MULTIFLO USER'S MANUAL
MULTIFLO VERSION 1.2

TWO-PHASE NONISOTHERMAL COUPLED THERMAL-HYDROLOGIC-CHEMICAL FLOW SIMULATOR

Prepared for

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1.3   THE MULTIFLO DRIVER

The MULTIFLO driver program controls the interaction of the submodules METRA and GEM. The code MULTIFLO is designed so that the submodules METRA and GEM may be run individually in stand-alone mode without coupling to one another, in which case, both codes have their own main driver programs. They may also be run from the MULTIFLO driver program in stand-alone or coupled mode by appropriately setting the parameter icode. There are four possible choices for icode:

icode = 1, METRA stand-alone
       = 2, GEM stand-alone
       = 3, Coupled METRA and GEM in transient mode
       = 4, Coupled METRA and GEM with steady-state flow field and GEM in transient model

The parameter icode is entered following a prompt from MULTIFLO:

```
→ read icode: (1-metra, 2-gem, 3-coupled, 4-coupled: steady-state)
```

With icode = 1 and 2, METRA and GEM are run in stand-alone mode. For icode = 3 and 4, METRA and GEM are coupled through the MULTIFLO driver. For icode = 3, GEM is called after each successfully completed METRA time step. For icode = 4, first METRA is run until a steady-state solution is obtained, and then GEM is called using the steady-state METRA solution. In coupled mode (icode = 3 and 4), the target time for writing plot files is taken from the GEM input file masin, whereas the grid spacing, porosity, temperature, pressure, and saturation are taken from the METRA input file multi.dat.

1.4   HARDWARE AND SOFTWARE REQUIREMENTS

The MULTIFLO code is written in the ANSI FORTRAN 77 programming language. The code was developed and tested on a SUN workstation and a PC running Windows NT. It can also be run under HP workstations, and on a PC with the DOS operating system using the Lahey-Fortran compiler. Version 1.2 of MULTIFLO contains approximately 80,000 lines of code including comment lines. The GEM submodule consists of 20,242 lines of code and the METRA submodule consists of 15,832 lines of code not including comment lines. The complete source code occupies 2.3 MB bytes of disk space uncompiled and 13.5 MB compiled, with full optimization on a SUN workstation, including the three executable files multiflo, metra, and gem. The size of executable modules will vary with compiler options.

The amount of RAM required to run the code depends on the size and complexity of the problem considered. Dynamic memory allocation provides flexible use of storage so that, generally, both small- and large-sized problems can be run with the same executable without unduly wasting memory resources. For large problems or if only relatively small problems are run, the user may easily tailor various array dimensions to the specific demands required. On completion of these changes it is necessary, of course, to recompile the code. Make files are provided which automate this task.

2.3.2.3   BOUNDARY CONDITIONS [BCON]

Initialization Data   Keyword: **BCON**

Required

This keyword reads in the boundary condition data for defining the composition of a multicomponent fluid. In this version of the code, only concentration, zero flux, and zero gradient boundary conditions are possible. Zero flux is the default boundary condition. The boundary condition is applied uniformly over the specified region of the face of the bounding surface. For a structure grid the boundary surface consists of one of the faces of a rectangular parallelepiped, or the faces of the bounding cylinder in cylindrical coordinates. The origin of coordinates for Cartesian coordinates is taken in the upper left corner of the parallelepiped at the front face with the z-axis pointing downward, the y-axis horizontal, and the x-axis perpendicular to the yz-plane forming a left-handed coordinate system (see figure 2-2). For the case of cylindrical geometry, the origin is at the top, centered on the axis of the cylinder.

Read: BCON

Read: IBNDTYP IFACE TMPBC DIST AREA VELL VELG POR SL PORM SLM IMTX

Unstructured Grid Read: M1 M2 INC

Structured Grid Read: I1 I2 J1 J2 K1 K2

Read: SPECIES ITYPE CTOT CONSPEC GUESS

DCM Matrix Read: SPECIES ITYPE CTOT CONSPEC GUESS

BCON   Keyword for specifying boundary conditions.

IBNDTYP   Type of boundary condition.

           = 1   Concentration boundary condition
           = 2   Not used
           = 3   Zero gradient boundary condition (no diffusive flux)

IFACE   Boundary at which solution composition is to be determined (see figure 2-2).

           IFACE is not used for unstructured grid.

           = 1   Left face or inner radius in cylindrical coordinates (I = 1, X = 0)
           = 2   Right face or outer radius in cylindrical coordinates (I = NX)
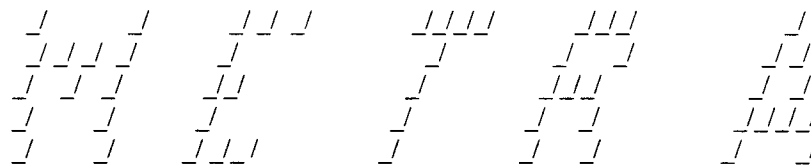
4 EXPLANATION OF OUTPUT RESULTS

Although most of the output is self-explanatory, some of the more important output variables requiring further explanation or clarification are described in this section.

4.1 SCREEN DISPLAY

During a run, information is displayed on the screen that shows the progress of the run and can aid the user in determining whether or not the run is progressing satisfactorily. The initial display gives the program (MULTIFLO, METRA, or GEM) the revision number and date and a copyright notice. Running METRA with the input file 1d.dat gives the screen output:

```
--> open input file 1d.dat
```

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```
  /      /    / /  /     / / / /    / / /        /
 / / / /    /        /      /    / /      / /
/ / /     / /       /      / / /      / /
/      /    /        /     /  /      / / / /
/      /   / / /    /     /  /      /    /
```

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MASS AND ENERGY TRANSPORT MODEL

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4.1.1 METRA Screen Display

When running METRA in its normal transient mode, the screen printout displays in order of appearance: step number, current time, time step size, number of Newton-Raphson iterations (with the cumulative number of iterations in parenthesis), number of time step cuts (with cumulative number of cuts in parenthesis), convergence criteria used, number of inner iterations for solver per Newtonian iterations changes in pressure, saturation, and temperature over the time step.

```
step    time [y]    dt [y]      newton   ncut   icnv <... solver (gmres) itrs...>
   1    1.000E-05   1.000E-05 2(    2)  0(   0)  1     4    4
dP( 1   1  72)=     1.13E+00  dS(   1  1    72)= -4.95E-07  dT( 1 1 72)= 2.55E-03
   2    3.000E-05   2.000E-05 2(    4)  0(   0)  1     4    4
dP( 1   1  72)=     1.72E-00  dS( 1 1 72)= -9.89E-07 dT(    1    1 72)= 5.09E-03
   3    7.000E-05   4.000E-05 2(    6)   0(  0)  2     4    4
dP(    1 1 72)= 2.37E-00 dS( 1 1    72)= -1.97E-06 dT( 1 1 72)= 1.1E-02
```

By inspection of output variables dpmx, dsmx, and dtmx it can usually be determined which variable is limiting the time step by comparing the displayed changes with those specified in the input file in the LIMIt keyword. The location of grid blocks are given by indices (i, j, k). For the unstructured grid option, only the linear index is printed with j and $k = 1$.

When invoking the STEAdy keyword, after 10 time steps an additional line appears on the screen showing how far the solution is from a steady-state based on the tolerances chosen on the STEAdy keyword:

```
  10    1.023E-02   5.120E-03  1(   10)   0(   0)   1    1
dP( 1 1    8)= -8.54E-03  dS( 1  1   72)=  3.19E-08 dT(    1    1 72)- -7.80E-06
  11    2.047E-02   1.024E-02  1(   11)   0(   0)   1    1
dP(   1 1  8)= -7.53E-03 dS(  1    1     72)=  6.12E-08   dT(    1    1 72)-8.14E-06
 dx/dt->

  12    4.095E-02   2.048E-02  1(   12)   0(   0)   1 1
dP(    1    1    4)=  7.90E-03 dS(    1    1 72)= 1.16E-07  dT( 1 1 86)= -807E-06
 dX.dt--->
```

When dX/dt becomes less than one for all three variables (pressure, saturation, and temperature), the solution has converged.

4.1.2 Screen Display

The GEM screen display appears as
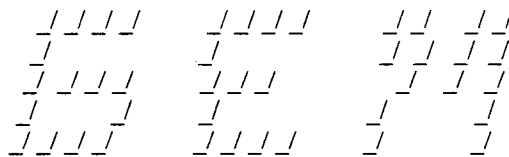
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At each time step the GEM screen display gives the number of steps (mcyc), iterations (iter), time step cuts (ihalve), convergence criteria (iconv), solution method (ifor), time, time step, maximum time step as specified on the DTSTep keyword and the species controlling the time step (maspec). A second line displays the maximum change in concentration in solution (dc) and the maximum time rate of change (dcdt) for the indicated node and species. A third line gives the maximum change in mineral concentration (dm) for the specified node and mineral. An example is shown:

```
 mcyc iter ihalve iconv ifor time    delt    dtmax [y]  maspec
    1   2    0     2    2  1.000   1.000    100.0    sio2  1
   --> watsolv:  1  1
   --> dc = -6.7763E-20 dcdt = -6.7763E-20 at node 40 sio2(aq)
   --> dm =    0.   at node = 1 quartz
........................................................................
 mcyc iter ihalve iconv ifor time    delt    dtmax [y]  maspec
   10   2    0     2    2  16.31   3.765    100.0    sio2  1   --> watsolv:  1  1
   --> dc =  2.4395E-19 dcdt =  6.4794E-20 at node 31 sio2(aq)
   --> dm =  1.9493E-18 at node = 6 quartz
.........................................................................
```
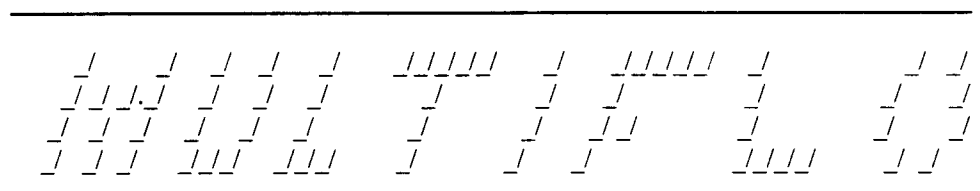
4.1.3 MULTIFLO Screen Display

Running MULTIFLO gives the screen display

```
--> read icode: (1-metra, 2-gem, 3-coupled, 4-coupled:
    steady-state) 3
```


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```
--> Initialization METRA
--> open input file multi.dat
--> read initial data from file init.int
--> Initialization GEM
--> call readat icode = 3
```

for Cartesian geometry,

$$= \pi\left(r_{i+1/2} + r_{i-1/2}\right)\left(r_{i+1/2} - r_{i-1/2}\right)DZ, \tag{4-4}$$

for cylindrical geometry, where

DX, DY, DZ	—	Block dimensions in x-, y-, and z-direction
π	—	3.14159
$r_{i+1/2}$	—	Outer radius of ith block
$r_{i-1/2}$	—	Inner radius of ith block

The pore volume of a block (PV) is computed as $VB - Por$.

4.2.1.2   Initial Conditions

Initial condition variables include pressure (P), temperature (T), gas saturation (S_g), and mole fraction of air component (X_g^a). In a two-phase region, X_g^a is a function of P and T, computed using the ideal gas law as

$$X_g^a = \left(P - P_v\right)/P, \tag{4-5}$$

where

$$P_v = \textbf{saturation pressure of water.} \tag{4-6}$$

Vapor pressure P_v is only a function of T if the effect of capillary pressure on vapor pressure is neglected. If the effect of capillary forces, on vapor pressure is taken into account P_v is a function of capillary pressure, liquid water density, temperature, and saturation pressure.

4.2.1.3   Transmissibility

The constant coefficients of fluid transmissibility (T_x, T_y, and T_z) are interblock properties and calculated in each direction as follows—for Cartesian Geometry

$$T_{x_i} = \frac{2\kappa_i\kappa_{i-1}\Delta y_j \Delta z_\kappa}{\Delta X_i \kappa_{i-1} + \Delta X_{i-1}\kappa_i} \tag{4-7}$$

$$T_{y_i} = \frac{2\kappa_j \kappa_{j-1} \Delta x_i \Delta z_\kappa}{\Delta y_j \kappa_{j-1} + \Delta y_{j-1}\kappa_j} \tag{4-8}$$

In 2D:

$$A_{fm}^{2D} = 2\left(1 - \varepsilon_f\right)\left[\frac{1}{l_x} + \frac{1}{l_y}\right], \qquad \text{(A-42)}$$

and in 1D:

$$A_{fm}^{1D} = 2\left(1 - \varepsilon_f\right)\frac{1}{l}. \qquad \text{(A-43)}$$

A.7 MINC IMPLEMENTATION

The multiple interacting continuum (MINC) model described by Pruess (1983) and Pruess and Narasimhan (1982) is not supported in this version. The MINC model differs from the DCM in that the matrix continuum is discontinuous rather than continuous. Each matrix block is discretized as a nested set of volume elements with only the outer most element connected to the fracture continuum. Distinct matrix blocks are not connected to one another. The MINC model can still be implemented by using the unstructured grid option with nodal connections defined in a manner consistent with nested matrix elements. However, the computational efficiency of this implementation of MINC will be poor compared to the decomposition procedure described in Seth and Hanano (1995).

A.8 REFERENCES

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The equilibrium constants K_i^π, in general, are functions of temperature and pressure. An extensive database is included with the program covering a temperature range of 0–300°C along the saturation curve of water based on the EQ3/6 database (Wolery, 1992). Log values are stored at temperatures of 0, 25, 60, 100, 150, 200, 250, and 300°C and interpolated according to the Mayer-Kelly expression

$$\log K(T) = \frac{a_{-2}}{T^2} + \frac{a_{-1}}{T} + a_0 \ln T + a_1 + a_2 T, \qquad (B\text{-}21)$$

where T denotes the absolute temperature in degrees Kelvin. Pressure lies along the steam saturation curve for temperatures above 100°C, otherwise it is set at 1 bar. Other databases may be generated for any desired temperature range and pressure using the computer code SUPCRT (Johnson et al., 1992). Because of the small variation in pressure, this is considered an adequate approximation. The density of pure water is determined using the equation of state provided by Haar et al. (1980) in uncoupled mode.

B.1.2.2 Kinetic Rate Law

Mineral reactions are assumed to be irreversible, with their rates of reaction described through a kinetic rate law. For simplicity and because of lack of knowledge of detailed reaction mechanisms, mineral reactions are represented by an overall reaction between the solid and aqueous solution. The form of the reaction rate is based on transition state theory. Precipitation or dissolution may occur depending on the sign of the affinity A_m of the reaction, defined by

$$A_m = -RT \ln K_m Q_m, \qquad (B\text{-}22)$$

where K_m denotes the corresponding equilibrium constant for the mineral reaction as written in Eq. (B-3), and Q_m the ion activity product, defined by

$$Q_m = \prod_{j=1}^{N_c} \left(\gamma_j^I C_j^I \right)^{v_{jm}}, \qquad (B\text{-}23)$$

with R the gas constant, and T the temperature. At equilibrium the affinity and the rate vanish. The expression for the reaction rate must take into account the moving boundary nature of the transport—reaction problem. This can be accomplished with the form

B.3   REFERENCES

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