ON PVT-DATA, WELL TREATMENT, AND PREPARATION OF INPUT DATA FOR AN ISOTHERMAL GAS-WATER-FOAM VERSION OF MULKOM

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On PVT - Data, Well Treatment, and Preparation of Input Data for an Isothermal Gas - Water - Foam Version of MULKOM

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Introduction

MULKOM is a multi-dimensional numerical model for simulating the coupled mass and heat transport of multiphase fluids in permeable media. Originally developed for geothermal reservoir simulation, MULKOM features a modular architecture (Fig. 1) which facilitates applications to a variety of flow systems of interest in subsurface resource recovery and storage. Table 1 lists presently available fluid property modules.

Because of the diverse research applications in the engineering of geothermal, oil, and gas reservoirs, as well as in the geologic isolation of nuclear wastes, and in groundwater contamination problems, MULKOM has proliferated into different versions with special features, limited compatibility, and generally sketchy documentation. The notes assembled in this report are intended to assist in applications of a particular version of MULKOM adapted for isothermal flow of gas-water-foam mixtures. Not all of these three phases need be present; for example, systems containing only gas and water may be simulated by setting foam saturation (volume fraction of foam) to a very small value. It is emphasized that the version of MULKOM described here is under continuing development; the chief shortcoming at the present time being the treatment of foam as an indestructible phase, rather than as an emulsion of gas and surfactant solution with texture changing in response to flow.

The section on PVT treatment highlights the correlations used to calculate thermophysical properties of the foam and gas phases, and gives detailed specifications of the relative permeability treatment used. The section on well treatment describes the formulation for production and injection wells with multi-layer completions operating under combined rate and pressure constraints. Subsequently, a detailed description of
input formats for specifying simulation problems is given. The appendices include statements of the governing equations for multiphase flow solved by the MULKOM simulator in continuum as well as in discretized form.

The information in these notes is not meant as a "stand alone"; it is to be used in conjunction with the TOUGH User's Guide (Pruess, 1987), which documents a particular version of MULKOM for nonisothermal flow of water-air mixtures (saturated-unsaturated flow), and with a recent report (Pruess, 1988) on the overall design and governing equations of MULKOM. Interested users are cautioned that familiarity with the source code is required for meaningful applications of MULKOM.
PVT - TREATMENT

The treatment of thermophysical properties for gas and water is similar to that used in other versions of the MULKOM and TOUGH simulators (Pruess, 1983, 1987, 1988). Special provisions are made to take into account the effects of pressure gradients upon effective foam viscosity and to handle foam relative permeability.

Water Phase

There are no provisions for user-input water properties, as all thermophysical properties of liquid water are computed, within experimental accuracy, from the steam table equations as given by the International Formulation Committee (1967).

Foam Phase

Foam is not a "phase" in the thermodynamic sense. It is a discontinuous fluid, comprised of gas bubbles separated by thin liquid lamellae. We treat foam in a phenomenological way, using conventional concepts of multi-phase flow of continua. At the present time no provisions are made to account for generation or destruction of foam in the porous medium. It is treated as a phase distinct from gas and water which obeys a separate conservation law.

1. Equation of State

The pressure dependence of foam density is parametrized with the real gas law (Ross, 1971),
Here $\rho_f$, $P_f$, $M_f$, and $Z_f$ are, respectively, the effective density, pressure, molar weight and compressibility factor of the foam phase. $R$ is the universal gas constant, and $T$ is temperature. $M_f$ is defined as:

$$M_f = \frac{1}{\frac{W_f}{M_g} + \frac{1 - W_f}{M_l}}$$  \hspace{1cm} (2)

where $M_g$ and $M_l$ are, respectively, the molar weights of the gaseous and liquid phases making up the foam. $W_f$ is the foam mass quality, i.e., the mass fraction of gas in the foam phase. It is defined in terms of the gas and liquid masses per unit volume of foam, $m_g$ and $m_l$, as follows

$$W_f = \frac{m_g}{m_g + m_l}$$  \hspace{1cm} (3)

Applying the real gas law to the gas phase inside the foam bubbles, and neglecting contributions from liquid compressibility and from surface effects, the foam compressibility factor $Z_f$ in (1) can be expressed as (Lord, 1981)

$$Z_f = M_f P_f Z_g \left[ W_f + (1 - W_f) \frac{\rho_g}{\rho_f} \right]/M_g P_g$$  \hspace{1cm} (4)

Values for the foam compressibility factor $Z_f$ can either be supplied from tabular input data obtained from laboratory experiments, or default values calculated internally from Equation (4) can be used.

2. Capillary Pressure

Capillary pressure between water and foam phases is defined as:

$$P_{cwf} = P_f - P_w = f(S_w, S_f)$$  \hspace{1cm} (5)
being a function of water saturation $S_w$ and foam saturation $S_f$, (no hysteresis), which is obtained by interpolation from user-supplied input data.

3. Viscosity

Effective foam viscosity is represented as a function of pressure gradient as follows:

$$\mu_f = \mu_\infty + \frac{\alpha}{[\max(0,|\nabla P_f| - P_b)]^\beta + \delta}$$

where $\mu_\infty$ is the asymptotic viscosity for large pressure gradient. $\alpha$ and $\beta$ are rheological constants of foam, to be supplied from measured data and $P_b$ is the threshold or blocking pressure gradient which must be exceeded before foam begins to flow. $\delta$ is a very small number ($10^{-10}$) introduced to avoid a singularity in effective viscosity for numerical calculations at small pressure gradient.

Gas Phase

The gas phase consists of methane and is assumed to obey the real gas law.

$$\rho_g = \frac{P_g M_g}{Z_g RT}$$

The gas compressibility factor $Z_g$ is calculated internally as function of pressure and temperature, based on tabulated properties of methane, (Vargaftik, 1975)

$$Z_g = Z_g (T, P_g)$$

Capillary pressure between water and gas phases

$$P_{cwg} = P_g - P_w = f(S_g)$$

is a single-valued function of gas saturation, (no hysteresis), which is obtained by interpolation from user-supplied input data or by the internal formulation of Leverett's function [TOUGH User's Guide, Pruess (1987)]. Viscosity is calculated internally as function of temperature and pressure, using interpolation from tabulated data for
methane (Vargaftik, 1975)

\[ \mu_g = \mu_g(T, P_g) \] (10)

Relative Permeability

It is assumed that all three phases (gas, foam, and water) are present in all volume elements at all times. When dealing with two-phase flow problems of gas-water, foam-water, or gas-foam flow, a very small value is specified for the saturation of the absent phase \( S = 10^{-5} \).

To prevent any of the three phases from disappearing, relative permeabilities are interpolated to zero at small values of saturation (see Figure 2). The following formulation is used.

When \( S_\beta \leq S_{\text{cut}2} \) (\( \beta = \text{gas, liquid, foam} \)),

\[
k_{r\beta} = \begin{cases} 
  k_{r\beta}^* + (S_\beta - S_{\text{cut}2}) / (S_{\text{cut}2} - S_{\text{cut}1}) & \text{for } S_\beta \geq S_{\text{cut}1} \\
  0 & \text{for } S_\beta < S_{\text{cut}1}
\end{cases}
\] (11)

The parameters \( S_{\text{cut}1} \) and \( S_{\text{cut}2} \) are taken as \( 5 \times 10^{-6} \) and \( 10^{-5} \), respectively. Water and gas relative permeabilities for water-gas two-phase flow are obtained as single-valued functions of water and gas saturation, respectively, by interpolating from user-supplied input data:

\[ k_{r_w} = k_{r_w}(S_w) \] (12)

\[ k_{r_g} = k_{r_g}(S_g) \] (13)

As an alternative, analytical expressions given by Fatt and Klikoff (1959) can be used. When dealing with three-phase flow, we have two options for foam relative permeability. One is to use Stone's second method (Stone, 1973) with the renormalization of Aziz and Settari (1979). The other is a sharp-front tracking technique which is discussed in the next section. For the former, foam relative permeability is specified in the foam-water and foam-gas two-phase systems:
\[ k_{\text{rfw}} = k_{\text{rfw}}(S_w) \]  
(14)

\[ k_{\text{rg}} = k_{\text{rg}}(S_g) \]  
(15)

Then foam relative permeability in three-phase conditions is:

\[ k_{\text{rf}} = k_{\text{rfc}} \left( \frac{k_{\text{rfw}}}{k_{\text{rfc}} + k_{\text{rfw}}} + k_{\text{rfw}} \right) \left( \frac{k_{\text{rg}}}{k_{\text{rfc}} + k_{\text{rg}}} + k_{\text{rg}} \right) - (k_{\text{rw}} + k_{\text{rg}}) \]  
(16)

where \( k_{\text{rfc}} \) is (two-phase) foam relative permeability at connate water saturation.

**Treatment of Sharp Displacement Fronts**

In order to model sharp fronts which may arise at gas-foam or foam-water interfaces, an optional front-tracking technique is available for one-dimensional flow, in which a suitable adjustment of relative permeabilities is performed to maintain the moving gas-foam or foam-water interfaces sharp. The relative permeabilities are considered as functions not only of saturations at the node, but also of those at the upstream and downstream nodes:

\[ k_{\text{rf}} = k_{\text{rf}}(S_f, S_{\text{up}}, S_{\text{down}}) \]  
(17)

\[ k_{\text{rw}} = k_{\text{rw}}(S_w, S_{\text{up}}, S_{\text{down}}) \]  
(18)

\[ k_{\text{rg}} = k_{\text{rg}}(S_g, S_{\text{up}}, S_{\text{down}}) \]  
(19)

Consider a process in which a foam bank is driven by gas to displace water. The foam-water interface is identified by \( S_{\text{f, up}} = 1 \) and \( S_{\text{w, down}} = 1 \). (For the "sharp interface" option irreducible saturations are ignored. If necessary, non-zero irreducible saturations can be accounted for by a suitable adjustment in porosity.) At the grid block boundary downstream from the foam-water interface relative permeability to water should be reduced and foam relative permeability should become non-zero only when upstream foam saturation approaches 1. The gas-foam interface is identified by \( S_{\text{g, up}} = 1 \) and \( S_{\text{f, down}} = 1 \). At the grid block boundary downstream from this interface, only foam can flow until gas saturation in the upstream node approaches 1.
The "sharp front" constraints on phase mobilities are implemented by means of appropriate relative permeability functions. We introduce two parameters, \( S_1 \) and \( S_2 \) (\( S_2 > S_1 \)), which typically are of order 0.01. The relative permeability at the grid block boundary downstream from the sharp front is then varied from 0 to 1 as the saturation of the invading phase in the upstream block increases from \( 1 - S_2 \) to \( 1 - S_1 \). Denoting the relative permeability of the invading phase by \( k_{r,\text{in}} \), we perform a linear interpolation as follows.

\[
\begin{cases}
  0 & S_{\text{in,up}} \leq 1-S_2 \\
  \frac{S_{\text{in,up}} - (1-S_2)}{(S_2-S_1)} & 1-S_2 < S_{\text{in,up}} < 1-S_1 \\
  1 & S_{\text{in,up}} > 1-S_1 
\end{cases}
\] (20)

The relative permeability of the displaced phase, denoted by \( k_{r,\text{dis}} \), is simply given by

\[
k_{r,\text{dis}} = 1 - k_{r,\text{in}}
\] (21)

The "sharp front" treatment can be applied at grid block boundaries where foam is either the invading phase (sweeping the upstream block) or the displaced phase (being swept from the downstream block).
WELL TREATMENT

The code does not contain a separate wellbore model which would permit modeling of the flow in the tubing between wellhead and sandface. Therefore, wells must be represented in terms of sandface conditions, such as pressure or flow rate from production wells (sinks), and flow rate or injection pressure for injection wells of gas, foam or water. Well operating conditions can be time-dependent, i.e., wells can be injected into, produced from, or shut in according to arbitrary user-specified schedules.

Production Wells

The code allows production wells to produce on deliverability by producing against a specified bottomhole pressure or under water or gas rate constraints. For specified bottomhole pressure $P_{wb}$, the mass production rate for a well from grid layer $l$ is expressed as (Fanchi, et al., 1982):

$$q_l = (PD)_l \sum_{\beta=1}^{NPH} \left( \frac{K_{\beta}P_{\beta}}{\mu_{\beta}} \right) (P_l - P_{wb} - f_l)$$

where $(PD)_l$ is the well productivity index in layer $l$; $P_l$ is the pressure in the well grid block; $f_l$ is a gravity correction for the flowing wellbore pressure; and $\beta$ is a phase index ($\beta = 1$: gas; 2: water; 3: foam). For a pseudo-steady state radial flow, the productivity index is given by (Coats, 1977):

$$(PI)_l = \frac{2\pi (kA\Delta Z)_l}{\ln(\frac{r_e}{r_w}) + \frac{s}{2}}$$

where $(kA\Delta Z)_l$ is the permeability-thickness product in layer $l$; $r_e$ is well grid block radius; $r_w$ is well radius; and $s$ is the van Everdingen skin factor. If the well is producing from a grid block which does not have cylindrical shape, an approximate productivity index can be computed by using an effective radius

$$r_e = \sqrt{A/\pi}$$
The gravity correction $f_l$ in the rate expression (22) is obtained as follows (Pruess, 1987). Assume the production well is open from layer $l = 1$ (bottom) to $l = L$ (top). The gravity correction in layer $l$, $f_l$, is then calculated from the gravity correction in layer $l + 1$ immediately above it by means of the following recursion formula:

$$f_l = f_{l+1} + \frac{g}{2} (\rho_l f \Delta Z_l + \rho_{l+1} f \Delta Z_{l+1})$$

where $\rho_l$ is the flowing density in the tubing opposite layer $l$. The gravity correction vanishes in the top layer, i.e., $f_L = 0$. Flowing densities $\rho_l$ are computed using a phase volume-weighting procedure. If wellbore pressure were zero, we would obtain the following volumetric flow rate of phase $\beta$ from layer $l$:

$$r_{l, \beta} = (\frac{k_{p \beta}}{\mu_{p \beta}}) (\text{PI})_l \rho_l$$

The total volumetric flow rate of phase $\beta$ opposite layer $l$ is, at zero wellbore pressure:

$$r_{l, \beta}^T = \sum_{m=1}^{l} r_{l, \beta}$$

Then flowing densities are obtained from the following approximate expression:

$$\rho_l^f = \frac{\sum_{\beta=1}^{NPH} \rho_{l, \beta} r_{l, \beta}^T}{\sum_{\beta=1}^{NPH} r_{l, \beta}^T}$$

It is possible to specify target rates (constraints) on water-production or gas production. If either target production is specified, the code computes a flowing wellbore pressure opposite the topmost open layer:

$$P_{wbc} = \frac{-Q_{con} + \sum_l (\text{PI})_l (\frac{k_{p \beta} \rho_{p \beta}}{\mu_{p \beta}}) L \frac{P_l - f_l}{\rho_{p \beta}}}{\sum_l (\text{PI})_l (\frac{k_{p \beta} \rho_{p \beta}}{\mu_{p \beta}}) L \frac{1}{\rho_{p \beta}}}$$

where phase $\beta$ is water or gas according to which rate constraint is in effect; $Q_{con}$ is the target rate; $\rho_{p \beta}$ is the density of phase $\beta$ at standard conditions. After obtaining the
wellbore pressure $P_{wbc}$ from (29) for a rate constraint, the code compares it to the input minimum flowing wellbore pressure $P_{wb}$. If $P_{wbc} > P_{wb}$ the well is able to deliver the target rate(s), and $P_{wbc}$ is used as flowing bottomhole pressure in (22). For $P_{wbc} < P_{wb}$ the target rate(s) cannot be achieved, and the well is placed on deliverability with bottomhole pressure $P_{wb}$. The code has the capability to switch from rate to pressure constraints (or vice versa) in the course of a simulation, as required in response to changing reservoir conditions.

**Injection Wells**

The treatment for injection wells is similar to that for production wells, except that no gravity correction is made for flowing wellbore pressure. For specified injection pressure $P_{in}$, the mass rate of injection of phase $\beta$ ($\beta = \text{gas, water or foam}$) into layer $l$ is given by:

$$W_l = (W_l) I \rho_l (P_{in} - P_l) \sum_{\beta=1}^{NPH} \left( \frac{k_{\beta}}{\mu_{\beta}} \right)_l$$  \hspace{1cm} (30)$$

where the injectivity index $(W_l)_I$ is defined exactly like the productivity index $(P_l)_I$. Note that the fluid mobility for injection is based on total mobility of all phases, as is customary when injecting into multi-phase systems (Fanchi et al., 1982). $\rho_l$ is the density of injected fluid at reservoir conditions. When injecting foam, a viscosity corresponding to the largest velocity is used in (30). When a target injection rate is specified, a flowing injection wellbore pressure is calculated as:

$$P_{in,c} = \frac{W_o + \sum_{l} (W_l) I \rho_l P_l \sum_{\beta} \left( \frac{k_{\beta}}{\mu_{\beta}} \right)_l}{\sum_{l} (W_l) I \rho_l \sum_{\beta} \left( \frac{k_{\beta}}{\mu_{\beta}} \right)_l}$$  \hspace{1cm} (31)$$

where $W_o$ is the specified target mass injection rate. If $P_{in,c} > P_{in}$ the target rate cannot be achieved, and a rate will be calculated from (30) for injection pressure $P_{in}$. For $P_{in,c} \leq P_{in}$ the target rate can be achieved, and injection pressure is equal to $P_{in,c}$. As in the case of production wells, the code has a capability to switch from pressure to rate...
constraint (or vice versa) in the course of a simulation.

All well equations given above are coded fully implicitly in the program, except for the gravity correction equation (25), which is obtained just once at the beginning of each time step. All derivative terms arising from the well equations are taken into account in the Jacobian matrix. The rate constraints are embedded in the source terms, so that they are automatically satisfied when solving the mass-balance equations.
INPUT FORMATS

The blocks ROCKS, ELEME, CONNE, GENER, and INCON can have a variable number of records, depending upon how many items the user wishes to specify. The end of these variable-length blocks is indicated with a blank record. (For CONNE, GENER, and INCON it is possible to have, instead of the blank record, a record with "+++" written in columns 1-3, followed by some element and source cross-referencing information in the case of CONNE and GENER, and followed by restart-information in the case of INCON; see below.)

We shall now explain the records and variables in detail.

All the input and output can be specified either in standard metric units, or in field units.

TITLE

is the first record of the deck, containing a header of up to 80 characters, to be printed on every page of output. This can be used to identify a problem. If no header is desired, leave this record blank.

ROCKS

introduces material parameters and initial conditions for up to 27 different reservoir domains

Record ROCKS.1

Format (A5, I3, I2, 5E10.4)

MAT, NADF, NAD, DM, POR, (PER(I) I = 1,3)

MAT material (domain) name.

NADF sequence number of relative permeability and capillary pressure function.
NAD = 0: will only read one data record per domain.

1: will read one additional record per domain with pore compressibility.

2: will read another record per domain with initial conditions.

DM rock grain density; lb/cuft (kg/m³).

POR default porosity (void fraction) for all grid blocks belonging to domain "MAT", for which no other porosity has been specified in block INCON.

PER(I), I = 1, 2, 3 absolute permeability along three principal axes, as specified by ISOT in block CONNE: md (m²).

Record ROCKS.1.1 (optional, NAD ≥ 1 only)

Format (1E10.4)

COM pore compressibility; 1/psi (1/Pa).

Record ROCKS.1.2 (optional, NAD ≥ 2 only)

This record introduces a set of primary variables which are used as default initial conditions in the domain specified in "MAT" (Record ROCKS.1) for all elements for which no other values are specified in block INCON (with option START only).

Format (3E20.14)

X1, X2, X3

X1 water pressure; psi (Pa).

X2 gas saturation.

X3 foam saturation.

Repeat records 1, 1.1, and 1.2 for up to 27 reservoir domains.
Record ROCKS.2  A blank record closes the ROCKS data block.

PARAM  introduces computation parameters

Record PARAM.1

Format (2I2, 3I4, 24I1, E10.4).

NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 24), T.

NOITE  specifies the maximum number of iterations per time step (default value is 8).

KDATA  specifies amount of printout (default = 1).

0 or 1:  print a selection of the most important variables.

2:  print fluxes.

3:  print primary variables and their changes.

If the above values for KDATA are increased by 10, printout will occur after each iteration (not just after convergence).

MCYC  maximum number of time steps to be calculated.

MSEC  maximum duration, in machine seconds, of the simulation (default is infinite).

MCYPR  printout will occur for every multiple of MCYPR steps (default is 1).

MOP(I),  I = 1,24 allows choice of various options.

MOP(1)  if ≠ 0, short printout for non-convergent iterations will be suppressed.

MOP(2) though MOP(6) generate additional printout in various subroutines, if set ≠ 0. The amount of printout increases with MOP(I).

MOP(2)  CYCIT (main subroutine).

MOP(3)  MULTI (flow- and accumulation-terms).
MOP(4) QU (sinks/sources).
MOP(5) EOS (equation of state).
MOP(6) LINEQ (linear equations).
MOP(7) if ≠ 0, a printout of input data will be provided.
MOP(8) not used.
MOP(9) not used.
MOP(10) not used.

Calculational choices are as follows:

MOP(11) determines evaluation of mobilities at interfaces.
        0: mobilities are upstream weighted with WUP (default is WUP = 1.).
        1: mobilities are spatially interpolated between adjacent elements.

MOP(12) not used

MOP(13) if ≠ 0, perform new matrix decomposition only when the number of pivot failures is a multiple of MOP(13). This option is available only with MOP(14) = 2.

MOP(14) determines handling of pivot failures in matrix decomposition.
        0: perform new decomposition.
        1: reduce time step, stay with old decomposition.
        2: ignore pivot failure and proceed (MOP(13) = 0, or number of pivot failures not a multiple of MOP(13)).

MOP(15) not used.

MOP(16) permits to choose time step selection option.
0: use time steps explicitly provided in INPUT.

>0: Increase time step by at least a factor 2, if convergence is achieved in a number of iterations not exceeding MOP (16)

MOP(17) permits to scale the matrix solved in MA28.

0: No scaling.

1: Scale after encountering a singular matrix.

2: Scale after pivot failure.

3: Scale after pivot failure or matrix singularity.

>4: Scale on first iteration in each time step.

>6: Scale all the time.

MOP(18) used to perform a permutation (reordering) of the Jacobian matrix.

0: no pre-ordering of Jacobian matrix.

1: Jacobian matrix is pre-ordered for block lower triangular form.

MOP(19) permits to choose relative permeability data and front-tracking techniques.

0: \( k_{rw}, k_{rg}, \) and \( k_{rf} \) are provided from tabular INPUT data.

1: \( k_{rw} \) and \( k_{rg} \) are calculated from the internally installed formulation [Fatt and Klikoff (1959)], only dealing with water-gas two phase flow.

2: relative permeabilities are calculated internally by the sharp-front technique. No capillary pressure data are needed, regardless of the choice of MOP(20).

MOP(20) permits to choose capillary pressure data.

0: \( P_{cwg} \) and \( P_{cwf} \) are provided from tabular INPUT data.
1: Use Leverett’s function [TOUGH User’s Guide, Pruess (1987)] to calculate capillary pressure $P_{cwg}$. $P_{cwf}$ is set to zero.

MOP(21) - not used.
MOP(24) - not used.

T reservoir temperature; °F (°C)

Record PARAM.2

Format (4E10.4, A5, 5X, 2E10.4)
TSTART, TIMAX, DELTEN, SCALE, ELST, GF, REDLT

TSTART starting time of simulation; seconds.

TIMAX time in seconds at which simulation should stop (default is infinite).

DELTEN length of time steps in seconds. If DELTEN is a negative integer, DELTEN = -NDLT, the program will proceed to read NDLT records with time step information.

SCALE scale factor to change the size of the mesh (default = 1.0).

ELST set equal to the name of one element to obtain a short printout after each time step.

GF magnitude (ft/sec² or m/sec²) of the gravitational acceleration vector. Blank or zero gives "no gravity" calculation.

REDLT factor by which time step is reduced in case of convergence failure (default is 4.).

Record PARAM.2.1, 2.2, etc.

Format (8E10.4)
(DLT(I), I = 1, 100)

DELT(I) length (in seconds) of time step I.

This set of records is optional for DELTEN = − NDLT, a negative integer: Up to 13 records can be read, each containing 8 time step sizes. If the number of simulated time steps exceeds the number of DLT(I), the simulation will continue with time steps equal to the last non-zero
Record PARAM.3

Format (8E10.4)
RE1, RE2, FOR, WUP, WNR, DFAC, SING, U

RE1 convergence criterion for relative error (default = 1.E-5)

RE2 convergence criterion for absolute error (default = 1.)

FOR weighting factor for time differencing (it is strongly recommended to use only default value = 1., i.e., fully implicit). Generally, 0 ≤ FOR ≤ 1.

WUP upstream weighting factor for mobilities at interfaces (default = 1.0). 0 ≤ WUP ≤ 1.

WNR weighting factor for increments in Newton/Raphson iteration (default = 1.0). 0 < WNR ≤ 1.

DFAC increment factor for computing derivatives (default = 1.E-8).

SING correction for matrix elements which are numerically zero (default = 0.).

U pivoting parameter (default = 0.1). 0 ≤ U ≤ 1; increased value for U will make criterion for pivot selection more stringent, resulting in better numerical stability at the expense of more storage for matrix decomposition.

Record PARAM.4

Format (3E20.14)
DEP(I), I = 1, 3

This record holds a set of primary variables completely analogous to record ROCKS.1.2. These variables are used as default initial conditions for all elements for which no other values are prescribed either in block ROCKS or in block INCON (with option START only).

DEP(1) water pressure; psi (Pa).
DEP(2)  gas saturation.

DEP(3)  foam saturation.

FIN  (optional).

A record with FIN punched in columns 1-3 indicates that all data are input in field units. In this case the file SAVE, holding thermodynamic parameters at the end of a MULKOM run, will also be written in field units, to permit restarting with the same input deck. If FIN is absent, input data and file SAVE are in SI units.

FOUT  (optional)

A record with FOUT punched in columns 1-4 will cause the main printed output to be written in field units. If FOUT is absent, printed output will be in SI units. In either case, dimensioned parameters are printed with their units displayed.

FIVEP  (optional)

A record with FIVEP punched in columns 1-5 will cause patterned printout to be generated for single- or multi-layer grids corresponding to 1/8 of a five- or nine-spot pattern.

Record FIVEP.1  (only for option "FIVEP")

Format (2I5)

NROW, LAY

NROW  number of grid block rows in the 1/8 five-spot mesh.

LAY  number of grid layers.

TIMES  (optional)

This data block specifies desired printout times.

Record TIMES.1

Format (2I5, 2E10.4)

ITI, ITE, DELAF, TINTER
ITI is the number of explicitly provided times at which printout is to be generated (restriction: ITI ≤ 100).

ITE is the total number of times at which printout is desired (restriction: ITE ≥ ITI).

DELAF is the maximum time step, in seconds, to be taken after any of the printout times have been reached (default is infinite).

TINTER is the time increment, in seconds, to be applied for printout times with index ITI+1, ITI+2,... , ITE.

Record TIMES.2, 3, 4, etc.

Format (8E10.4)

TIS(I), I = 1, ITI

TIS(I) Printout times, in seconds.

A maximum of 100 printout times can be specified, in ascending order. Time steps will be automatically adjusted to let the program reach the desired printout times.

ELEME introduces element information.

Record ELEME.1

Format (A3, I2, 2I5, A3, A2, E10.4)

EL, NE, NSEQ, NADD, MA1, MA2, VOLX

EL, NE 5-character code name of an element. The first three characters are arbitrary, the last two characters must be numbers.

NSEQ number of additional elements having the same volume and belonging to the same reservoir domain.

NADD increment between the code numbers of two successive elements. (Note: the maximum permissible code number NE + NSEQ * NADD is <99.).

MA1, MA2 a five character material identifier corresponding to one of the reservoir domains as specified in block ROCKS. If the first three characters are
blanks, the last two characters must be numbers in which case they would indicate the sequence number of the domain as entered in ROCKS.

VOLX  element volume, ft$^3$ (m$^3$).

Repeat record ELEME.1 for the number of elements desired.

Record ELEME.2 A blank record closes the ELEME data block.

CONNE introduces information for the connections (interfaces) between elements.

Record CONNE.1

Format (A3, I2, A3, I2, 315, I5, 4E10.4)

EL1, NE1, EL2, NE2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX

EL1, NE1  code name of the first element.

EL2, NE2  code name of the second element.

NSEQ  number of additional connections in the sequence.

NAD1  increment of the code number of the first element between two successive connections.

NAD2  increment of the code number of the second element between two successive connections.

ISOT  set equal to 1, 2, or 3; specifies absolute permeability to be $\text{PER(\text{ISOT})}$ for the materials in elements (EL1, NE1) and (EL2, NE2), where PER is read in block ROCKS. This allows assignment of different permeabilities, e.g., in the horizontal and vertical direction.

D1, D2  distance ft (m) from center of first and second element, respectively, to their common interface.

AREAX  interface area ft$^2$ (m$^2$).
BETAX is the cosine of the angle between the gravitational acceleration vector and the line between the two elements. $GF \times \text{BETAX} > 0$ ($<0$) corresponds to the first element being above (below) the second element.

Repeat record CONNE.1 for the number of connections desired.

Record CONNE.2 a blank record closes the CONNE data block.

GENER provides specifications for multilayer production and injection wells. It is possible to specify arbitrary well schedules, by providing up to 20 data blocks beginning with a record having GENER written in columns 1-5, followed by specifications of all production and injection well feeds, and terminated by a blank record. Subsequent GENER blocks will be read at times as specified in block GENTI (see below).

Record GENER.1.1 (production wells)

- **ELEG**: code name of element containing well feed (bottommost layer must be specified first).
- **SOURCE**: code name of the well. The first three characters are arbitrary; the last two characters are numbers.
- **WAT**: rate constraint (target rate) of water production from well (to be specified for record with bottommost feed only); STB/D (m$^3$/s).
- **LTABG**: number of open layers (to be specified for bottommost feed only).
- **TYPE**: set equal to "DELV", to indicate a production well is being specified.
- **PI**: productivity index for the particular layer; RB·cp/D/psi (m$^3$).
- **PWB**: flowing bottomhole pressure opposite topmost open layer (to be specified for last -top- layer only); psi (Pa).
- **HG**: vertical thickness of layer in which the well is open; ft (m).
- **QGAS**: gas target rate from well (to be specified for bottommost feed only); MMCF/D, (m$^3$/D).
Repeat record GENER.1.1 for all LTABG open layers of a multilayer well. The feeds must be entered sequentially, going from bottom up. After all feeds of one production well have been entered, additional production well data may be specified.

Record GENER.1.2 (gas, foam or water injection wells)

- Format (2A5, E10.4, 5X, I5, 5X, A4, 1X, E10.4, 20X, E10.4)

- ELEG, SOURCE, WI, LTABG, TYPE, G, PIN

ELEG: code name of element containing an open interval of the injection well (open layers can be specified in arbitrary order).

SOURCE: code name of the well. The first three characters are arbitrary; the last two characters must be numbers.

WI: injectivity index of the well (to be specified separately for each layer); RB·cp/D/psi (m³).

LTABG: number of open layers (to be specified on first record for each injection well).

TYPE: set equal to "GASI", "FOAM", "WATI" to indicate that an injection well for gas, foam or water, respectively, is being specified.

G: total (maximum) rate of entire injection well (to be specified on first record for each injection well); STB/D (kg/s) for foam or water injection, MMCF/D (kg/s) for gas injection.

PIN: injection pressure; psi (Pa).

Repeat record GENER.1.2 for all LTABG open layers of a multi-layer injection well. The feeds can be entered in arbitrary order. After all feeds of one well have been entered, injection data for additional wells may be specified.

Record GENER.2

A blank record closes a set of generation data. Additional sets of generation data may be specified, which will be read at times specified in block GENT!, below.
This data block introduces information on times at which new generation data will be read. If GENTI is absent, only one GENER block will be read, and the well data provided in that block will be used throughout the entire run.

Record GENTI.1

Format (I5)

IGEN

number of generation data sets.

Record GENTI.2

Format(8E10.4)

GENT(I), I = 1, IGEN

times, in seconds, at which generation data will be read.

A maximum of 20 times can be specified, in ascending order. For each of these times, a new data block GENER will be read.

START (optional)

A record with START punched in columns 1-5, allows a more flexible assignment of initial conditions.

INCON introduces initial conditions.

Record INCON.1

Format (A3, I2, 2I5, E15.9)

EL, NE, NSEQ, NADD, PORX

EL, NE code name of element.

NSEQ number of additional elements with same initial conditions.
increment between the code numbers of two successive elements with identical initial conditions.

PORX porosity (void fraction); if zero or blank, porosity will be taken as specified in block ROCKS if option START is used.

Record INCON.2

<table>
<thead>
<tr>
<th>Format (3E20.14)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1, X2, X3</td>
</tr>
</tbody>
</table>

Set of primary variables for the element specified in record INCON.1.

X1 water pressure; psi (Pa).

X2 gas saturation.

X3 foam saturation.

Record INCON.3 A blank record closes the INCON data input block. (For an alternative, see note below).

Note on closure of blocks CONNE, GENER, and INCON.

The "ordinary" way to indicate the end of any of the above data blocks is by means of a blank record. There is an alternative available if the user makes up an input deck from the files MESH, GENER, or SAVE, which have been generated by a previous MULKOM run. These files are written exactly according to the specifications of data blocks ELEME and CONNE (file MESH), GENER (file GENER), and INCON (file SAVE), except that the blocks CONNE, GENER, and INCON terminate with a record with "+++" in columns 1-3 followed by some cross-referencing and restart information. MULKOM will accept this type of input, and in this case there is no blank record at the end of the indicated data blocks.

PVT Data Input.

RELATive permeability

A record with RELAT written in columns 1-5 indicates beginning of relative permeability and capillary pressure information. Up to ten data sets can be specified, each of which provides two-phase water-foam and
foam-gas relative permeability data, and optional capillary pressure data. A data set can be attached to a certain reservoir domain by setting the parameter NADF in record ROCKS.1 for that domain equal to the sequence number of the data set.

Record RELAT.1

Format (2(I1,I4))

NCW, NSW, NCG, NSG

NCW = 0: no water-foam-capillary pressure data will be read; $P_{cfw}$ is assumed to be zero.

1: water-foam capillary pressure data will be read.

NSW number of water saturations provided in data set (restriction: $NSW \leq 20$).

NCG = 0: no gas-water-capillary pressure data will be read; $P_{cwg}$ is assumed to be zero.

1: gas-water-capillary pressure data will be read.

NSG number of gas saturations provided in data set (restriction: $NSG \leq 20$).

Record RELAT.2

Format (8E10.4)

$ASW(I)$, $I = 1, NSW$

$I = 1, NSW$ specifies an array of $NSW$ water saturations, in ascending order, for which relative permeability and (optional) capillary pressure data will be tabulated. $ASW(1)$ is irreducible water saturation for $MOP(19) \neq 2$. $ASW(1)$ and $ASW(2)$ are the two parameters $S_1$ and $S_2$ for performing an interpolation of "sharp front" relative permeabilities for water and foam if $MOP(19) = 2$.

Record RELAT.3

Format(8E10.4)

$AKRW(I)$, $I = 1, NSW$
AKRW(I), \( I = 1,\) NSW provides water relative permeabilities in two-phase water-foam system at the water saturations read in array ASW, above.

Record RELAT.4

Format (8E10.4)

AKRFW(I), \( I = 1,\) NSW

AKRFW(I), \( I = 1,\) NSW provides foam relative permeabilities in two-phase water-foam-system at the water saturations read in array ASW, above.

Record RELAT.4.1 (optional, NCW \( \geq 1 \) only)

Format (8E10.4)

PCFW(I), \( I = 1,\) NSW

PCFW(I), \( I = 1,\) NSW provides foam capillary pressures in two-phase water-foam-system at the water saturations read in array ASW, above.

Record RELAT.5

Format (8E10.4)

ASG(I), \( I = 1,\) NSG

ASG(I), \( I = 1,\) NSG specifies an array of NSG gas saturations, in ascending order, for which relative permeability and (optional) capillary pressure data will be tabulated. ASG(1) is irreducible gas saturation for MOP(19) \( \neq 2. \) ASG(1) and ASG(2) are the two parameters \( S_1 \) and \( S_2 \) used for performing an interpolation of "sharp front" relative permeabilities for gas and foam if MOP(19) \( = 2. \)

Record RELAT.6

Format (8E10.4)

AKRG(I), \( I = 1,\) NSG

AKRG(I), \( I = 1,\) NSG provides gas relative permeabilities in two-phase foam-gas system at the gas saturations read in array ASG, above.
Record RELAT.7

Format (8E10.4)

AKRFG(I), I = 1,NSG

AKRFG(I), I = 1,NSG provides foam relative permeabilities in two-phase foam-gas system at the gas saturations read in array ASG, above.

Record RELAT.7.1 (optional, NCG ≥ 1 only)

Format (8E10.4)

PCOG(I), I = 1,NSG

PCOG(I), I = 1,NSG provides gas capillary pressures in two-phase gas-water system at the gas saturations read in array ASG, above.

Repeat records RELAT.1 through RELAT.7.1 for up to ten data sets.

Record RELAT.8 a blank record closes the RELAT data block.

REOLG introduces information on rheological properties of foam

Record REOLG.1

Format (8E10.4)

ALPHA, BETA, VISI, DPB, QF, RMWF

ALPHA rheological constant of foam, cp·(psi/ft)^BETA (Pa·s(Pa/m)^BETA)

BETA rheological exponent of foam

VISI foam viscosity at large pressure gradient; cp (Pa·s)

DPB blocking pressure gradient; psi/ft (Pa/m)

QF foam mass quality (gas mass fraction)

RMWF effective molecular weight of foam

ENDCY closes the MULKOM input file and initiates the simulation.
Acknowledgement

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References


Coats, K. H., Geothermal Reservoir Modelling, paper SPE-6892, presented at the 52nd Annual Fall Technical Conference and Exhibition of the SPE, Denver, CO, October 1977.


Appendix A. Mass and Energy Balances

The basic mass- and energy-balance equations(*) solved by MULKOM can be written in the following general form:

\[ \frac{d}{dt} \int_{V_n} M^{(\kappa)} \, dV = \int_{\Gamma_n} F^{(\kappa)} \cdot n \, d\Gamma + \int_{V_n} q^{(\kappa)} \, dV \]  

(A.1)

The integration here is over an arbitrary subdomain \( V_n \) of the flow system under study, which is bounded by the closed surface \( \Gamma_n \). The quantity \( M \) appearing in the accumulation term denotes mass or energy per unit volume, with \( \kappa = 1, \ldots, NK \) labeling the mass components, and \( \kappa = NK + 1 \) for the heat “component”.

The mass accumulation term is written in a general way, to allow for the presence of several components (chemical species) in the fluid.

\[ M^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_{\beta} \rho_{\beta} X^{(\kappa)}_{\beta} \]  

(A.2)

The total mass of component \( \kappa \) is obtained by summing over all fluid phases \( \beta = 1, \ldots, NPH \). \( S_{\beta} \) is the saturation (volume fraction) of phase \( \beta \), \( \rho_{\beta} \) is density of phase \( \beta \), and \( X^{(\kappa)}_{\beta} \) is the mass fraction of component \( \kappa \) present in phase \( \beta \). Similarly, the heat accumulation term in a multi-phase system is(*)

\[ M^{(NK+1)} = \phi \sum_{\beta=1}^{NPH} S_{\beta} \rho_{\beta} u_{\beta} + (1-\phi) \rho_R C_R T \]  

(A.3),

where \( u_{\beta} \) denotes internal energy of fluid phase \( \beta \).

The mass flux term is a sum over phases

\[ F^{(\kappa)} = \sum_{\beta=1}^{NPH} X^{(\kappa)}_{\beta} F_{\beta} \]  

(A.4)

for \( \kappa = 1, \ldots, NK \). Individual phase fluxes are given by a multi-phase version of

(*) The heat balance equation is ignored in the isothermal gas-water-foam version of MULKOM.
Darcy’s law:

\[ F_\beta = -k \frac{k_{f\beta}}{\mu_\beta} \rho_\beta (\nabla P_\beta - \rho_\beta g) \]  
(A.5)

Here \( k \) is absolute permeability, \( k_{f\beta} \) is relative permeability of phase \( \beta \), \( \mu_\beta \) is viscosity, and

\[ P_\beta = P + P_{\text{cap,}\beta} \]  
(A.6)

is the pressure in phase \( \beta \), which is the sum of the pressure \( P \) of a reference phase, and the capillary pressure of phase \( \beta \) relative to the reference phase. In addition to Darcy flow, MULKOM also includes binary diffusion in the gas phase for fluids with two gaseous (or volatile) components \( \kappa, \kappa' \).

\[ f^{(x)}_{\beta, \text{gas}} = -\phi \mathsf{S}_g \tau D_{\kappa,\kappa'} \rho_g \nabla X^{(x)}_g \]  
(A.7)

\( D_{\kappa,\kappa'} \) is the coefficient of binary diffusion which depends on the nature of the gaseous components and on pressure and temperature. \( \tau \) is a tortuosity factor. When binary diffusion is present the flux-term (A.7) simply gets added to that of (A.4).

Heat flux contains conductive and convective components (no dispersion)

\[ F^{(\text{NK+1})} = -K \nabla T + \sum_\beta h_\beta F_\beta \]  
(A.8)

where \( K \) is thermal conductivity of the medium, and \( h_\beta = u_\beta + P/\rho_\beta \) is the specific enthalpy of phase \( \beta \).

MULKOM can model vapor pressure lowering due to capillary and phase adsorption effects. This is represented by Kelvin’s equation (Edlefsen and Anderson, 1943):

\[ P_v (T, S_I) = P_{\text{sat}} (T) \cdot \exp \left\{ \frac{m_l \cdot P_{\text{cap}}(S_I)}{\rho_l \cdot R(T + 273.15)} \right\} \]  
(A.9)

where \( P_{\text{sat}} \) is saturated vapor pressure of bulk liquid, \( P_{\text{cap}} \) is the difference between liquid and gas phase pressures, \( m_l \) is the molecular weight of the liquid, and \( R \) is the universal gas constant.
Appendix B. Space and Time Discretization

The continuum equations (A.1) are discretized in space using the "integral finite difference" method (Edwards, 1972; Narasimhan and Witherspoon, 1976). Introducing appropriate volume averages, we have

$$\int_{V_n} M \, dV = V_n \, M_n$$

(B.1)

where $M$ is a volume-normalized extensive quantity, and $M_n$ is the average value of $M$ over $V_n$. Surface integrals are approximated as a discrete sum of averages over surface segments $A_{nm}$:

$$\int_{f_{n}} F \cdot n \, d\Gamma = \sum_{m} A_{nm} \, F_{nm}$$

(B.2)

Here $F_{nm}$ is the average value of the (inward) normal component of $F$ over the surface segment $A_{nm}$ between volume elements $V_n$ and $V_m$. This is expressed in terms of averages over parameters for elements $V_n$ and $V_m$. For the basic Darcy flux term, Eq. (A.5), we have

$$F_{\beta, nm} = -k_{nm} \left( \frac{k_{\beta}}{\mu_{\beta}} \right)_{nm} \left[ \frac{p_{\beta, n} - p_{\beta, m}}{D_{nm}} - \rho_{\beta, nm} g_{nm} \right]$$

(B.3)

where the subscripts $(nm)$ denote a suitable averaging (interpolation, harmonic weighting, upstream weighting). $D_{nm}$ is the distance between the nodal points $n$ and $m$, and $g_{nm}$ is the component of gravitational acceleration in the direction from $m$ to $n$.

The discretized form of the binary diffusive flux in the gas phase is

$$f_{\beta g, nm}^{(k)} = -\phi_{nm} S_{g, nm} \tau_{nm} (D_{kk'})_{nm} \rho_{g, nm} \frac{x_{g, n} - x_{g, m}}{D_{nm}}$$

(B.4)

Substituting Eqs. (B.1) and (B.2) into the governing Eq. (A.1) a set of first-order ordinary differential equations in time is obtained.

$$\frac{dM_{n}^{(k)}}{dt} = \frac{1}{V_n} \sum_{m} A_{nm} \, F_{nm}^{(k)} + q_{n}^{(k)}$$

(B.5)
Time is discretized as a first order finite difference, and the flux and sink and source terms on the right hand side of Eq. (B.5) are evaluated at the new time level, $t^{k+1} = t^k + \Delta t$, to obtain the numerical stability needed for an efficient calculation of multi-phase flow. This treatment of flux terms is known as "fully implicit," because the fluxes are expressed in terms of the unknown thermodynamic parameters at time level $t^{k+1}$, so that these unknowns are only implicitly defined in the resulting equations; see e.g. Peaceman (1977). The time discretization results in the following set of coupled non-linear, algebraic equations:

$$R_n^{(k)k+1} = M_n^{(k)k+1} - \frac{\Delta t}{V_n} \left\{ \sum_m A_{nm} F_n^{(k)k+1} + V_n q_n^{(k)k+1} \right\}$$

$$= 0$$

(B.6)

The entire geometric information of the space discretization in Eq. (B.6) is provided in the form of a list of grid block volumes $V_n$, interface areas $A_{nm}$, nodal distances $D_{nm}$, and components $g_{nm}$ of gravitational acceleration along nodal lines. There is no reference whatsoever to a global system of coordinates, or to the dimensionality of a particular flow problem. The discretized equations are in fact valid for arbitrary irregular discretizations in one, two or three dimensions, and for porous as well as for fractured media. This flexibility should be used with caution, however, because the accuracy of solutions depends upon the accuracy with which the various interface parameters in equations such as (B.3, B.4) can be expressed in terms of average conditions in grid blocks. A sufficient condition for this to be possible is that there exists approximate thermodynamic equilibrium in (almost) all grid blocks at (almost) all times (Pruess and Narasimhan, 1985). For systems of regular grid blocks referenced to global coordinates (such as $r - z$, $x - y - z$), Eq. (B.6) is identical to a conventional finite difference formulation (e.g. Peaceman, 1977).

For each volume element (grid block) $V_n$ there are $NK+1$ equations ($k=1, \ldots, NK, NK+1$), so that for a flow system with $N$ grid blocks (B.6) represents a total of $N \cdot (NK+1)$ coupled non-linear equations. The unknowns are the $N \cdot (NK+1)$
independent primary variables \( x_i \) \( [i = 1, \ldots, N \cdot (NK+1)] \) which completely define the state of the flow system at time level \( t^{k+1} \). These equations are solved by Newton/Raphson iteration, which is implemented as follows. We introduce an iteration index \( p \) and expand the residuals \( R_n^{(k)k+1} \) in Eq. (B.6) at iteration step \( p+1 \) in a Taylor series in terms of those at index \( p \):

\[
R_n^{(k)k+1} (x_{i,p+1}) = R_n^{(k)k+1} (x_{i,p})
+ \sum_i \frac{\partial R_n^{(k)k+1}}{\partial x_i} \bigg|_p (x_{i,p+1} - x_{i,p}) + \ldots = 0
\]  

(B.7)

Retaining only terms up to first order, we obtain a set of \( N \cdot (NK+1) \) linear equations for the increments \( (x_{i,p+1} - x_{i,p}) \):

\[
- \sum_i \frac{\partial R_n^{(k)k+1}}{\partial x_i} \bigg|_p (x_{i,p+1} - x_{i,p}) = R_n^{(k)k+1} (x_{i,p})
\]  

(B.8)

All terms \( \partial R_n/\partial x_i \) in the Jacobian matrix are evaluated by numerical differentiation. Eq. (B.8) is solved with the Harwell subroutine package "MA28" (Duff, 1977). Iteration is continued until the residuals \( R_n^{(k)k+1} \) are reduced below a preset convergence tolerance.
Table 1. MULKOM fluid property modules.

<table>
<thead>
<tr>
<th>components</th>
<th>number of components</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>1</td>
</tr>
<tr>
<td>water at near-critical conditions</td>
<td>1</td>
</tr>
<tr>
<td>two waters*</td>
<td>2</td>
</tr>
<tr>
<td>water, CO₂†</td>
<td>2</td>
</tr>
<tr>
<td>water, NaCl</td>
<td>2</td>
</tr>
<tr>
<td>water, air</td>
<td>2</td>
</tr>
<tr>
<td>water, SiO₂‡</td>
<td>2</td>
</tr>
<tr>
<td>water, volatile hydrocarbon,</td>
<td>3</td>
</tr>
<tr>
<td>non-volatile hydrocarbon</td>
<td></td>
</tr>
<tr>
<td>water, natural gas, foam</td>
<td>3</td>
</tr>
</tbody>
</table>

*water with tracer
† with mineral buffer
‡ includes dissolution and precipitation, as well as associated changes in porosity and permeability.
Solution of Linear Equations

Data Input and Initialization

Assembling and Iterative Solution of Transport Equations

Primary Variables
Secondary Parameters

Printed Output

"EOS-Module"

Equation of State

Figure 1. Modular architecture of MULKOM and TOUGH.
Figure 2. Schematic of linear interpolation of relative permeability for a phase with small saturation.