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Equivalence of two models in single-phase multicomponent flow simulations

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ABSTRACT

In this work, two models to simulate the single-phase multicomponent flow in reservoirs are introduced: single-phase multicomponent flow model and two-phase compositional flow model. Because the single-phase multicomponent flow is a special case of the two-phase compositional flow, the two-phase compositional flow model can also simulate the case. We compare and analyze the two models when simulating the single-phase multicomponent flow, and then demonstrate the equivalence of the two models mathematically. An experiment is also carried out to verify the equivalence of the two models.

1. Introduction

Much work has contributed to the field of single-phase and multi-phase flow simulations in reservoirs. Such flow simulations can be applied in broad regimes such as enhancing oil and gas recovery from hydrocarbon reservoirs by injection of chemicals [1–3], storing greenhouse gases in saline aquifers and oil fields [4,5], monitoring the transport of contaminants in groundwater flow [6–8] among others.

The study of the flows in reservoirs can be traced back to the year 1856 when Frenchman Henry Darcy investigated the flow characteristics of sand filters for water purification. He established the foundation of the quantitative theory for the flow of homogeneous fluids in porous media [9]. Then Muskat and Wyckoff [10–13] studied the flow of reservoir fluids in 1930's, and their work was instrumental in advancing the knowledge of reservoir dynamics to its present state.

Algorithmically, many schemes have been developed to simulate the multi-phase flow such as the fully implicit scheme and implicit–explicit hybrid scheme. The use of fully implicit schemes in reservoir simulations can be traced back to the work of Roebuck et al. [14], where they developed an implicit numerical method to simulate the differential and algebraic relations governing one-dimensional three-phase flows in porous media. Then much work to improve the solution procedure of implicit scheme was carried out such as [15,16]. The first application of an implicit–explicit scheme in reservoir simulations can be found in [17], where an implicit equation for the oil-phase pressure and two explicit equations for the over-all composition and water saturation were obtained. Further investigation on implicit–explicit hybrid scheme can be observed in [18–22]. A fully implicit scheme can solve for the pressures, velocities, saturations etc. simultaneously, and its time step can be set larger than the implicit–explicit hybrid scheme. However, the fully implicit scheme requires significantly more computing resources than the implicit–explicit hybrid scheme when solving the discretized linear system. The implicit–explicit hybrid scheme solves for the pressures implicitly, then solves for the saturations or concentrations explicitly. Its computing cost is lower compared to the fully implicit scheme, but to achieve convergence its time step is

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limited by the CFL condition and the splitting error from decoupling pressure and saturation/concentration equations. In many large-scale simulations, the number of unknowns in the discretized linear system of the fully implicit scheme becomes very large, and it is not efficient to solve the system, thus an implicit–explicit hybrid scheme is preferred.

Moreover, many discretization schemes have been proposed in the multi-phase flow simulation. Popular methods include finite difference method (FDM) [23,24], finite element method (FEM) [25–28] and Lattice-Boltzmann method (LBM) [29–38]. Traditional FDM dominates both theoretical and practical work in the multi-phase flow simulation. It is based on the physical concepts such as mass conservation law, energy conservation law, Darcy's law and the isothermal fluid phase behavior. Both structured and unstructured grids can be used in discretization to represent the geometry of the reservoir accurately. FDM is simple and easy to implement, but it is not very versatile in dealing with boundaries and achieving stable results. Some restrictive mesh refinement has to be imposed to get a nonsingular system. However, FEM can get well-posedness results easily, and its variational framework is very amenable to a posteriori error estimation. But the sparsity patterns from FEM are less structured and can be more difficult to parallelize efficiently. Although FDM and FEM achieve much success in the multi-phase flow simulation, they cannot tackle the complex pore space and inherent free-boundary issues such as breaking and merging of interfaces in the reservoir. Thus, LBM is proposed to capture the microscopic effects and reproduce the macroscopic behavior. LBM does not track interfaces but rather maintains the sharp interfaces automatically. Macroscopic behavior such as interface dynamics can arise naturally from the microscopic effects. FDM is the discretization method of choice in this work, considering its ready realization of parallelization.

Based on the algorithmic scheme and discretization scheme mentioned above, a series of models to simulate the flows have been proposed. Two of them are the single-phase multicomponent flow model and the two-phase compositional flow model. Because the single-phase multicomponent flow is a special case of the two-phase compositional flow, the two-phase compositional flow model can also simulate the single-phase multicomponent flow. However, it is unknown that whether the two models would output the same simulation results. To the best of our knowledge, no work has ever tried to compare and analyze the two models when simulating the single-phase multicomponent flow. Thus, whether the two models are equivalent with each other in such condition is a work deserved to do. In this work, we firstly establish the two models under some assumptions, and then we derive the condition to achieve the equivalence mathematically. Finally, we verify the equivalence by a numerical experiment.

2. Single-phase multicomponent flow model

2.1. Basic equations

In the single-phase multicomponent flow model, the flow is in either oil phase or gas phase. Suppose there are c components, then the c mass conservation equations can be expressed as

$$\frac{\partial(\phi x_m \xi)}{\partial t} = \nabla\cdot\left(\frac{x_m\xi}{\mu}\boldsymbol{k}\left(\nabla p-\rho\boldsymbol{g}\right)\right)+q_m,\quad m=1,2,\ldots,c. \tag{2.1}$$

In the above equation, ϕ is the porosity of the porous medium, x_m stands for the molar fraction of component m, ξ is the molar density of the flow, t is the time, μ is the viscosity, p is the pressure, ρ is the mass density of the flow, $\boldsymbol{g}$ is the gravity vector, q_m is the source or sink term of component m, and c is the number of components. $\boldsymbol{k}$ is the permeability tensor, and in 2D condition it can be expressed as

$$\boldsymbol{k}=\begin{pmatrix} k_{xx} & k_{xy}\\ k_{yx} & k_{yy}\end{pmatrix}.$$

Diffusion and dispersion effect is omitted in the model. We add the c equations of (2.1) together and have

$$\frac{\partial(\phi\xi)}{\partial t} = \nabla\cdot\left(\frac{\xi}{\mu}\boldsymbol{k}\left(\nabla p-\rho\boldsymbol{g}\right)\right)+q, \tag{2.2}$$
$$q=\sum_{m=1}^{c} q_m.$$

Because ξ is the function of p and N_m with N_m being the molar amount of component m, the left-hand side of (2.2) can be derived further as

$$\begin{aligned}\frac{\partial(\phi\xi)}{\partial t} &= \phi\frac{\partial\xi}{\partial t}+\xi\frac{\partial\phi}{\partial t}\\ &= \phi\left(\frac{\partial\xi}{\partial p}*\frac{\partial p}{\partial t}+\sum_{m=1}^{c}\frac{\partial\xi}{\partial N_m}*\frac{\partial N_m}{\partial t}\right)+\xi\frac{\partial\phi}{\partial t}\\ &= \phi\left(\frac{\partial\xi}{\partial p}*\frac{\partial p}{\partial t}+\sum_{m=1}^{c}\frac{\partial\xi}{\partial N_m}*\frac{\partial N_m}{\partial t}\right).\end{aligned}$$