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MUFITS CODE FOR ANALYSIS OF BINARY MIXTURE FLOWS IN POROUS MEDIA

Andrey Afanasyev[1]
[1]Institute of Mechanics Moscow State University; 1 Mitchurinskiy prospekt, Moscow, 119192, Russia
e-mail: afanasyev@imec.msu.ru

ABSTRACT MUFITS (MUltiphase FIltration Transport Simulator) is a noncommercial developing code intended for analysis of nonisothermal multiphase flows of binary mixture in porous media. A nonclassical approach for mixture properties calculation is implemented in MUFITS. The approach facilitates simulation of flows subjected to wide pressure and temperature variations, flows close to critical conditions and three-phase nonisothermal flows of binary mixture. Transport equations and Darcy correlation are closed by conditional extremum problem for mixture properties calculation. This problem corresponds to maximum entropy condition in thermodynamic equilibrium. Such approach allows determining not only single-phase states and two-phase states of liquid-gas type as in classical models but also two phase states of liquid-liquid type and three-phase states and allows the corresponding flows in porous media simulation.

Keywords: multiphase flow, compositional simulation

INTRODUCTION

Multiphase flows in porous media with a transition between sub- and supercritical thermodynamic conditions occur in many natural and technological processes (e.g. in deep regions of geothermal reservoirs where temperature reaches critical point of water or in gas-condensate fields where subject to critical conditions retrograde condensation occurs and even in underground carbon dioxide sequestration processes at high formation pressure). Simulation of these processes is complicated due to degeneration of conservation laws under critical conditions and requires non-classical mathematical models and methods.

A new mathematical model is proposed for analysis of binary mixture flows in porous media subjected to wide pressure and temperature variations and critical thermodynamic conditions. The distinctive feature of the model lies in the methodology for mixture properties determination. Transport equations and Darcy law are solved together with calculation of the entropy maximum that is reached in thermodynamic equilibrium and determines mixture composition. To define and solve the problem only one function – mixture thermodynamic potential – is required. Such approach allows determination not only single-phase states and two-phase states of liquid-gas type as in classical models but also two-phase states of liquid-liquid type and three-phase states.

For water-carbon dioxide binary mixture flows in geothermal reservoirs or in the CO_2 storage processes the proposed model can be applied for analysis of single-phase water, water vapor, gaseous CO_2 or liquefied CO_2 flows and two-phase or three-phase flows of any combination of these phases with allowance for phase transitions. The approach can handle flows in shallow and deep regions of geothermal reservoir under sub- and supercritical thermodynamic conditions.

The proposed model was implemented in MUFITS (MUltiphase FIltration Transport Simulator) code for hydrodynamic simulations. As opposed to classical approaches pressure, enthalpy and composition variables together with fully implicit method and cascade procedure are used. The code is capable of unstructured grids, heterogeneous porous media, relative permeability and capillary pressure dependence on temperature and pressure, multiphase diffusion, optional number of sinks and sources, etc. There is a developed module for mixture properties specification. The starting point for the simulation is a cubic equation of state that is used for mixture thermodynamic potential – entropy – calculation in pressure, enthalpy and composition variables. A polynomial spline is implemented to save the potential for subsequent hydrodynamic simulations. At this stage the majority of complicated thermodynamic procedures are performed prior to hydrodynamic that results in sufficient acceleration of calculations.

GOVERNING EQUATIONS

Equations of State

A cubic equation of state is used for binary mixture thermodynamic potential definition prior to multiphase flash calculation (multiphase equilibrium problem). Entropy σ depending on pressure P, enthalpy h and mixture composition x (x is the components molar fractions) is defined

$$\sigma(P,h,x) \tag{1}$$

For a given potential (1) the binary mixture multiphase flash problem is defined by the relations

$$\sum_{i=1}^{3} \sigma(P,h_i,x_i)V_i \to \max \tag{2}$$

$$\sum_{i=1}^{3} V_i = 1, \qquad \sum_{i=1}^{3} h_i V_i = h_t, \qquad \sum_{i=1}^{3} x_i V_i = x_t, \tag{3}$$

$$0 \le V_i \le 1 \tag{4}$$

Here, index t denotes total, summed over all phases parameters, V is the phase molar fraction. Index i is the phase number. According to Gibbs phase rule, the maximum number of phases in binary mixture thermodynamic equilibrium is equal to 3. That's why $i = 1 \ldots 3$.

Relation (2) is the maximum entropy condition while (3), (4) are restrictions for this condition. Following (3), summed over all phases enthalpy and composition are equal to h_t, x_t respectively. The phase molar fraction is a value between 0 and 1 (4).

The conditional extremum problem (2)-(4) is applicable for single-, two- and three-phase states of binary mixture detection. There is a single-phase state if entropy reaches maximum at $V_1 = 1$, $V_2 = 0$, $V_3 = 0$ conditions. In this case phases $i = 2,3$ are absent in thermodynamic equilibrium. There is a two-phase state if entropy reaches maximum at $0 < V_{1,2} < 1$, $V_3 = 0$ conditions implying that only phase $i = 3$ is absent. There is a three-phase state if entropy reaches maximum at $0 < V_i < 1$, $i = 1 \ldots 3$ conditions.

According to the problem (2)-(4) formulation, P, h_t, x_t are known while h_i, x_i, V_i, $i = 1 \ldots 3$ are unknown parameters determined by the problem solution.

Transport Equations

Binary mixture flow in porous media is considered under the following restrictions

- the porous media is under thermal equilibrium. The rock and fluid temperatures are equal
- the binary mixture is under thermodynamic equilibrium
- pore-scale parameters of rock reservoir and capillary pressure are supposed to have no affect on thermodynamic equilibrium
- no solid-liquid, solid-gas phase transitions. No chemical reactions
- relatively slow flows. The Darcy correlation can be applied
- no saturation functions hysteresis

The flow is described by the following equations

$$\frac{\partial}{\partial t}\left(\frac{1-m}{v_s}\right) = 0 \tag{5}$$

$$\begin{aligned} &\frac{\partial}{\partial t}\left(m \sum_{i=1}^{3} \frac{M_{(j)} x_{i(j)}}{v_i} s_i \right) + \\ &\quad + div\left(\sum_{i=1}^{3} \frac{M_{(j)} x_{i(j)}}{v_i} \mathbf{w}_i + \mathbf{D}_{(j)} \right) = Q_{(j)} \end{aligned} \tag{6}$$

$$\begin{aligned} &\frac{\partial}{\partial t}\left(m \sum_{i=1}^{3} \frac{e_i}{v_i} s_i + (1-m)\frac{e_s}{v_s} \right) + \\ &\quad + div\left(\sum_{i=1}^{3} \frac{h_i}{v_i} \mathbf{w}_i + \mathbf{D}_e \right) = A_g + Q_e \end{aligned} \tag{7}$$

$$\mathbf{w}_i = -K \frac{f_i}{\mu_i}\left(\mathbf{grad} P_i - \frac{M_i}{v_i}\mathbf{g} \right) \tag{8}$$

Equation (5) is mass conservation equation for rock material. Here, m is the porosity, v is the molar volume, index s denotes parameters of rock.

Relations (6) are mass conservation equations for each component of the binary mixture $j = 1,2$. Equation (7) is energy balance equation. Here, M is the molar density, s is the saturation, $\mathbf{w}$ is the Darcy velocity, e is the internal energy, $\mathbf{D}$ denotes fluxes caused by diffusion and heat conduction, Q are a given sinks and sources rates, A_g is the work done by the force of gravity

$$A_g = \sum_{i=1}^{3} \frac{M_i}{v_i} \mathbf{w}_i \mathbf{g},$$

$\mathbf{g}$ is the gravity acceleration. Index $i = 1 \ldots 3$ denotes phase parameters, index (j) denotes $j = 1,2$ component parameters.

Equation (8) is the Darcy correlation. Here, K is the rock permeability, f is the relative permeability, μ is the viscosity.

The transport equations (5)-(8) are closed by the conditional extremum problem (2)-(4).

METHODS OUTLINE

Primary Simulation Variables

MUFITS uses pressure, molar enthalpy and mixture composition as primary hydrodynamic simulation variables. These variables have an advantage because

- single-phase, two-phase and three-phase states of binary mixture can be determined (if temperature is used instead of enthalpy then three-phase states can't be determined)
- hydrodynamic equations are not degenerated under critical conditions if these variables are used

Mixture Properties Design

The MUFITS simulator distinctive feature from both commercial and open source codes lies in mixture properties calculation method. Nowadays two approaches to mixture equation of state treatment are marked out

- explicit formulation is used individually for every phase properties (TOUGH2 code, black oil model formulation)
- mixture thermodynamic equilibrium is determined implicitly by an iterative procedure (flash calculation in compositional simulator)

The first approach allows fast properties calculation giving an opportunity of implicit hydrodynamic simulations on high resolution grids. However, the properties explicit formulation usually makes impossible their determination in wide region of thermobaric conditions and close to critical conditions. Thus the first approach can't be applied to simulation of flows subjected to complicated thermodynamic effects like retrograde condensation and gases liquefaction.

In general case the second approach implementation demands application of nested iterative procedures leading to slow properties calculation. This results in slow hydrodynamic simulation even by an explicit method. However, this approach has an advantage because it can be applied to simulation of flows subjected to complicated thermodynamic effects.

A modified approach is applied in MUFITS merging some features of each treatment. This approach can be divided in two steps

- firstly, cubic equation of state is used for mixture thermodynamic potential (1) calculation (entropy depending on primary simulation variables - pressure, enthalpy and composition). This time consuming step is performed only once before hydrodynamic simulation. The majority of nested iterative procedures are implemented at this step.
- secondly, the potential is used for fast multiphase flash calculation (2)-(4) using a single iterative procedure. This fast step is executed scores of times during hydrodynamic simulation.

This approach makes possible relatively fast compositional hydrodynamic simulations by fully implicit method implemented in the MUFITS code.

Grid

Flow geometry is specified by two arrays. The first array defines parameters of cells (volume, location depth, porosity) while the second array defines parameters of flow connections (interface area, distance between cell centers, permeability). This formulation can handle simulation of flows on both structured and unstructured grids in one, two and three dimensions. Reservoir heterogeneity can be easily specified.

Numeric methods

The following methods are implemented in MUFITS for hydrodynamic simulations

- FIM: finite volume method with fully implicit upwind approximation of fluxes
- MPI+DVBR: message passing interface and distributed variable block format for matrix storage
- Newton's method preconditioned by the cascade procedure for nonlinear equations solution
- ILUT+GMRES: generalized minimum residual linear solver with domain decomposition preconditioner and ILUT subdomain solver
- Numeric differentiation: numeric calculation of derivatives for matrix filling

APPLICATIONS

MUFITS code is supposed to be applicable to

Underground carbon dioxide storage

- liquified CO_2 phase;
- three-phase flows of liquid H_2O liquid CO_2 and gaseous CO_2

Gas condensate fields exploration

- three-phase compositional hydrocarbon flows;
- sub- and supercritical flows;
- retrograde condensation in porous media;
- cycling process

Geothermal energy

- sub- and supercritical flows, deep and shallow processes;
- transition through critical point of water

SAMPLE SIMULATIONS

Water-Carbon Dioxide Phase Diagram

In Fig. 1, the characteristic points are shown and the regions with various numbers of phases for the CO_2-H_2O binary mixture are restricted. The phase diagram is obtained from the solution of problem (2)–(4) for $P \in [0.1, 150]$ MPa, $h \in [-10, 55]$ kJ/mole and $x \in [0,1]$. Here, x is the CO_2 molar fraction, $U = \ln(P / P_a)$ and $P_a = 0.1$ MPa.

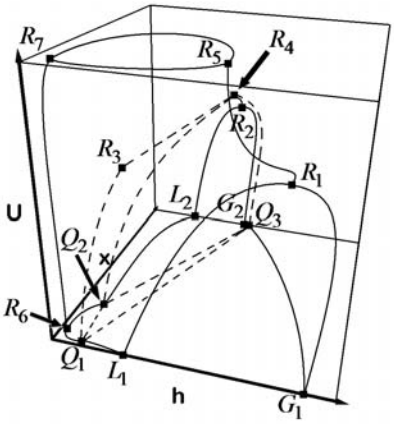

Fig. 1. CO_2-H_2O binary mixture phase diagram

The solid lines are located on the surface separating the regions of single-phase and two-phase equilibriums of the mixture and the dashed lines, which are also located on the surface, limit the three-phase equilibriums. Inside the region $Q_1Q_2Q_3R_4R_3$, the mixture is in the three-phase state (liquid H_2O and CO_2 in liquid and gaseous state), outside of it but inside the region limited by solid lines, it is in the two-phase state. $R_1(R_2)$ is the critical point of H_2O (CO_2). R_1R_5 and R_2R_4 are the critical conditions lines for the binary mixture.

CO_2 Injection in Water Saturated Reservoir

The MUFITS code was used for test studies of CO_2 injection in reservoir initially saturated with water (fig. 2). A realistic geology is used with folds and rock properties heterogeneity. The injection well-1 is under constant injection rate conditions while well-2 is under constant bottom hole pressure. CO_2 molar fraction x_t (fig. 2) has a non uniform distribution caused by phase transitions and reservoir heterogeneity.

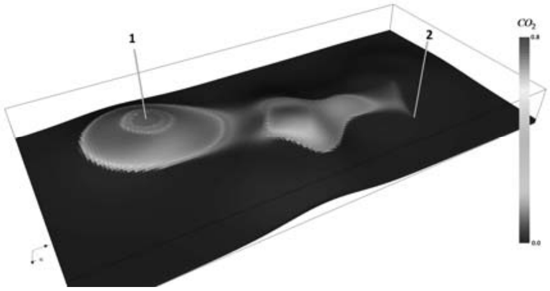

Fig. 2. Distribution of CO_2 in the reservoir

The grid contains 8 layers and about 10^5 cells in this case study. The numeric simulation of flow takes about 115 minutes using 64 MPI processes.

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REFERENCES

Afanasyev A.A. Mathematical model of nonisothermal multiphase binary mixture flow through a porous medium. Fluid Dynamics, 2011, Volume 46, Number 1, Pages 80-89.

Afanasyev A.A. Binary-mixture flows in a porous medium at high pressure and temperature. Doklady Physics, 2011, Volume 56, Number 4, Pages 224-226.