66667          0.00000          0.00000
        64       1828.00000          0.00000          0.00000
         0          0.00000          0.00000          0.00000
elem
   4,   49,     0
        1     9      10      2      1
        2    10      11      3      2
        3    11      12      4      3
        4    12      13      5      4
        5    13      14      6      5
        6    14      15      7      6
        7    15      16      8      7
        8    17      18     10      9
        9    18      19     11     10
       10    19      20     12     11
       11    20      21     13     12
       12    21      22     14     13
       13    22      23     15     14
       14    23      24     16     15
       15    25      26     18     17
       16    26      27     19     18
       17    27      28     20     19
       18    28      29     21     20
       19    29      30     22     21
       20    30      31     23     22
       21    31      32     24     23
       22    33      34     26     25
       23    34      35     27     26
       24    35      36     28     27
       25    36      37     29     28
```

Fig. 17. (Continued)

26	37	38	30	29
27	38	39	31	30
28	39	40	32	31
29	41	42	34	33
30	42	43	35	34
31	43	44	36	35
32	44	45	37	36
33	45	46	38	37
34	46	47	39	38
35	47	48	40	39
36	49	50	42	41
37	50	51	43	42
38	51	52	44	43
39	52	53	45	44
40	53	54	46	45
41	54	55	47	46
42	55	56	48	47
43	57	58	50	49
44	58	59	51	50
45	59	60	52	51
46	60	61	53	52
47	61	62	54	53
48	62	63	55	54
49	63	64	56	55
0	0	0	0	0

stop

Fig. 17. Continued.

```
fehm.4.0     12/11/90

**** toronyi example ****

output file,wt tape,rd tp,user call parameter
    12   44    0    0


  storage for geometric coefficients 218,   in common(nr) 48000
  pressures and temperatures set by gradients
  storage needed for ncon 353,  available 80000
  storage needed for nop 353,  available 100000
  storage needed for a matrix 1152,  available 300000
  storage needed for b matrix 1152,  available 720000
  storage needed for gmres 1152,  available 187200

 time for reading input,forming coefficients  6.94

  **** analysis of input data on file fe.chk ****


time step         1

        3       8.0       64.0

years       0.227e-01 days   0.8300000e+01 ts size    8.300e+00
 cpu sec for step    0.1750e+00 total time   0.2091e+00
  node       p(mpa)       e(mj)   l sat    temp(c)    well dis dis ent     r eql  r eq2
    10       4.300        1.27   0.200    254.600  0.000e+00    0.000 -0.3e-12 -0.7e-13
    11       4.299        1.27   0.199    254.585  0.000e+00    0.000 -0.2e-12 -0.2e-12
    12       4.293        1.28   0.196    254.507  0.000e+00    0.000 -0.2e-11 -0.1e-11
    13       4.265        1.29   0.182    254.123  0.000e+00    0.000  0.3e-12 -0.7e-12
    14       4.293        1.28   0.196    254.506  0.000e+00    0.000  0.4e-11  0.2e-11
    15       4.298        1.27   0.199    254.580  0.000e+00    0.000 -0.9e-12 -0.4e-12
    18       4.300        1.27   0.200    254.600  0.000e+00    0.000 -0.1e-11 -0.6e-12
    19       4.299        1.27   0.199    254.585  0.000e+00    0.000 -0.4e-12 -0.2e-12
    20       4.293        1.28   0.196    254.507  0.000e+00    0.000 -0.6e-11 -0.3e-11
    21       4.264        1.29   0.181    254.101  0.000e+00    0.000  0.3e-12  0.2e-12
    22       4.293        1.28   0.196    254.506  0.000e+00    0.000  0.2e-10  0.9e-11
    23       4.298        1.27   0.199    254.580  0.000e+00    0.000 -0.3e-11 -0.2e-11
    26       4.300        1.27   0.200    254.600  0.000e+00    0.000 -0.1e-11 -0.6e-12
    27       4.299        1.27   0.199    254.585  0.000e+00    0.000 -0.2e-12 -0.1e-12
    28       4.293        1.28   0.196    254.507  0.000e+00    0.000  0.7e-11  0.4e-11
    29       4.261        1.29   0.179    254.055  0.820e-01    2.792 -0.4e-12  0.2e-11
    30       4.293        1.28   0.196    254.506  0.000e+00    0.000  0.8e-11  0.4e-11
    31       4.298        1.27   0.199    254.580  0.000e+00    0.000 -0.5e-11 -0.3e-11
    34       4.300        1.27   0.200    254.600  0.000e+00    0.000 -0.1e-11 -0.5e-12
    35       4.299        1.27   0.199    254.585  0.000e+00    0.000  0.8e-13  0.1e-12
    36       4.293        1.28   0.196    254.508  0.000e+00    0.000  0.2e-10  0.8e-11
    37       4.265        1.29   0.182    254.118  0.000e+00    0.000  0.4e-13  0.2e-12
    38       4.293        1.28   0.196    254.507  0.000e+00    0.000 -0.8e-11 -0.4e-11
    39       4.298        1.27   0.199    254.580  0.000e+00    0.000 -0.5e-11 -0.3e-11
    42       4.300        1.27   0.200    254.600  0.000e+00    0.000 -0.1e-11 -0.7e-12
    43       4.299        1.27   0.199    254.585  0.000e+00    0.000 -0.3e-12 -0.3e-12
    44       4.293        1.28   0.196    254.508  0.000e+00    0.000  0.7e-11  0.4e-11
    45       4.268        1.29   0.183    254.158  0.000e+00    0.000  0.2e-12 -0.6e-12
    46       4.293        1.28   0.196    254.507  0.000e+00    0.000 -0.1e-10 -0.6e-11
    47       4.298        1.27   0.199    254.580  0.000e+00    0.000 -0.5e-11 -0.3e-11
    50       4.300        1.27   0.200    254.600  0.000e+00    0.000 -0.7e-12 -0.4e-12
    51       4.299        1.27   0.199    254.585  0.000e+00    0.000 -0.4e-12 -0.2e-12
    52       4.293        1.28   0.196    254.509  0.000e+00    0.000 -0.6e-11 -0.3e-11
    53       4.269        1.29   0.184    254.178  0.000e+00    0.000 -0.2e-12 -0.5e-12
    54       4.293        1.28   0.196    254.508  0.000e+00    0.000 -0.7e-11 -0.3e-11
    55       4.298        1.27   0.199    254.580  0.000e+00    0.000 -0.3e-11 -0.2e-11

res mass0.287727e+07 kg vap mass 290027.      kq energy0.212729e+09 mj

net discharge      58812.     kg net energy discharge    0.16422e+06 mj
conservation errors:mass    -0.66302e-08 energy   -0.66939e-08

this time step discharges : ,mass,enthalpy,power
      5.881e+04 kg       1.642e+05 mj       2.290e-01 mw

cumulative discharges : ,mass,enthalpy,avg power
      5.881e+04 kg       1.642e+05 mj       2.290e-01 mw
  number of region changes this time step 0
```

Fig. 18. Output for the Toronyi example.

```
 time step         9

          1       1.0       64.0


years        0.214e+00 days   0.7830010e-02 ts size    1.000e-04
 cpu sec for step    0.5129e-01 total time   0.1539e+01
  node      p(mpa)      e(mj)   l sat   temp(c)   well dis dis ent    r eq1  r eq2
    10       4.267        1.29   0.183   254.151  0.000e+00   0.000  0.3e-13  0.4e-14
    11       4.249        1.30   0.173   253.895  0.000e+00   0.000 -0.2e-13 -0.2e-14
    12       4.209        1.32   0.153   253.336  0.000e+00   0.000  0.2e-12 -0.5e-14
    13       4.146        1.37   0.120   252.441  0.000e+00   0.000  0.4e-13  0.5e-16
    14       4.203        1.32   0.149   253.242  0.000e+00   0.000  0.7e-13 -0.3e-14
    15       4.232        1.31   0.164   253.650  0.000e+00   0.000  0.3e-13 -0.5e-14
    18       4.267        1.29   0.183   254.151  0.000e+00   0.000 -0.7e-13 -0.9e-15
    19       4.249        1.30   0.173   253.895  0.000e+00   0.000 -0.2e-13  0.5e-14
    20       4.209        1.32   0.153   253.336  0.000e+00   0.000 -0.7e-13 -0.2e-15
    21       4.145        1.37   0.119   252.421  0.000e+00   0.000 -0.9e-13 -0.5e-14
    22       4.203        1.32   0.149   253.242  0.000e+00   0.000 -0.7e-13  0.8e-14
    23       4.232        1.31   0.164   253.650  0.000e+00   0.000 -0.1e-12 -0.5e-15
    26       4.267        1.29   0.183   254.151  0.000e+00   0.000  0.5e-13 -0.7e-14
    27       4.249        1.30   0.173   253.895  0.000e+00   0.000  0.5e-13  0.5e-14
    28       4.209        1.32   0.153   253.336  0.000e+00   0.000 -0.3e-14  0.2e-14
    29       4.142        1.38   0.118   252.382  0.820e-01   2.799 -0.6e-13 -0.2e-14
    30       4.203        1.32   0.149   253.242  0.000e+00   0.000  0.7e-14 -0.6e-14
    31       4.232        1.31   0.164   253.650  0.000e+00   0.000 -0.5e-13 -0.1e-13
    34       4.267        1.29   0.183   254.151  0.000e+00   0.000 -0.5e-13  0.4e-14
    35       4.249        1.30   0.173   253.895  0.000e+00   0.000 -0.1e-13 -0.9e-15
    36       4.210        1.32   0.153   253.337  0.000e+00   0.000 -0.1e-13  0.1e-14
    37       4.146        1.37   0.120   252.439  0.000e+00   0.000 -0.1e-13  0.7e-14
    38       4.203        1.32   0.149   253.243  0.000e+00   0.000  0.8e-14 -0.7e-14
    39       4.232        1.31   0.164   253.650  0.000e-00   0.000  0.8e-13 -0.3e-14
    42       4.267        1.29   0.183   254.151  0.000e+00   0.000 -0.3e-13 -0.4e-14
    43       4.249        1.30   0.173   253.895  0.000e+00   0.000  0.1e-13  0.6e-14
    44       4.210        1.32   0.153   253.338  0.000e+00   0.000  0.4e-13 -0.9e-15
    45       4.149        1.37   0.121   252.477  0.000e+00   0.000 -0.7e-13  0.4e-15
    46       4.203        1.32   0.149   253.243  0.000e+00   0.000  0.5e-13  0.4e-14
    47       4.232        1.31   0.164   253.650  0.000e+00   0.000  0.1e-12 -0.5e-14
    50       4.267        1.29   0.183   254.151  0.000e+00   0.000 -0.2e-13 -0.8e-15
    51       4.249        1.30   0.173   253.895  0.000e+00   0.000  0.8e-13 -0.1e-14
    52       4.210        1.32   0.153   253.339  0.000e+00   0.000  0.2e-12  0.2e-14
    53       4.150        1.37   0.122   252.496  0.000e+00   0.000  0.4e-13  0.5e-14
    54       4.203        1.32   0.149   253.244  0.000e+00   0.000 -0.1e-12 -0.4e-15
    55       4.232        1.31   0.164   253.650  0.000e+00   0.000 -0.7e-13 -0.7e-15

res mass0.238127e+07 kg vap mass 298427.     kq energy0.211341e+09 mj

net discharge     0.55481e+06 kg net energy discharge    0.15518e+07 mj
conservation errors:mass    -0.29266e-08 energy   -0.43337e-08

this time step discharges : ,mass,enthalpy,power
      7.086e-01 kg      1.983e+00 mj      2.295e-01 mw

cumulative discharges : ,mass,enthalpy,avg power
      5.548e+05 kg      1.552e+06 mj      2.294e-01 mw
  number of region changes this time step 0

simulation ended: days  7.830e+01 timesteps      9
                  contour plt:fe.con , history plt:fe.his
  total newton-raphson iterations- 19
```

Fig. 18. (Continued)

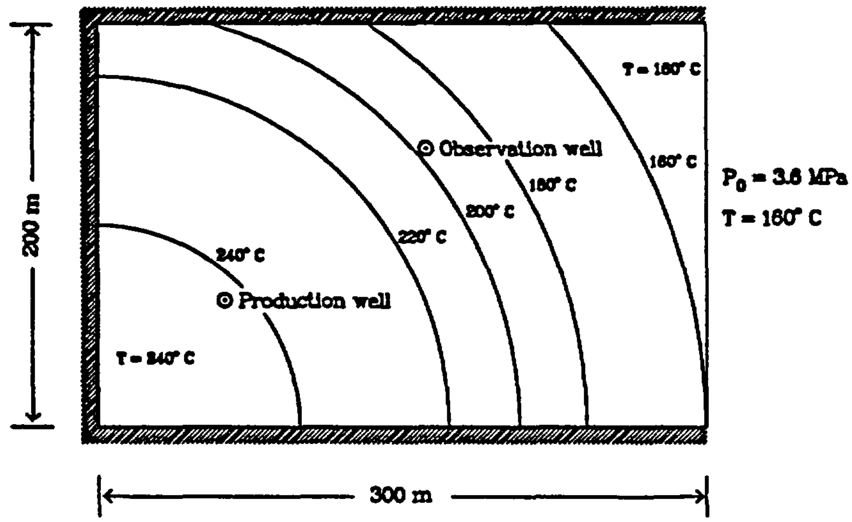

Fig. 19. Schematic diagram of the geometry and boundary conditions for the DOE code comparison project problem.

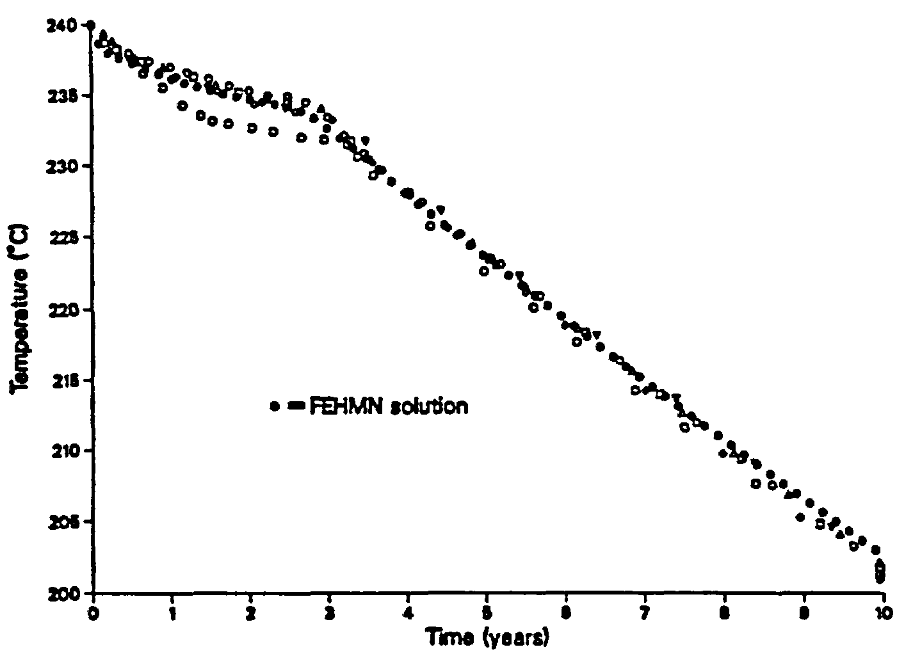

Fig. 20. Comparison of FEHMN production well temperatures with results from other codes.

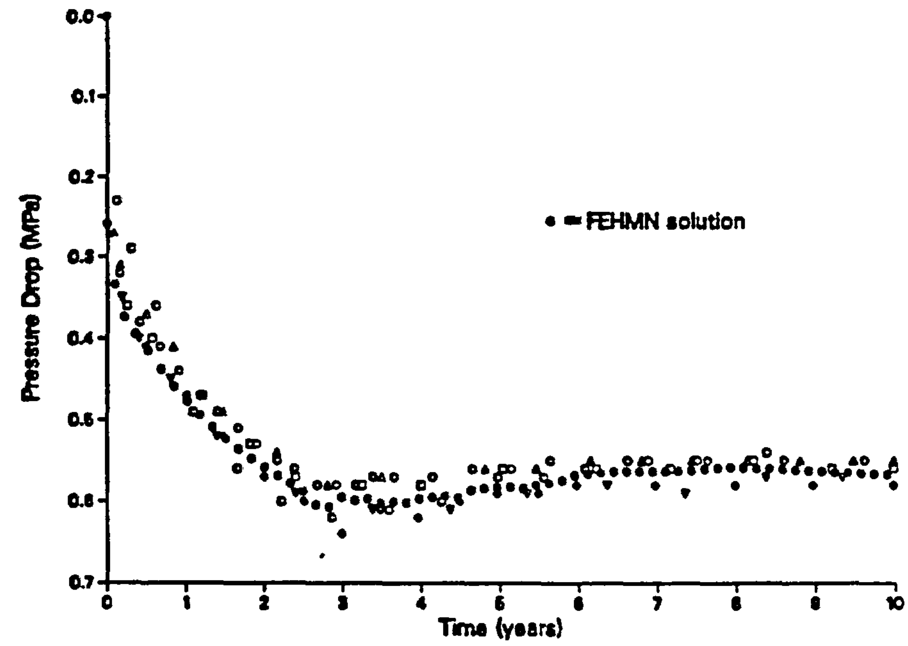

Fig. 21. Comparison of FEHMN production well pressure with results from other codes.

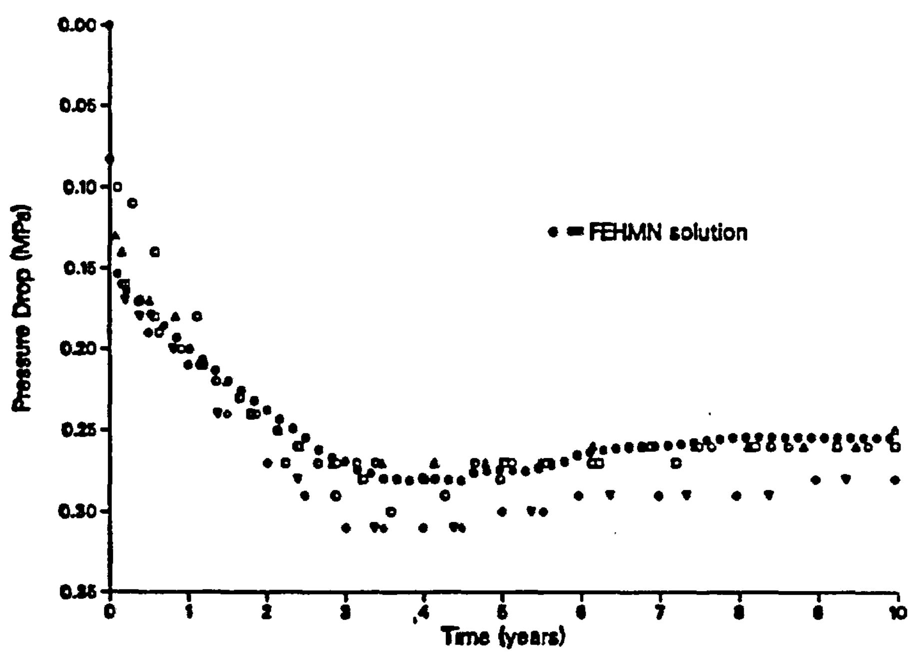

Fig. 22. Comparison of FEHMN observation well pressure with results from other codes.

```
DOE Code Comparison Project, Problem 5, Case A
8 1 8 0 2 1 0
1 1 2 3 4 5 6 7 8
0. 150. 300. 300. 300. 150. 0. 0.
0. 0. 0. 100. 200. 200. 200. 100.
1 13 9 1
.5 1 1 1 1 1 1 1 1 1 1 1 .5
.5 1 1 1 1 1 1 1 .5
```

Fig. 23. Input for GENMSH for the DOE example.

```
*** DOE Code Comparison Project, Problem 5, Case A ***
node
2
88 50
sol
    1    1
init
    3.6000    0.00    240.    0.     0.    240.    0.    0.
rlp
    2    0.3    0.1    0.0    0.0
0
1 140 1 1
0 0 0 0
rock
    1   140     1      2563.      1010.    0.3500
    0     0     0        0.         0.     0.
cond
    1   140     1   1.00e-00   1.00e-00   0.00e-00
    0     0     0   0.00e-00   0.00e-00   0.00e-00
perm
    1   140     1   2.50e-14   2.50e-14   0.00e-00
    0     0     0   0.00e-00   0.00e-00   0.00e-00
flow
   88    88     1     0.050      -25.     0.
   14   140    14     3.600      -160.0   1.
    0     0     0     0.         0.       0.
```

Fig. 24. Input for FEHMN for the DOE example.

```
time
   30.0     3650.     10000     1000  1989     10
1.0 -1.2 1.0 1000
    0.     0.     0.     0
ctrl
   40      1.e-7      8
    1   140      1    1
    0     0      0    0
    1.0   0.0    1.00
   40     1.2    .1    60.000
    1     0
coor
  140
            1          0.00000       200.00000          0.00000
            2         12.50000       200.00000          0.00000
            3         37.50000       200.00000          0.00000
            4         62.50000       200.00000          0.00000
            5         87.50000       200.00000          0.00000
            6        112.50000       200.00000          0.00000
            7        137.50000       200.00000          0.00000
            8        162.50000       200.00000          0.00000
            9        187.50000       200.00000          0.00000
           10        212.50000       200.00000          0.00000
           11        237.50000       200.00000          0.00000
           12        262.50000       200.00000          0.00000
           13        287.50000       200.00000          0.00000
           14        300.00000       200.00000          0.00000
           15          0.00000       187.50000          0.00000
           16         12.50000       187.50000          0.00000
           17         37.50000       187.50000          0.00000
           18         62.50000       187.50000          0.00000
           19         87.50000       187.50000          0.00000
           20        112.50000       187.50000          0.00000
           21        137.50000       187.50000          0.00000
           22        162.50000       187.50000          0.00000
           23        187.50000       187.50000          0.00000
           24        212.50000       187.50000          0.00000
           25        237.50000       187.50000          0.00000
           26        262.50000       187.50000          0.00000
           27        287.50000       187.50000          0.00000
           28        300.00000       187.50000          0.00000
           29          0.00000       162.50000          0.00000
           30         12.50000       162.50000          0.00000
           31         37.50000       162.50000          0.00000
           32         62.50000       162.50000          0.00000
           33         87.50000       162.50000          0.00000
           34        112.50000       162.50000          0.00000
           35        137.50000       162.50000          0.00000
           36        162.50000       162.50000          0.00000
           37        187.50000       162.50000          0.00000
           38        212.50000       162.50000          0.00000
           39        237.50000       162.50000          0.00000
           40        262.50000       162.50000          0.00000
           41        287.50000       162.50000          0.00000
           42        300.00000       162.50000          0.00000
           43          0.00000       137.50000          0.00000
           44         12.50000       137.50000          0.00000
           45         37.50000       137.50000          0.00000
```

Fig. 24. (continued)

46	62.50000	137.50000	0.00000
47	87.50000	137.50000	0.00000
48	112.50000	137.50000	0.00000
49	137.50000	137.50000	0.00000
50	162.50000	137.50000	0.00000
51	187.50000	137.50000	0.00000
52	212.50000	137.50000	0.00000
53	237.50000	137.50000	0.00000
54	262.50000	137.50000	0.00000
55	287.50000	137.50000	0.00000
56	300.00000	137.50000	0.00000
57	0.00000	112.50000	0.00000
58	12.50000	112.50000	0.00000
59	37.50000	112.50000	0.00000
60	62.50000	112.50000	0.00000
61	87.50000	112.50000	0.00000
62	112.50000	112.50000	0.00000
63	137.50000	112.50000	0.00000
64	162.50000	112.50000	0.00000
65	187.50000	112.50000	0.00000
66	212.50000	112.50000	0.00000
67	237.50000	112.50000	0.00000
68	262.50000	112.50000	0.00000
69	287.50000	112.50000	0.00000
70	300.00000	112.50000	0.00000
71	0.00000	87.50000	0.00000
72	12.50000	87.50000	0.00000
73	37.50000	87.50000	0.00000
74	62.50000	87.50000	0.00000
75	87.50000	87.50000	0.00000
76	112.50000	87.50000	0.00000
77	137.50000	87.50000	0.00000
78	162.50000	87.50000	0.00000
79	187.50000	87.50000	0.00000
80	212.50000	87.50000	0.00000
81	237.50000	87.50000	0.00000
82	262.50000	87.50000	0.00000
83	287.50000	87.50000	0.00000
84	300.00000	87.50000	0.00000
85	0.00000	62.50000	0.00000
86	12.50000	62.50000	0.00000
87	37.50000	62.50000	0.00000
88	62.50000	62.50000	0.00000
89	87.50000	62.50000	0.00000
90	112.50000	62.50000	0.00000
91	137.50000	62.50000	0.00000
92	162.50000	62.50000	0.00000
93	187.50000	62.50000	0.00000
94	212.50000	62.50000	0.00000
95	237.50000	62.50000	0.00000
96	262.50000	62.50000	0.00000
97	287.50000	62.50000	0.00000
98	300.00000	62.50000	0.00000
99	0.00000	37.50000	0.00000
100	12.50000	37.50000	0.00000
101	37.50000	37.50000	0.00000
102	62.50000	37.50000	0.00000

Fig. 24. (continued)

```
          103        87.50000       37.50000        0.00000
          104       112.50000       37.50000        0.00000
          105       137.50000       37.50000        0.00000
          106       162.50000       37.50000        0.00000
          107       187.50000       37.50000        0.00000
          108       212.50000       37.50000        0.00000
          109       237.50000       37.50000        0.00000
          110       262.50000       37.50000        0.00000
          111       287.50000       37.50000        0.00000
          112       300.00000       37.50000        0.00000
          113         0.00000       12.50000        0.00000
          114        12.50000       12.50000        0.00000
          115        37.50000       12.50000        0.00000
          116        62.50000       12.50000        0.00000
          117        87.50000       12.50000        0.00000
          118       112.50000       12.50000        0.00000
          119       137.50000       12.50000        0.00000
          120       162.50000       12.50000        0.00000
          121       187.50000       12.50000        0.00000
          122       212.50000       12.50000        0.00000
          123       237.50000       12.50000        0.00000
          124       262.50000       12.50000        0.00000
          125       287.50000       12.50000        0.00000
          126       300.00000       12.50000        0.00000
          127         0.00000        0.00000        0.00000
          128        12.50000        0.00000        0.00000
          129        37.50000        0.00000        0.00000
          130        62.50000        0.00000        0.00000
          131        87.50000        0.00000        0.00000
          132       112.50000        0.00000        0.00000
          133       137.50000        0.00000        0.00000
          134       162.50000        0.00000        0.00000
          135       187.50000        0.00000        0.00000
          136       212.50000        0.00000        0.00000
          137       237.50000        0.00000        0.00000
          138       262.50000        0.00000        0.00000
          139       287.50000        0.00000        0.00000
          140       300.00000        0.00000        0.00000
            0         0.00000        0.00000        0.00000
elem
  4  117  0
         1      15      16       2       1
         2      16      17       3       2
         3      17      18       4       3
         4      18      19       5       4
         5      19      20       6       5
         6      20      21       7       6
         7      21      22       8       7
         8      22      23       9       8
         9      23      24      10       9
        10      24      25      11      10
        11      25      26      12      11
        12      26      27      13      12
        13      27      28      14      13
        14      29      30      16      15
        15      30      31      17      16
        16      31      32      18      17
```

Fig. 24. (continued)

17	32	33	19	18
18	33	34	20	19
19	34	35	21	20
20	35	36	22	21
21	36	37	23	22
22	37	38	24	23
23	38	39	25	24
24	39	40	26	25
25	40	41	27	26
26	41	42	28	27
27	43	44	30	29
28	44	45	31	30
29	45	46	32	31
30	46	47	33	32
31	47	48	34	33
32	48	49	35	34
33	49	50	36	35
34	50	51	37	36
35	51	52	38	37
36	52	53	39	38
37	53	54	40	39
38	54	55	41	40
39	55	56	42	41
40	57	58	44	43
41	58	59	45	44
42	59	60	46	45
43	60	61	47	46
44	61	62	48	47
45	62	63	49	48
46	63	64	50	49
47	64	65	51	50
48	65	66	52	51
49	66	67	53	52
50	67	68	54	53
51	68	69	55	54
52	69	70	56	55
53	71	72	58	57
54	72	73	59	58
55	73	74	60	59
56	74	75	61	60
57	75	76	62	61
58	76	77	63	62
59	77	78	64	63
60	78	79	65	64
61	79	80	66	65
62	80	81	67	66
63	81	82	68	67
64	82	83	69	68
65	83	84	70	69
66	85	86	72	71
67	86	87	73	72
68	87	88	74	73
69	88	89	75	74
70	89	90	76	75
71	90	91	77	76
72	91	92	78	77
73	92	93	79	78

Fig. 24. (continued)

74	93	94	80	79
75	94	95	81	80
76	95	96	82	81
77	96	97	83	82
78	97	98	84	83
79	99	100	86	85
80	100	101	87	86
81	101	102	88	87
82	102	103	89	88
83	103	104	90	89
84	104	105	91	90
85	105	106	92	91
86	106	107	93	92
87	107	108	94	93
88	108	109	95	94
89	109	110	96	95
90	110	111	97	96
91	111	112	98	97
92	113	114	100	99
93	114	115	101	100
94	115	116	102	101
95	116	117	103	102
96	117	118	104	103
97	118	119	105	104
98	119	120	106	105
99	120	121	107	106
100	121	122	108	107
101	122	123	109	108
102	123	124	110	109
103	124	125	111	110
104	125	126	112	111
105	127	128	114	113
106	128	129	115	114
107	129	130	116	115
108	130	131	117	116
109	131	132	118	117
110	132	133	119	118
111	133	134	120	119
112	134	135	121	120
113	135	136	122	121
114	136	137	123	122
115	137	138	124	123
116	138	139	125	124
117	139	140	126	125
0	0	0	0	0

```
stop
```

Fig. 24. (continued)

```
fehm.4.0     12/11/90

*** DOE Code Comparison Project, Problem 5, Case A ***

output file,wt tape,rd tp,user call parameter
    13   44    0    0


  storage for geometric coefficients 170,   in common(nr) 48000
  pressures and temperatures set by gradients
  storage needed for ncon 1261,  available 80000
  storage needed for nop 1261,  available 100000
  storage needed for a matrix 4480,  available 300000
  storage needed for b matrix 4480,  available 720000
  storage needed for gmres 2520,  available 187200

 time for reading input,forming coefficients  7.31

  **** analysis of input data on file fe.chk ****


time step         1

         4      16.7     140.0

years       0.274e-02 days   0.1000000e+01 ts size    1.000e+00
 cpu sec for step    0.7846e+00 total time   0.8199e+00
  node      p(mpa)      e(mj)   l sat    temp(c)   well dis dis ent      r eq1  r eq2
    46       3.341       1.04   0.999    239.971  0.500e-01    1.037 -0.2e-09  0.5e-10
    92       3.529       1.04   1.000    239.993  0.000e+00    0.000  0.4e-11 -0.8e-12

res mass0.170833e+08 kg vap mass 5.06828     kq energy0.418642e+08 mj

net discharge     2633.7     kg net energy discharge     3335.4      mj
conservation errors:mass    0.20321      energy    0.24829

this time step discharges : ,mass,enthalpy,power
      4.320e+03 kg      4.478e+03 mj       5.183e-02 mw

cumulative discharges : ,mass,enthalpy,avg power
      4.320e+03 kg      4.478e+03 mj       5.183e-02 mw
  number of region changes this time step 0

time step        63

         3      10.3     140.0

years       0.999e+01 days   0.3650000e+04 ts size    3.796e+01
 cpu sec for step    0.4888e+00 total time   0.3765e-02
  node      p(mpa)      e(mj)   l sat    temp(c)   well dis dis ent      r eq1  r eq2
    46       3.015       1.02   0.783    234.252  0.500e-01    1.016  0.3e-11 -0.6e-11
    92       3.353       0.93   1.000    218.169  0.000e+00    0.000  0.1e-11  0.4e-10

res mass0.169256e+08 kg vap mass 19184.9     kq energy0.360994e+08 mj

net discharge    0.16031e+06 kg net energy discharge    0.57681e+07 mj
conservation errors:mass    0.54996e-04 energy    0.67599e-04

this time step discharges : ,mass,enthalpy,power
      1.640e+05 kg      1.667e+05 mj       5.082e-02 mw

cumulative discharges : ,mass,enthalpy,avg power
      1.577e+07 kg      1.634e+07 mj       5.182e-02 mw
  number of region changes this time step 0

simulation ended: days  3.650e+03 timesteps    63
                  contour plt:fe.con , history plt:fe.his
  total newton-raphson iterations= 211
```

Fig. 25. Output from FEHMN for the DOE problem.

```
2
 temp contours for doe problem
0 0
0 300 0 200
0 0
6.5 6.5
1 -1. 0.0 0.0 0.0
8 160. 180. 200. 210. 220. 225. 230. 235.
```

Fig. 26. Instruction file (CON.INS) for the postprocessor FECPLTR for the DOE problem.

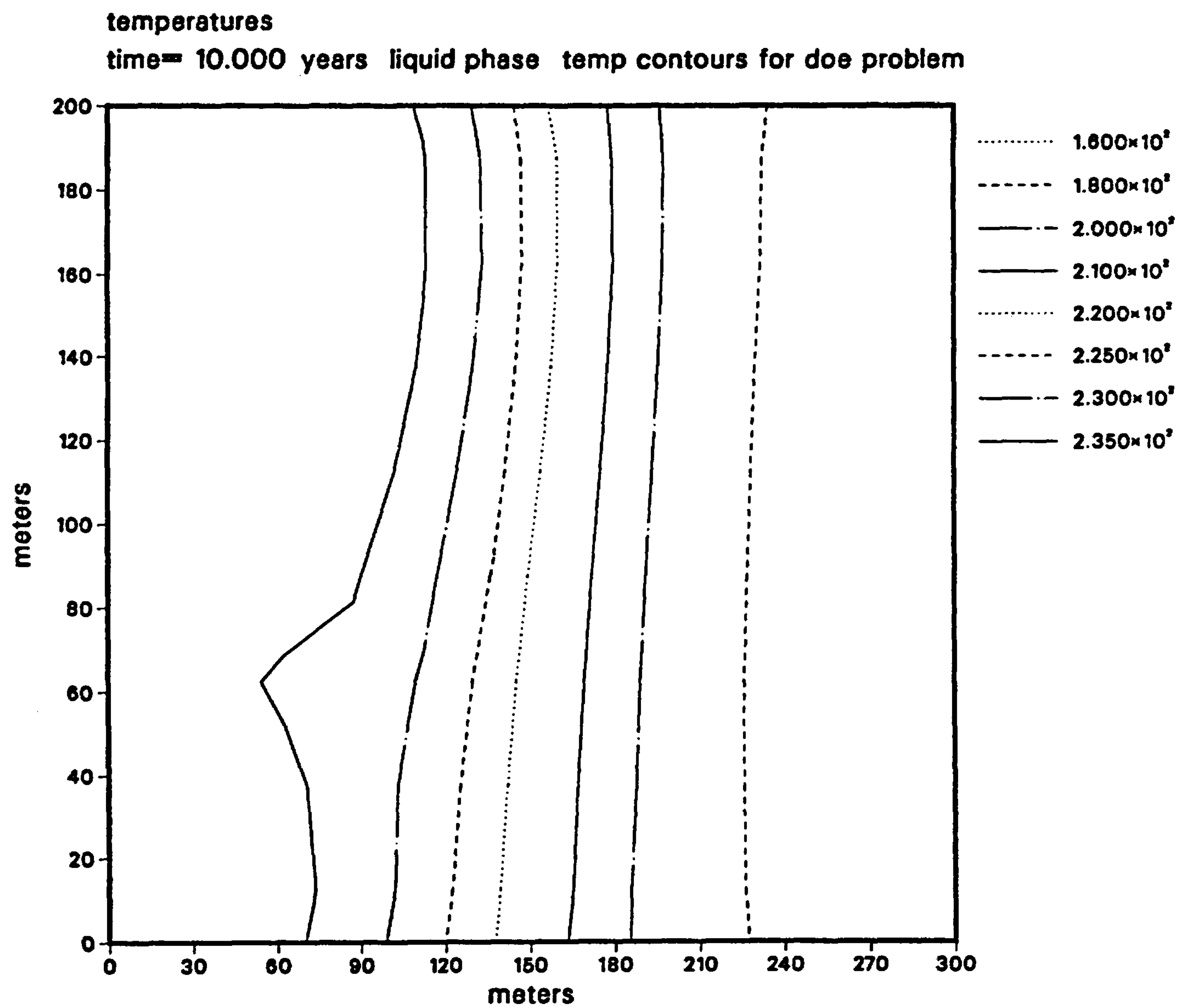

Fig. 27. Contour plot of temperature for the DOE problem.

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DISCLAIMER

The software documented in this report was not verified, validated, or otherwise subjected to the controls of a Yucca Mountain Site Characterization Project Office-approved quality program.

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