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An implicit numerical model for multicomponent compressible two-phase flow in porous media

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ABSTRACT

We introduce a new implicit approach to model multicomponent compressible two-phase flow in porous media with species transfer between the phases. In the implicit discretization of the species transport equation in our formulation we calculate for the first time the derivative of the molar concentration of component i in phase α ($c_{\alpha,i}$) with respect to the total molar concentration (c_i) under the conditions of a constant volume V and temperature T. The species transport equation is discretized by the finite volume (FV) method. The fluxes are calculated based on powerful features of the mixed finite element (MFE) method which provides the pressure at grid-cell interfaces in addition to the pressure at the grid-cell center. The efficiency of the proposed model is demonstrated by comparing our results with three existing implicit compositional models. Our algorithm has low numerical dispersion despite the fact it is based on first-order space discretization. The proposed algorithm is very robust.

1. Introduction

In two-phase compositional flow, most of the numerical models in the literature are based on explicit approximation of the species balance equation [1]. The nonlinearity between the phase molar and/or mass concentration and the total concentration in the implicit method requires some complicated derivatives that do not appear in an explicit scheme. In the explicit scheme, one of the major drawbacks is time step selection based on the Courant–Freidrichs–Levy condition, known as the CFL condition. The CFL condition requires the time step to be less than the necessary time for flow to pass through one mesh block. The impact of this condition becomes severe when one grid-block has a relatively small size compared to the size of the simulation domain. Numerical modeling of fractured reservoirs is a clear example of small and large grid-cells. Most of the numerical simulators that deal with fractures require either to have small mesh elements to explicitly model the fractures (e.g. single-porosity models) [2–4], or to have very small elements near the fractures (e.g. cross-flow-equilibrium approach) [5–8]. In this case the numerical simulation becomes – computational wise – expensive, if an explicit scheme is used in the numerical model. In compositional multiphase flow, the use of an explicit method is preferred for the following reasons: (i) significant numerical dispersion usually consorted with the implicit approximation, and (ii) complexity of applying a straightforward Newton method to solve the nonlinear system of equations in the compositional multiphase flow. The importance of using implicit scheme arises when the use of an explicit scheme is – CPU wise – expensive as mentioned above. This will be demonstrated in the core of this manuscript when we compare computational cost of both implicit and explicit schemes using the same gridding and then reducing the size of one or multiple grid-blocks to study how the CFL condition would affect the CPU time in the explicit scheme. Evidently, the CPU cost of the implicit scheme will not be affected by the size of the grid-block as much as by the number of the grid-blocks instead.

Despite the fact the implicit approximations are incorporated in all of the commercial models, very few publications could be found when an implicit scheme are discussed in compressible multiphase flow. Most of the literature goes back to early publications. Coats [9] presented a fully implicit scheme for compositional multiphase flow. In his model the set of unknowns consist of pressure, and phase mole fractions. These variables are referred to as natural-type variables. Fussel and Fussel [10] presented a formulation that uses a different set of variables based on phase compositions. These variables are referred to as the mass variables. Later, Chien et al. [11] proposed using the equilibrium ratios as a set of unknowns beside the pressure and the overall concentrations rather than saturations and phase compositions.

In Fig. 1 we show a comparison of our model to two different commercial models that we denote by CM-1 and CM-2. The comparison is based on a modified 3-component mixture example presented in

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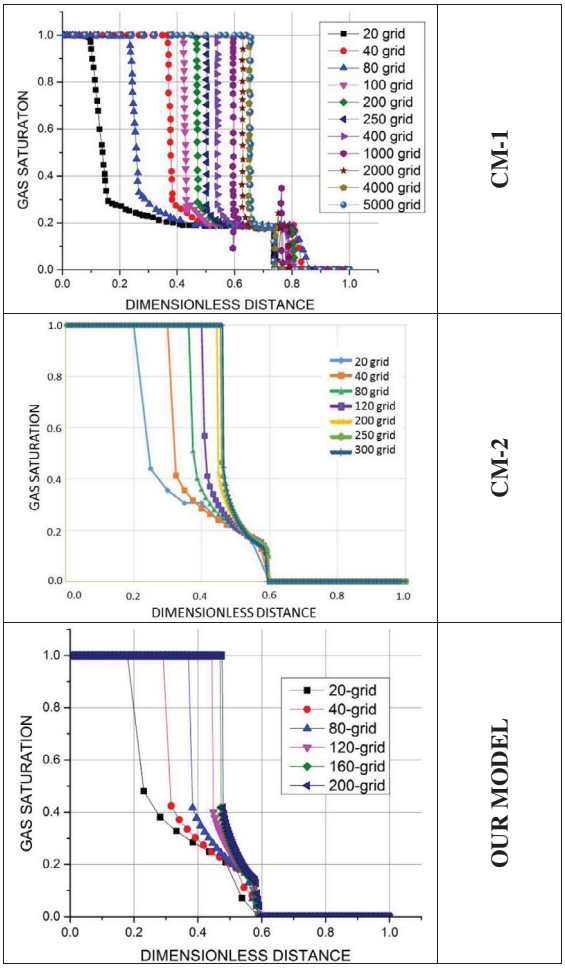

Fig. 1. Comparison of our model to CM-1 and CM-2 with different mesh refinements; modified coats example.

[9]. The modified example is in two-phase flow in 1-D. Results show high numerical dispersion from CM-1, even with very fine mesh compared to CM-2. Only CM-2, after removing the over and under-shoots gives comparable results to our model. We should note that we also compared the results to a third commercial model (CM-3). We do not show the results of CM-3 since it does not converge when a more refined mesh than 120 grid-blocks is used in the modified Coats example. All of the three commercial models (CM-1, 2 and 3) are based on first order finite difference discretization in space and time. To demonstrate the low numerical dispersion in our model, we compare results of 1-D and 2-D examples (with our model) to an explicit higher-order method (discontinuous Galerkin method) in Section 4.

The most recent work on compositional multiphase implicit scheme is reported in [12]. These authors chose the set of unknowns based on the overall molar density of species and the pressure. The phase compositions are updated in a post-processing step using constant volume and temperature flash routines.

In this paper we present a new model that solves implicitly the species balance equation. The species transport equation is discretized by using a finite volume (FV) approximation. The Newton–Raphson (NR) method is used to solve implicitly the species transport equation. The calculation of the derivatives in our formulation will be discussed later in detail. The total flux is calculated by the hybridized mixed finite element method (MFE). The latter provides accurate calculation of the velocity field even in highly heterogeneous media when compared to the traditional finite element and finite volume methods [1,5,7,13–20]. The strength of the MFE method is from the calculation of the pressure inside a finite element and the traces of the pressures at the interfaces of each finite element in the computational domain. The flux of each phase is deduced from the total flux by using the phase mobility coefficient as will be discussed later. In this paper the effect of gravity is taken into account. In two-phase flow, the calculation of the phase fluxes is not trivial with gravity effect. The difficulty arises from up-streaming the mobility of each phase. Without gravity, both phases flow in the same direction as the total flux. With gravity, however, counter-current flow may develop at the finite element interfaces due to the density contrast. Updating the phase mobilities based on the values at the previous time step is not consistent. A phase could appear/disappear from one time step to another. To resolve this complexity, we have developed an efficient method to upstream the phase derivatives based on the updated phase mobilities and phase fluxes at the current time step. In this paper we use the same upstreaming technique of the phase mobilities as in [1,7]. Once evaluated, the phase fluxes are then coupled with our upstreaming technique of the phase derivatives discussed in details in Section 3.

The compressible behavior of each phase is described by the Peng–Robinson equation of state [21]. The computation of composition of each phase is provided by the equality of fugacities of each component in both (vapor and liquid) phases. This calculation is commonly known in the literature by flash [22]. For a given pressure P and temperature T the flash calculation is performed at each finite element of the computational domain and the calculation is known as PT-flash calculation. However, when an implicit scheme is used to solve the species transport equation, the derivatives of concentration of each component of each phase is computed with respect to the total concentration at constant volume V and temperature T. In this work we will show how the derivatives can be calculated without the VT-flash.

In addition to the new derivatives that appear in the species transport equation in the implicit scheme, we couple the volumetric fluxes to the species equation differently from the work of [9,12] and others. The pressure in our formulation is calculated in a preprocessing step in order to update the fluxes based on the converged values of the molar densities. We believe that this approach reduces the number of iterations per time step when compared to the implicit update of the pressures with the molar densities and compositions. The numerical examples in this work will be compared to a higher-order explicit method, that is, the discontinuous Galerkin (DG) method. The DG method is based on a linear approximation of the molar density inside each grid cell. As a result, we have three degrees of freedom in each grid cell for the transport variable. A finite difference time discretization is used in both models. The aim of this work is to show that our implicit model can produce accurate results even when compared to a higher-order method such as the DG. We believe that the implicit scheme can be more efficient than the explicit scheme in problems that the CFL condition has a severe constraint on the time step as we mentioned above.

The rest of the paper is organized as follows: in the next section we provide the differential equations describing the multicomponent compressible two-phase flow in porous media. Then we present the discretization of the pressure and the species balance equations. We present seven numerical examples to demonstrate the efficiency and accuracy of the proposed algorithm.

2. Mathematical model

2.1. Species balance equation

The mass balance of component i in compressible two-phase (gas and oil) flow of n_c-component mixture is given by the following equations: