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SHAFT, MULKOM, TOUGH: A Set of Numerical Simulators for Multiphase Fluid and Heat Flow

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ABSTRACT

Numerical simulation of fluid and heat flow has become a widely accepted technique for studying and evaluating geothermal reservoirs and other subsurface flow systems. This article discusses several interrelated simulation codes which were developed at Lawrence Berkeley Laboratory with a capability to model multiphase flow and phase change effects. We review some of the early concepts in geothermal reservoir simulation, and summarize the development of the SHAFT79 and MULKOM codes. We also describe the architecture of MULKOM and TOUGH and give a detailed statement of the governing equations.

INTRODUCTION

In response to the 1973 OPEC oil embargo the U.S. Department of Energy initiated a number of Research and Development programs intended to improve energy technologies which could provide alternatives to hydrocarbon fuels. One of the major alternative energy programs was launched in the field of geothermal energy, with participation from National Laboratories, the U.S. Geological Survey, universities, and private companies. A substantial effort was made to develop geothermal reservoir simulators, i.e., computer software capable of simulating the behavior of geothermal reservoirs in their natural state as well as in response to exploitation. It was hoped that a computer simulation capability could help to improve our understanding of geothermal resources, and could thereby contribute to their more rapid and efficient utilization.

During the last decade, as a result of this development effort, reservoir simulation has become an accepted tool for studying fluid and heat flow in geothermal systems. It has provided important insights into the dynamics of geothermal reservoirs, and has come into routine use in the geothermal industry. Furthermore, techniques developed in geothermal reservoir simulation are finding applications in other areas, such as in the geologic disposal of high-level nuclear wastes, and in thermally enhanced oil recovery.

A number of computer programs for the simulation of geothermal reservoirs are available at the present time (see e.g. the recent review by O'Sullivan, 1985). In this article we review the development and architecture of several reservoir simulation codes which were developed at Lawrence Berkeley Laboratory (LBL) with a capability to handle multiphase flow with phase change effects. The codes dealt with include SHAFT78, SHAFT79, MULKOM, and TOUGH. It is hoped that the present review will clarify the relationship between these codes, and will provide useful background for applications.*

*Source codes and documentation for SHAFT79 and TOUGH are available, for a nominal fee, from the National Energy Software Center, c/o Argonne National Laboratory, 9700 South Cass Ave., Argonne, Ill.

SHAFT

Early efforts at developing a geothermal reservoir simulation capability at the Lawrence Berkeley Laboratory (LBL) are associated with the name "SHAFT", which is an acronym for "simultaneous heat and fluid transport." Preliminary results in the development of SHAFT were presented by Lasseter, Witherspoon, and Lippmann (1975). These authors discussed concepts for the important material constituents and physical processes in geothermal reservoirs. They presented governing heat and mass balance equations, as well as numerical techniques for their solution. Much of the mathematical and numerical concepts of SHAFT were borrowed from a heat flow code "TRUMP," which had been developed by A. Edwards at Lawrence Livermore Laboratory (Edwards, 1972). Lasseter et al. (1975) also gave examples of SHAFT runs for two-phase flow systems without phase transitions. A detailed study on the governing heat, mass and momentum balance equations to be used in SHAFT was made by Assens (1976).

The approach and methods on which SHAFT was based can be briefly summarized as follows. Geothermal reservoirs were conceptualized as systems of porous rock with a single-component fluid (water) filling the pore space. The fluid could be present as single-phase liquid or vapor, or as a two-phase liquid-vapor mixture. Physical processes considered for these systems included fluid flow, driven by pressure and body forces, and heat flow via conduction and convection, including latent heat effects as well as mechanical work. Rock and fluid were assumed compressible and in thermal equilibrium locally. The physical processes modeled by SHAFT were described by means of mass- and energy-balance equations, with a multiphase version of Darcy's law governing fluid flow (see appendix A). For numerical solution the equations were discretized by means of integral finite differences for the space variables (Narasimhan and Witherspoon, 1976; see appendix B), and by first-order finite differences in the time domain. The coupled non-linear mass and energy balance equations were replaced by approximate linearized equations, which were obtained by averaging over a time step. The resulting equations were then solved sequentially for a given time step; first all energy balances, followed by a solution to all mass balances. Either set

of approximate linear equations was solved by means of a variant of point-Jacobi iteration with an acceleration parameter (Varga, 1962).

An interesting aspect of SHAFT was the choice and treatment of thermodynamic variables. The program was intended to handle both single- and two-phase states and therefore could not use the variables (pressure, temperature), because in two-phase conditions these are not independent, being related by the saturated vapor pressure relationship for water. One possible way of dealing with this would be to use the variables (pressure, temperature) only for single phase conditions, and "switch" to variables (pressure, saturation) when a transition to two-phase conditions occurs. This variable switching was later implemented in the MULKOM and TOUGH codes, and has proven a very robust and satisfactory method for treating multiphase systems. An alternative approach is the use of a "persistent" pair of variables which remain independent of each other throughout the entire single- and two-phase regions, such as (pressure, enthalpy) or (density, internal energy). In the early days of geothermal reservoir simulation the prevailing opinion among researchers was that use of persistent variables would be advantageous (e.g., Lasseter et al., 1975; Pritchett, 1975; Faust and Mercer, 1975). In particular the choice of (density, internal energy) was believed to facilitate overall mass and energy conservation, because it results in the simplest expressions for the accumulation terms (see Eqs. (A.2) and (A.3)); this is the choice made in SHAFT. However, there is no useful closed-form expression for obtaining all other thermophysical parameters appearing in the governing equations, such as temperature, pressure, viscosity, gas saturation, in terms of density and internal energy. Therefore, SHAFT employed a table lookup procedure, in which all parameters were obtained by interpolation from values tabulated over a regular grid of density and internal energy values. The table was generated by a preprocessor program using steam table equations for water properties.

SHAFT78

As the development of the SHAFT code progressed some changes had to be made in the original concepts. The author and coworkers achieved a first workable implementation embodying most of the original SHAFT concepts in a code known as SHAFT78 (Pruess et al., 1979a, b). The most significant revision was in the coupling between mass- and energy-balance equations. The sequential scheme could not in general guarantee a sufficiently accurate local thermal equilibrium between rocks and fluid. Therefore, after the completion of a (relatively large) energy time step and associated (several smaller) density steps an explicit rock-fluid equilibration was performed to ensure local thermal equilibrium. If this equilibration could not be carried out within a certain user-specified accuracy the entire time step was repeated with reduced time increment. This procedure enabled phase transitions to be performed with acceptable accuracy through a number of automatically adjusted small time steps. The concept of tabulating all thermophysical properties as functions of internal energy and density of water could be made to work satisfactorily. Special procedures were set up to select points for tabulation as well as for table lookup so that interpolation would not occur across the saturation line. This was necessary for achieving accurate and stable phase transitions, during which the derivatives of thermodynamic state variables can change by several orders of magnitude.

SHAFT78 was applied successfully for studying a number of problems in geothermal reservoir engineering, including well tests and pressure decline in two-phase reservoirs. An important insight gained from SHAFT78 simulations was that pressure decline in response to production from boiling reservoirs does not in general permit estimation of fluid reserves (Pruess et al., 1979a). Attempts at modeling producing vapor-dominated reservoirs with SHAFT78, however, soon revealed that the time step limitations inherent in the sequential solution scheme were forbidding. Further analysis made clear that in two-phase systems with phase transitions and strong latent heat effects the coupling between fluid and heat flow can be so strong that only a fully coupled simultaneous solution of mass- and energy-balance equations will permit satisfactory time steps and accuracy. Mathematically, the coupling terms between mass-

and energy-balance equations increase proportional to time step size. Iterative matrix techniques for obtaining a fully coupled solution are then not satisfactory. They require the matrix of the equation system to be diagonally dominant (Varga, 1962), which imposes severe time step limitations.

Another difficulty arises from the extreme non-linearities during phase transitions. The concept of approximating the non-linear governing equations by a time-averaged linear system for each time step works fine as long as no phase transitions are encountered. During phase transitions, however, averaging leads to unstable behavior, because the averages over a time step can change dramatically for relatively small variations in the final state.

SHAFT79

In agreement with other workers active in geothermal reservoir simulation development at that time (Coats, 1977; Garg et al., 1977; Faust and Mercer, 1979; Zyvoloski et al., 1979) we concluded that in order to obtain a practically viable simulation methodology, the following techniques were needed: (1) solve all mass- and energy-balance equations in a fully coupled simultaneous manner; (2) evaluate all flow terms fully implicitly at the incremented time level; (3) do not linearize the equations, but use Newton-Raphson iteration to handle the non-linearities; and (4) solve the linear equations arising at each Newton-Raphson iteration step by means of direct matrix methods.

These techniques were implemented in a program known as ''SHAFT79'' (Pruess and Schroeder, 1980). Direct solution of the linear equations is accomplished with the program package ''MA28'' from the United Kingdom Atomic Energy Authority, Harwell (Duff, 1977). MA28 performs a sparse version of LU-decomposition with partial pivoting and back substitution. It is ideally suited for interfacing with SHAFT79 because it handles matrices with random sparsity structure, allowing to exploit the geometric flexibility of the integral finite difference method to its fullest extent. SHAFT79 solves the same governing equations as SHAFT78, but due to the

improved mathematical and numerical methods it can take much larger time steps, and it can accomplish transitions between single- and two-phase conditions in a stable and efficient manner. This has made possible applications to difficult multiphase flow problems (Pruess and Truesdell, 1980; Pruess et al., 1982a), as well as to actual field problems with difficult flow geometry and many years of production history (Pruess et al., 1983). For a number of years SHAFT79 was the "workhorse" of LBL's geothermal reservoir modeling effort, and it remains in use in a number of organizations to this day.

Although originally conceived for flow in porous media, subsequent development of a "multiple interacting continua" (MINC) technique has made it possible to apply the unmodified SHAFT79 code to simulations of multiphase flow in fractured media as well (Pruess and Narasimhan, 1982b; Pruess, 1983a; Pruess and Narasimhan, 1985). This extension was possible because of the great flexibility for specifying flow geometry offered by the integral finite difference method.

The diverse applications have proven the mathematical and numerical methods used in SHAFT79 to be robust and efficient. However, a number of limitations existed which prompted the development of another more powerful code, MULKOM. A minor inconvenience arises from the handling of thermophysical properties by interpolation from tabulated data as functions of (density, internal energy). Because of the extremely small compressibility of liquid water (of the order of $5 \cdot 10^{-10}$/Pa) very small density changes translate into large pressure changes. Initialization of a flow problem in terms of (density, internal energy) will then in general return a slightly different pressure than desired by the code user (discrepancies are of the order of 0.1 bar). A more severe limitation arises from the fact that SHAFT79 is written for a single-component fluid, whereas geofluids are typically multi-component mixtures often containing appreciable amounts of non-condensible gases and dissolved solids.

MULKOM

"MULKOM" is an acronym for "multi-component model," a family of computer modules for simulating the flow of multicomponent, multiphase fluids and heat in permeable (porous or fractured) media (Pruess, 1983b). The flow equations solved and the mathematical and numerical methods employed in MULKOM are similar to those in SHAFT79 (see appendix A and B).

The numerical approach in MULKOM is based on the integral finite difference method. The difference equations are formulated fully implicitly, providing stability and time step tolerance in highly non-linear flow problems. All mass- and energy-balance equations are solved simultaneously, using Newton/Raphson iteration. As in SHAFT79, the linear algebra is performed with the Harwell solver MA28 (Duff, 1977). The essential differences between MULKOM and SHAFT79 are in the code architecture, which allows for a flexible interfacing of modules representing different fluid mixtures, and provides for a variety of process capabilities (well specifications and schedules).

MULKOM was built on the recognition that the transport equations governing flow of heat and multicomponent multiphase fluids in porous or fractured rock masses have the same form, regardless of the number of fluid components and phases present (see appendix A). From the mathematical point of view, a reservoir containing an H_2O/CO_2 mixture, for example, differs from a system with pure water in only two respects: (1) compositional systems require additional mass-balance equations, namely, one for each component, and (2) the thermodynamic and thermophysical properties of mixtures are different from those of pure substances. Therefore, when modeling fluid and heat flow in compositional systems, it is desirable to employ a flexible program structure that can be easily adapted to handle different mixtures. MULKOM features a modular architecture (Figure 1), with separate modules for (1) initializing simulation problems, (2) representing PVT properties (equation of state) for the desired fluid mixtures, (3) assembling the nonlinear transport equations, and (4) solving the set of linear equations arising in the iterative solution process for the nonlinear equations. The

coding is done in such a way that the number of fluid components and phases to be treated can be provided as a variable input parameter.

Calculation of thermophysical properties by table lookup, as in SHAFT79, would lead to excessive storage requirements when there are more than two primary variables (more than one fluid component). Therefore, MULKOM employs closed-form expressions such as steam-table equations or suitable regression formulas. Phase transitions are handled by means of variable-switching, which leads to a very efficient and robust algorithm. For example, in simulations for pure water, (pressure, temperature) are used as primary variables throughout the single-phase regions. A phase transition from single phase liquid to two-phase conditions is diagnosed when pressure drops below the saturated vapor pressure for prevailing temperature. In analogous fashion, a vapor state begins to evolve liquid when pressure rises above the saturated vapor pressure at prevailing temperature. In either case the second primary variable is switched from temperature to vapor saturation, being initialized as slightly larger than zero when the transition occurred from a liquid state, and slightly smaller than one when the transition occurred from a vapor state. A transition from two-phase conditions to either single phase liquid or single phase vapor occurs when the vapor saturation variable goes outside of the range (0,1). In this case the second primary variable is switched back to (the latest) temperature, and pressure is reset to a value slightly above (for liquid) or below (for vapor) the corresponding saturation pressure. Analogous procedures are employed for fluid mixtures with more than two phases.

The nature of the fluids and their thermophysical properties are specified by means of equation of state modules (''EOS''), which also perform phase transition diagnostic and appropriate variable switching during a simulation. The EOS expresses all thermodynamic and thermophysical properties (''secondary parameters'') of multicomponent multiphase fluid mixtures in terms of a set of ''primary'' dependent variables, which uniquely define the thermodynamic state of the flow system. For a system with NK components, the number of primary variables (degrees of freedom) per grid block is NK + 1, i.e., there is one variable for each mass component and one variable for the heat ''component.''

The EOS module communicates with the other modules of MULKOM by means of two large arrays. The array fed to the EOS module contains the latest values of all primary variables for all grid blocks. The EOS then computes an array which contains a complete set of secondary parameters for the given primary variables. (In fact, it also provides parameters pertaining to each of the primary variables incremented by a small amount; these are needed for numerically computing all derivatives for the Jacobian matrix in the Newton/Raphson process, see appendix B). By convention, the first primary variable is always chosen to be the total pressure of a reference phase (usually the non-wetting phase). All other primary variables can be chosen freely for maximum convenience in the EOS-module, as they are not being used in the other modules. Therefore, primary variables can be chosen (and changed during a flow simulation) in such a way that accuracy and efficiency of the thermophysical property calculations and phase transition diagnostics are optimized. This has permitted better absolute and relative accuracy in parameters controlling flow, so that convergence can be obtained for larger time steps (often by factors of 5 to 10) than was possible with SHAFT79. The larger time step tolerance more than compensates for the increased time used in thermophysical property calculations from the full steam table equations (e.g., International Formulation Committee, 1967; Haar, Gallagher, and Kell, 1984), as compared with the fast table lookup in SHAFT79. We have found that accurate mass- and energy-balances can be easily maintained for any choice of primary variables that we have tried; there appears to be no particular advantage in this regard with the choice of (density, internal energy) as variables.

A list of presently used EOS modules for MULKOM is given in Table 1. Table 2 lists all the secondary parameters provided by these EOS modules for assembling the transport equations. The array of secondary parameters as provided by the EOS modules has a specific data structure that enables the transport module of MULKOM to obtain the needed thermophysical properties in definite storage locations, regardless of the number of fluid components and phases present. It is the special structure of the primary and secondary parameter arrays--and the architecture of the interface for the EOS module--that gives MULKOM the flexibility to represent different mixtures of

nonreactant fluids.

MULKOM has been used extensively for fundamental and applied studies of geothermal reservoirs, oil and gas fields, nuclear waste repositories, and for the design and analysis of laboratory experiments. A considerable number of modules with specialized capabilities and options has been developed for various research applications. These are not always mutually compatible; furthermore, internal and external documentation of MULKOM is sketchy so that at the present time the code remains a research tool which is not easily transferable to a would-be user.

TOUGH

A thorough effort at internal and external documentation and code cleanup and testing was undertaken for a set of MULKOM modules that simulate non-isothermal flow of water-air mixtures. This work was motivated by a desire to provide a capability for modeling the thermohydrologic conditions in a high-level nuclear waste repository in partially water saturated geologic formations. To set this particular version of MULKOM apart it was given a special name, "TOUGH," which is an acronym for "transport of unsaturated groundwater and heat," and is also an allusion to the tuff-formations at Yucca Mountain, Nevada, which are presently being evaluated by the U.S. Department of Energy for their suitability as a host medium for a high-level nuclear waste repository.

The TOUGH User's Guide (Pruess, 1987) gives a technical description of the code and its architecture. It also provides complete documentation for preparing input decks, and includes a set of sample problems which illustrate code applications. TOUGH can perform all the "conventional" geothermal simulations for pure water simply by setting air mass fraction equal to zero in the input deck.

CONCLUDING REMARKS

The SHAFT and SHAFT78 codes are now obsolete; they have been reviewed here primarily for historical reasons, and because they are forerunners of the program SHAFT79 as well as the MULKOM family of codes. SHAFT79 remains of interest for geothermal applications, because it has received widespread application and testing and is well documented. MULKOM is a versatile general-purpose research tool for studying nonisothermal flows of multicomponent multiphase fluids. Its flexibility has resulted in a proliferation of modules and options which require intimate familiarity with the source code for use. TOUGH is a well documented code for non-isothermal flow of water and air. It can be applied to problems in high-level nuclear waste storage and for geothermal reservoir simulations, offering an alternative to SHAFT79 for users interested in a basic geothermal simulation capability.

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Appendix A. Mass and Energy Balances

The basic mass- and energy-balance equations solved by SHAFT78, SHAFT79, MULKOM and TOUGH can all be written in the following general form:

$$\frac{D}{Dt}\int_{V_n} M^{(\kappa)}dv = \int_{\Gamma_n} \mathbf{F}^{(\kappa)} \cdot \mathbf{n}\, d\Gamma + \int_{V_n} q^{(\kappa)}\, dv \qquad (A.1)$$

The integration here is over an arbitrary subdomain V_n of the flow system under study, which is bounded by the closed surface Γ_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". For time differentiation we have written a "substantial derivative" D/Dt, which provides the most convenient way for dealing with flow in deformable media (Bird et al., 1960; Narasimhan and Witherspoon, 1977). In SHAFT78 and SHAFT79 we have only one mass component, water, and an energy component. We have for the mass accumulation term

$$M^{(1)} = \phi\rho \qquad (A.2).$$

The heat accumulation term contains fluid and rock contributions

$$M^{(2)} = \phi\rho u + (1-\phi)\rho_R\, C_R\, T \qquad (A.3),$$

where ϕ is porosity, ρ is density of the the (single- or two-phase) fluid, u is internal energy of the fluid, ρ_R and C_R are rock density and specific heat, respectively, and T is temperature.

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

$$M^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_\beta\, \rho_\beta\, X_\beta^{(\kappa)} \qquad (A.4)$$

The total mass of component κ is obtained by summing over all fluid phases $\beta = 1, \ldots, NPH$. S_β is the saturation (volume fraction) of phase β, ρ_β is density of phase β, and $X_\beta^{(\kappa)}$ is the mass fraction of component κ present in phase β. Similarly, the heat

accumulation term in a multi-phase system is

$$M^{(NK+1)} = \phi \sum_{\beta=1}^{NPH} S_\beta \rho_\beta u_\beta + (1-\phi) \rho_R C_R T \qquad (A.5),$$

where u_β denotes internal energy of fluid phase β.

The mass flux term is a sum over phases

$$\mathbf{F}^{(\kappa)} = \sum_{\beta=1}^{NPH} X_\beta^{(\kappa)} \mathbf{F}_\beta \qquad (A.6)$$

for $\kappa = 1, \ldots, NK$. Individual phase fluxes are given by a multi-phase version of Darcy's law:

$$\mathbf{F}_\beta = - k \frac{k_{r\beta}}{\mu_\beta} \rho_\beta (\nabla P_\beta - \rho_\beta \mathbf{g}) \qquad (A.7)$$

Here k is absolute permeability, $k_{r\beta}$ is relative permeability of phase β , μ_β is viscosity, and

$$P_\beta = P + P_{cap,\beta} \qquad (A.8)$$

is the pressure in phase β, which is the sum of the pressure P of a reference phase, and the capillary pressure of phase β relative to the reference phase. Capillary pressures are taken into account in MULKOM and TOUGH, but not in SHAFT78 and SHAFT79. $\mathbf{g}$ denotes the vector of gravitational acceleration. In addition to Darcy flow, MULKOM and TOUGH also include binary diffusion in the gas phase for fluids with two gaseous (or volatile) components κ, κ'

$$\mathbf{f}_{\beta = gas}^{(\kappa)} = - \phi S_g \tau D_{\kappa\kappa'} \rho_g \nabla X_g^{(\kappa)} \qquad (A.9)$$

$D_{\kappa,\kappa'}$ is the coefficient of binary diffusion which depends on the nature of the gaseous components and on pressure and temperature. τ is a tortuosity factor. When binary diffusion is present the flux-term (A.9) simply gets added to that of (A.6).

Heat flux contains conductive and convective components (no dispersion)

$$\mathbf{F}^{(NK+1)} = -K\nabla T + \sum_\beta h_\beta \mathbf{F}_\beta \qquad (A.10)$$

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

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

$$P_v\,(T, S_l) = P_{sat}\,(T) \cdot \exp\left\{\frac{m_l \cdot P_{cap}(S_l)}{\rho_l\ R(T + 273.15)}\right\} \qquad (A.11)$$

where P_{sat} is saturated vapor pressure of bulk liquid, P_{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

$$\int_{V_n} M dV = V_n M_n \tag{B.1}$$

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}:

$$\int_{\Gamma_n} \mathbf{F} \cdot \mathbf{n} \, d\Gamma = \sum_m A_{nm} F_{nm} \tag{B.2}$$

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.7), we have

$$F_{\beta,nm} = - k_{nm} \left[\frac{k_{r\beta} \rho_\beta}{\mu_\beta} \right]_{nm} \left[\frac{P_{\beta,n} - P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm} g_{nm} \right] \tag{B.3}$$

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 (MULKOM and TOUGH only)

$$f^{(\kappa)}_{\beta=gas,nm} = - \phi_{nm} S_{g,nm} \tau_{nm} (D_{\kappa\kappa'})_{nm} \rho_{g,nm} \frac{X_{g,n} - X_{g,m}}{D_{nm}} \tag{B.4}$$

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.

$$\frac{dM_n^{(\kappa)}}{dt} = \frac{1}{V_n} \sum_m A_{nm} F_{nm}^{(\kappa)} + q_n^{(\kappa)} \tag{B.5}$$

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:

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

$$= 0 \qquad \text{(B.6)}$$

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 (κ=1, . . ., 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, ..., N · (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 $R_n^{(\kappa)k+1}$ in Eq. (B.6) at iteration step p+1 in a Taylor series in terms of those at index p:

$$R_n^{(\kappa)k+1}(x_{i,p+1}) = R_n^{(\kappa)k+1}(x_{i,p}) + \sum_i \left.\frac{\partial R_n^{(\kappa)k+1}}{\partial x_i}\right|_p (x_{i,p+1} - x_{i,p}) + \ldots = 0 \qquad \text{(B.7)}$$

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

$$-\sum_i \left.\frac{\partial R_n^{(\kappa)k+1}}{\partial x_i}\right|_p (x_{i,p+1} - x_{i,p}) = R_n^{(\kappa)k+1}(x_{i,p}) \qquad \text{(B.8)}$$

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 $R_n^{(\kappa)k+1}$ are reduced below a preset convergence tolerance.

Table 1. MULKOM fluid property modules.

components	number of components
water	1
water at near-critical conditions	1
two waters*	2
water, CO_2†	2
water, NaCl	2
water, air	2
water, SiO_2‡	2
water, volatile hydrocarbon, non-volatile hydrocarbon	3
water, natural gas, foam	3

*water with tracer

† with mineral buffer

‡ includes dissolution and precipitation, as well as associated changes in porosity and permeability

Table 2. Secondary parameters.

Parameter	Meaning (units)
S_β	Saturation of phase β (dimensionless)
$k_{r\beta}$	Relative permeability (dimensionless)
μ_β	Viscosity (Pa-s)
ρ_β	Density (kg/m^3)
h_β	Specific enthalpy (J/kg)
$P_{cap,\beta}$	Capillary pressure (Pa)
$X_\beta^{(\kappa)}$	Mass fraction of component κ in phase β (dimensionless)
T	Temperature (°C)
K	Heat conductivity (W/m°C)

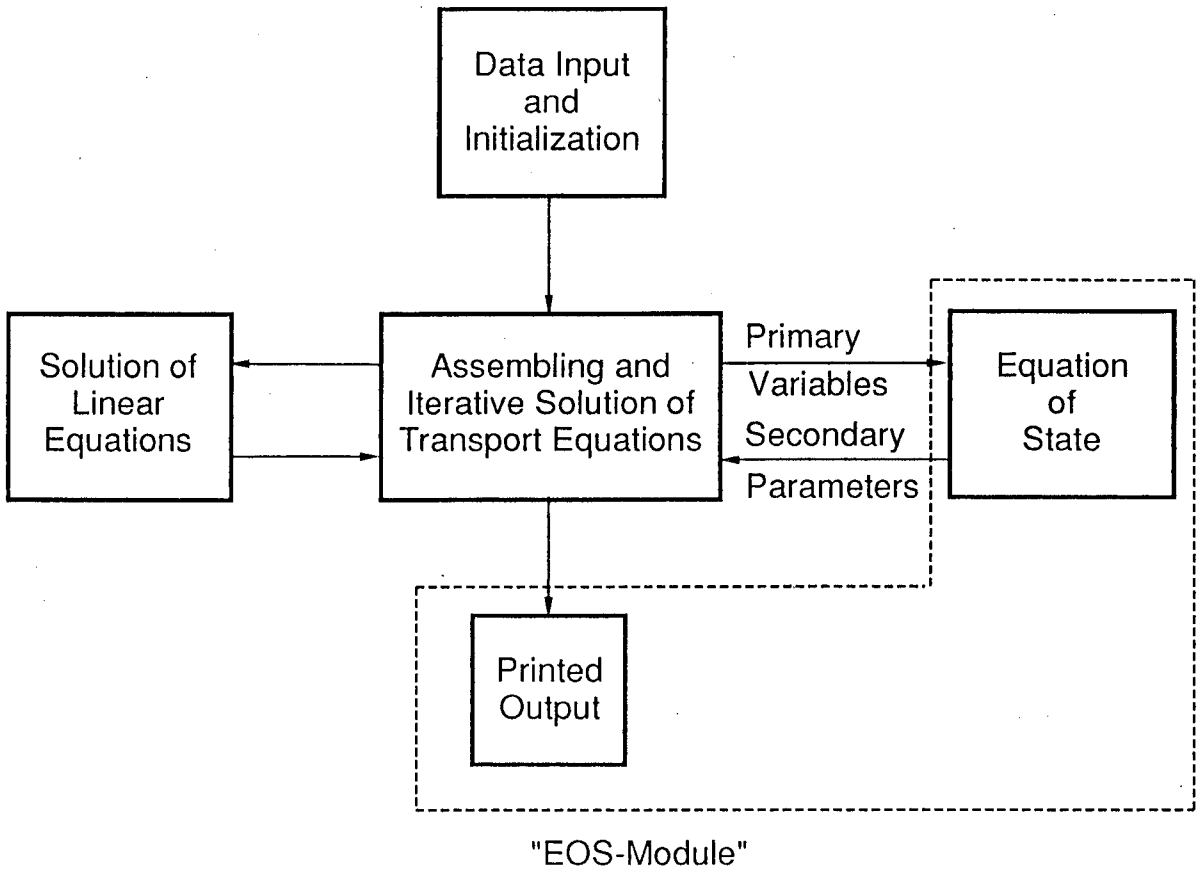

Figure 1. Modular architecture of MULKOM and TOUGH.

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