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EFFICIENT ENERGY-STABLE DYNAMIC MODELING OF COMPOSITIONAL GRADING

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Abstract. Compositional grading in hydrocarbon reservoirs caused by the gravity force highly affects the design of production and development strategies. In this paper, we propose a novel mathematical modeling for compositional grading based on the laws of thermodynamics. Different from the traditional modeling, the proposed model can dynamically describe the evolutionary process of compositional grading, and it satisfies the energy dissipation property, which is a key feature that real systems obey. The model is formulated for the two scales of free spaces without solids (laboratory scale) and porous media (geophysical scale). For the numerical simulation, we propose a physically convex-concave splitting of the Helmholtz energy density, which leads to an energy-stable numerical method for compositional grading. Using the proposed methods, we simulate binary and tenary mixtures in the free spaces and porous media, and demonstrate that compared with the laboratory scale, the simulation at large geophysical scales has more advantages in simulating the features of compositional grading.

Key words. Compositional grading, dynamic modeling, energy stability, Peng-Robinson equation of state.

1. Introduction

In the hydrocarbon reservoirs, gravity can cause a considerable compositional variation with depth. This phenomenon is known as compositional grading [6, 8, 10, 18, 20], and it has been observed in various oil and gas-condensate reservoirs (see [6, 17] and the references therein). Accurate modeling and simulation of composition variation have significant contributions to the correct design of production and development strategies [6, 20].

Because of its importance, the compositional grading phenomenon has been modeled and numerically simulated in the literature. Gibbs [7] proposed a model to calculate compositional variation under the force of gravity for an isothermal system. A formulation for non-isothermal compositional grading has also been proposed in [8] based on the stationary system assumption and theory of irreversible processes. In [20], a nonisothermal model was used to predict compositional variation in a petroleum fluid column. In [17], a continuous thermodynamic framework was presented to calculate compositional grading in hydrocarbon reservoirs, and the effect of the gravity field on the segregation characteristics of heavy fractions in the oil was established analytically using the method of moments.

The existing modeling and simulation so far can well predict the features of compositional grading at the steady states. As the PVT (pressure, volume, and temperature) conditions of a hydrocarbon reservoir are changed by the surrounding environment, the hydrocarbon mixtures shall immigrate and mix towards a new steady state. There may exist incomplete hydrocarbon mixing since complete mixing may take a long time. So in this case, a dynamic modeling is necessary since it can provide the information about the states during evolution. Moreover, the dynamic modeling is also a useful instrument to obtain the solutions at the steady

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state. In this paper, we treat the total (free) energy as a summation of the fluid Helmholtz energy and gravitational potential energy, and based on the first law of thermodynamics, we derive an entropy equation, which yields the requirement of total energy dissipation by the second law of thermodynamics. Furthermore, combining the diffusion equations for multiple components, we derive a dynamic model for compositional grading. The proposed model satisfies the energy dissipation property, which means that a thermodynamics-consistent steady state can be achieved after a time evolution period.

Physical experiments are often applied to study the features of compositional grading. For the laboratory scale, a free space without solids is often used, and the space size may not be large due to restricted space. The proposed model is first derived for the free space, and then it is extended to the scale of porous media. Different from the free space, a porous medium usually has multi-scale structures including various porosity and geometric tortuosity, which have significant effects on this mixing process of hydrocarbon mixtures. These multi-scale physical properties are also considered in the proposed model, and as a result, the simulated results can reflect the effects of multi-scale structures.

An analytical solution is obtained for the ideal gas equation of state that describes the PVT relation by a simple linear equation. By this analytical solution, we clearly show that heavy components are concentrated toward the bottom while light components are concentrated toward the top. For realistic hydrocarbon fluids, the numerical simulation is required in practical applications since the realistic equation of state (e.g. Peng-Robinson equation of state (PR-EOS) [21]) is strongly nonlinear, and the solutions are also essentially different from the ideal gas. Phase transition also increases the complexity of compositional grading; in fact, the mixture may be split into gas and liquid phases due to gravity effect. Numerical modeling and simulation of multi-phase fluid flow at the Darcy scale and at the pore scale have been active and challenging research topics [1, 4, 5, 26–28]; this is especially true for multi-phase flow based on a realistic equation of state, which is a very challenging but also attractive research subject in recent years [11,12,15,19,23]. To simulate such problems efficiently, a stable numerical method is demanded to satisfy the energy-dissipation principle. Here, we construct a convex-concave splitting form for the Helmholtz free energy density, which leads to an efficient, energy-stable numerical method. Finally, we simulate the compositional grading of binary and tenary mixtures at a laboratory scale and a porous medium scale, and we conclude with some analysis and comments on the simulation results.

2. Energy formulations for compositional grading

We assume that hydrocarbon mixtures in a closed reservoir have fixed total moles and constant temperature. The conditions of the fixed volume, moles and temperature have been applied in the literature [9, 14, 16, 22] for instance. For a mixture composed of N components, we denote by n_i the molar density of component i, and let $\mathbf{n} = (n_1, n_2, \cdots, n_N)^T$ and $n = \sum_{i=1}^{N} n_i$. For compositional grading in the free spaces, the total (free) energy is a summation of two contributions: the Helmholtz free energy F_b, and the gravitational potential energy F_g as

$$F(\mathbf{n}) = F_b(\mathbf{n}) + F_g(\mathbf{n}), \tag{1}$$

where

$$F_b(\mathbf{n}) = \int_\Omega f_b(\mathbf{n}) d\mathbf{x}, \; F_g(\mathbf{n}) = \int_\Omega f_g(\mathbf{n}) d\mathbf{x}. \tag{2}$$