

AN EULERIAN-LAGRANGIAN FORMULATION FOR COMPOSITIONAL FLOW IN POROUS MEDIA

HONG WANG ^{*}, RICHARD E. EWING AND GUAN QIN [†], AND S.L. LYONS [‡]

Abstract. We derive an Eulerian-Lagrangian formulation for two-phase, multicomponent compositional flow in porous media with sources and sinks. The formulation can be used by many Eulerian-Lagrangian methods in solving the component mass balance equations. It can be combined with different types of pressure solvers in solving the coupled systems of compositional models. A full thermodynamic flash calculation is carried out to determine phase stability and composition.

Numerical experiments are presented to investigate the performance of the formulation and to compare it with widely used upwind method for compositional flow. These results indicate that the Eulerian-Lagrangian formulation generates stable and accurate solutions that resolve moving steep fronts and are physically reasonable, even if it uses a time step of at least two orders of magnitude larger than that used by the upwind method.

Key words.

AMS subject classifications.

1. Introduction. Compositional models describe the simultaneous transport of multiple components flowing in different phases in porous media. Mathematical models that describe the flow and transport processes consist of strongly coupled systems of time-dependent nonlinear partial differential equations of convection-diffusion type together with constraining equations describing the phase behavior. In industrial applications, upstream weighting techniques have commonly been used to stabilize the numerical approximations [1, 2]. These methods generate numerical solutions with qualitatively correct trend, but often produce excessive numerical diffusion that smears out the propagation fronts. For processes with high adverse mobility ratios, the traditional application upwind methods on structured grids may lead to strong grid orientation effects [2, 3]. These can sometimes be alleviated by the use of higher-order upwind schemes, or the use of grids that have better alignment with the flow.

One class of such methods is the class of streamline methods. Streamline methods solve the transport equations on a grid that is aligned with the flow, and handle convection along streamlines. They decouple three-dimensional mass transport into a large set of parallelizable one-dimensional problems. Therefore, streamline methods are highly efficient in convection and heterogeneity dominated flow regimes, and have been widely used in petroleum reservoir simulations [4]. In the context of two-phase compositional flow and transport, operator splitting is applied to separate processes that are not aligned with total flow (gravity, capillary effects, and other diffusive processes). Then the one-dimensional mass transport is solved along each streamline using nonlinear hyperbolic methods [5]. However, streamline methods have several potential shortcomings with respect to modeling compositional flows, e.g., difficulty in modeling mass transfer across streamlines, numerical diffusion caused by the projection of streamline solutions to a fixed mesh (for solving the pressure equation), and clustering and/or missing streamline coverage over some simulation cells. Further difficulties could arise when gravity segregation, diffusive or capillary effects are

^{*}Department of Mathematics, University of South Carolina, Columbia, South Carolina 29208; Fax: (803)777-3783; hwang@math.sc.edu

[†]Institute for Scientific Computation, Texas A&M University, College Station, Texas 77843-3404; Fax: (979) 845-5827; richard-ewing@tamu.edu

[‡]ExxonMobil Upstream Research Company, Houston, Texas 77252-2189

important drive mechanisms.

Another closely related class of methods is the class of Eulerian-Lagrangian methods. Eulerian-Lagrangian methods combine the convection and capacity terms in the mass transport equations to carry out the temporal discretization in a Lagrangian coordinate, and discretize the diffusion-dispersion term on a fixed mesh. Eulerian-Lagrangian methods symmetrize the mass transport equations and stabilize their numerical approximations. They generate accurate numerical solutions and significantly reduce the numerical diffusion and grid-orientation effect present in upwind methods, even if large time steps are used. Eulerian-Lagrangian methods have been developed for miscible displacement in enhanced oil recovery [6, 7, 8, 9, 10] and for immiscible displacement in water flooding [11, 12]. Because of increased efficiency, more components can be modeled using Eulerian-Lagrangian methods. This is very attractive in many cases. Eulerian-Lagrangian methods potentially provide a means to accurately deal with gravity at the same time as convection. This could be very important in CO₂ or gas injection processes.

In this paper we present an Eulerian-Lagrangian method for two-phase multi-component flow and transport processes in porous media, which has high potential to improve efficiency and accuracy of numerical simulations to compositional flow and transport processes. The method retains the numerical advantages of earlier Eulerian-Lagrangian methods for single-phase flow. In addition, the accurate solution of the mass transport equations by the Eulerian-Lagrangian method provides an accurate initial guess for and so speeds up flash calculation. Conversely, the accurate flash calculation improves the solutions to the mass transport equations in the next iterative or time step. Finally, larger time steps can be used, leading to further reduction of computational storage and cost. Preliminary numerical simulation of two-phase multi-component compositional flow in a two-dimensional reservoir reveals the following observations: (1) on the same spatial partition, using a timestep $\lesssim 100$ times larger, the Eulerian-Lagrangian method generates more accurate solutions with steeper fronts than the upwind method; (2) both methods use comparable CPU time per time step.

Finally, we will explore the idea on how to integrate compositional streamline methods with Eulerian-Lagrangian methods to develop a mass-conservative local-streamline Eulerian-Lagrangian method. The integrated method combines the advantages of streamline and Eulerian-Lagrangian methods and provides a mass-conservative framework. In this formulation, we track streamlines from certain quadrature points in each cell during a time step. We then use a streamline method locally in the current time interval. The advantages are as follows: (1) the tracking is needed only in evaluating the right-hand side, both the pressure and component mass transport equations are solved on the fixed mesh. Thus, no grid distortion or mapping is needed; (2) the choice of quadrature points can vary from cell to cell and from time step to time step. This adaptive feature naturally avoids the formation of clusters of points or missing cells; (3) the underlying Eulerian-Lagrangian formulation conserves mass in a systematic manner.

2. Mathematical model. We consider the simultaneous transport of multiple hydrocarbon components indexed as $i = 1, 2, \dots, n_c$, each of which can exist in a liquid phase l and a vapor phase v , flowing through a porous medium reservoir Ω . Let ϕ be the porosity of the medium, ρ^α and s^α be the molar density and saturation of phase α , and c_i^α be the mole fraction of component i in phase α . Then the mass

transport equation of component i is of the form [1, 13, 14]

$$\{s2a:e1\} \quad (2.1) \quad \frac{\partial}{\partial t} \sum_{\alpha=l,v} (\phi s^\alpha \rho^\alpha c_i^\alpha) + \nabla \cdot \sum_{\alpha=l,v} (\mathbf{u}^\alpha \rho^\alpha c_i^\alpha) - \nabla \cdot \sum_{\alpha=l,v} (\rho^\alpha \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla c_i^\alpha) = \sum_{\alpha=l,v} \bar{c}_i^\alpha \bar{\rho}^\alpha q^\alpha.$$

where q^α is the volumetric flow rate per unit bulk volume that accounts for external supplies of phase α . \bar{c}_i^α is prescribed at sources and $\bar{c}_i^\alpha = c_i^\alpha$ at sinks. The hydrodynamic dispersion tensor $\mathbf{D}(\mathbf{u}^\alpha, s^\alpha)$ is of the expression [1, 13]

$$(2.2) \quad \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) = s^\alpha d_m \phi \mathbf{I} + d_t |\mathbf{u}^\alpha| \mathbf{I} + \frac{d_l - d_t}{|\mathbf{u}^\alpha|} (u_i^\alpha u_j^\alpha). \quad \{s2a:e2\}$$

Here \mathbf{I} is the identity tensor, d_m is the molecular diffusion coefficient, and d_t and d_l are the transverse and longitudinal dispersivities. Here we have included the diffusion-dispersion in the mathematical model because of its potential importance in applications of miscible displacement [7].

Darcy's law establishes a relationship between Darcy velocity \mathbf{u}^α and the pressure gradient ∇p^α of phase α [1, 13]

$$(2.3) \quad \mathbf{u}^\alpha = -\frac{k^{r,\alpha}}{\mu^\alpha} \mathbf{K}(\nabla p^\alpha - \tilde{\rho}^\alpha \mathbf{g}). \quad \{s2b:e1\}$$

Here $k^{r,\alpha}$, μ^α , p^α are the relative permeability, viscosity, and pressure of phase α for $\alpha = l, v$; \mathbf{g} is acceleration due to gravity vector; $\mathbf{K} = (k_{ij})$ is the intrinsic permeability tensor of the medium. $\tilde{\rho}^\alpha$ is mass density of phase α , which is related to molar mass density ρ^α by $\tilde{\rho}^\alpha = (\sum_{i=1}^{n_c} MW_i c_i^\alpha) \rho^\alpha$ where MW_i is molecular weight of component i for $i = 1, 2, \dots, n_c$.

Compositional modeling requires thermodynamic flash calculation to determine phase partition and composition and other phase properties. The real gas law is often used to describe the relationship between molar density ρ^α , pressure p^α of phase α and temperature T of the fluid mixture [15]

$$(2.4) \quad \rho^\alpha = \frac{p^\alpha}{Z^\alpha RT}. \quad \{s2c:e1\}$$

Here R is the universal gas constant. $Z^\alpha = Z^\alpha(c_1^\alpha, \dots, c_{n_c}^\alpha, p^\alpha, T)$ is the compressibility factor of phase α ; it measures deviation of phase α from ideality. Z^α can be computed, for example, by using Peng-Robinson equation [16]

$$(2.5) \quad Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0. \quad \{s2c:e2\}$$

The coefficients $A = A^\alpha = (a^\alpha p^\alpha)/(R^2 T^2)$ and $B = B^\alpha = b^\alpha p^\alpha/(RT)$. The constants a^α and b^α are calculated from phase composition c_i^α , the binary interaction coefficients κ_{ij} between components i and j , and the attraction and repulsion parameters a_i and b_i of component i that are expressed in terms of critical pressure P_i and critical temperature T_i for $i = 1, \dots, n_c$ [15, 16].

Given the overall fluid composition c_1, c_2, \dots, c_{n_c} of a fluid mixture, phase pressure p^α , and temperature T , the goal of flash is to compute phase mole fraction Y^α and phase composition $c_1^\alpha, c_2^\alpha, \dots, c_{n_c}^\alpha$ for each phase α . The Gibbs free energy of the

fluid mixture is at its minimum at an equilibrium state, leading to the fundamental equations of thermodynamic phase equilibrium [15]

$$(2.6) \quad f_i^l(c_1^l, \dots, c_{n_c}^l, p^l, T) = f_i^v(c_1^v, \dots, c_{n_c}^v, p^v, T), \quad 1 \leq i \leq n_c. \quad \{\text{s2c:e4}\}$$

Here the fugacity $f_i^\alpha = f_i^\alpha(c_1^\alpha, \dots, c_{n_c}^\alpha, p^\alpha, T)$ of component i in phase α is given by

$$(2.7) \quad \begin{aligned} f_i^\alpha &= \frac{c_i^\alpha p^\alpha}{Z^\alpha - B^\alpha} \exp \left[\frac{b_i}{b^\alpha} (Z^\alpha - 1) \right] \left[\frac{Z^\alpha + (\sqrt{2} + 1)B^\alpha}{Z^\alpha - (\sqrt{2} - 1)B^\alpha} \right]^{-l_i^\alpha}, \\ l_i^\alpha &= \frac{A^\alpha}{2\sqrt{2}B^\alpha} \left[\frac{2}{a^\alpha} \sum_{j=1}^{n_c} \sqrt{a_i a_j} c_j^\alpha (1 - \kappa_{ij}) - \frac{b_i}{b^\alpha} \right]. \end{aligned} \quad \{\text{s2c:e5}\}$$

3. An Eulerian-Lagrangian method and a local streamline method for single-phase flow and transport. To illustrate the idea we begin by looking at an Eulerian-Lagrangian method for single-phase flow and transport. We present numerical experiments in section 5 to show the potential of the method. Then we demonstrate how to integrate this method with the streamline method to develop a mass-conservative local streamline method in the context of miscible displacement.

3.1. An Eulerian-Lagrangian method. In this case the mass transport equations (2.1) are reduced to be follows

$$\{\text{s3a:e1}\} \quad (3.1) \quad \frac{\partial(\phi \rho c_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} c_i - \rho \mathbf{D}(\mathbf{u}) \nabla c_i) = \bar{\rho} \bar{c}_i q, \quad i = 1, 2, \dots, n_c.$$

Here we have dropped the phase index α since it is assumed that there is only one phase present.

To reflect the Lagrangian nature of the mass transport, we choose the weighting function $z(\mathbf{x}, t)$ to be constant along each characteristic curves of the governing equation [17, 18, 19]. We then multiply equation (3.1) by these weighting functions $z(\mathbf{x}, t)$ and integrate the resulting equation to obtain an Eulerian-Lagrangian method [17, 8, 10, 19]

$$\{\text{s3a:e2}\} \quad (3.2) \quad \begin{aligned} &\int_{\Omega} \phi \rho c_i(\mathbf{x}, t_n) z(\mathbf{x}, t_n) d\mathbf{x} + \Delta t_n \int_{\Omega} \nabla z(\mathbf{x}, t_n) \cdot (\rho \mathbf{D} \nabla c_i)(\mathbf{x}, t_n) d\mathbf{x} \\ &= \int_{\Omega} \phi \rho c_i(\mathbf{x}, t_{n-1}) z(\mathbf{x}, t_{n-1}^+) d\mathbf{x} + \Delta t_n \int_{\Omega} \bar{\rho} \bar{c}_i(\mathbf{x}, t_n) q(\mathbf{x}, t_n) z(\mathbf{x}, t_n) d\mathbf{x}. \end{aligned}$$

The Eulerian-Lagrangian scheme symmetrizes the governing mass transport equation and generates a symmetric and positive-definite coefficient matrix. Thus, the scheme stabilizes the numerical approximation. We note that in the scheme (3.2) all the terms but the first one on the right-hand side are defined on the fixed spatial grid and are standard integrals in finite element or finite volume methods for heat equations. These integrals can be evaluated in a fairly straightforward manner.

In the first term on the right-hand side of the scheme (3.2), the trial function $c(\mathbf{x}, t_{n-1})$ is known from the solution at the previous time step t_{n-1} . The evaluation of the weighting function $z(\mathbf{x}, t_{n-1}^+)$ requires extra attention. To evaluate z at spatial location \mathbf{x} at time step t_{n-1} , we need to solve the initial-value problem of the differential equation

$$\{\text{s3a:e3}\} \quad (3.3) \quad \frac{d\mathbf{x}}{dt} = \frac{\mathbf{u}}{\phi}$$

to track the characteristic curve $\mathbf{r}(t; \mathbf{x}, t_{n-1})$ from the spatial location \mathbf{x} at time step t_{n-1} to the spatial location $\tilde{\mathbf{x}} = \mathbf{r}(t_n; \mathbf{x}, t_{n-1})$ at time step t_n . Here the Darcy velocity \mathbf{u} can be computed from any pressure solver. Then we calculate $z(\mathbf{x}, t_{n-1}^+)$ by the relation $z(\mathbf{x}, t_{n-1}^+) = z(\tilde{\mathbf{x}}, t_n)$, where the weighting function z is defined as a standard shape function at time step t_n . It has been shown that the Eulerian-Lagrangian scheme (3.3) is mass-conservative [17, 19, 21]. We will present the numerical results in section 5 to show the strong potential of the Eulerian-Lagrangian method.

3.2. An integrated local streamline method. The Eulerian-Lagrangian formulation (3.2) provides an ideal platform for the development of an integrated local streamline method. We note that the mass contained in each finite element cell $e \subset \Omega$ at time step t_{n-1} is $\int_e \phi \rho c_i(\mathbf{x}, t_{n-1}) d\mathbf{x}$. To evaluate this integral or the mass of the cell, we enforce an integration quadrature on this cell e with respect to the fixed spatial grid. In this way, discrete quadrature points \mathbf{x}_j ($j = 1, \dots, j_e$) are chosen in the cell and the integral $\int_e \phi \rho c_i(\mathbf{x}, t_{n-1}) d\mathbf{x}$ can be computed by the quadrature as follows

$$(3.4) \quad \begin{aligned} \int_e \phi \rho c_i(\mathbf{x}, t_{n-1}) d\mathbf{x} &= \sum_k \int_e \phi \rho c_i(\mathbf{x}, t_{n-1}) z_k(\mathbf{x}, t_{n-1}^+) d\mathbf{x} \\ \int_e \phi \rho c_i(\mathbf{x}, t_{n-1}) z_k(\mathbf{x}, t_{n-1}^+) d\mathbf{x} &= \sum_{j=1}^{j_e} \omega_j \phi \rho c_i(\mathbf{x}_j, t_{n-1}) z_k(\mathbf{x}_j, t_{n-1}^+). \end{aligned} \quad \{\text{s3b:e1}\}$$

In other words, the cell e is decomposed as a set of particles \mathbf{x}_j for $j = 1, \dots, j_e$ in a systematical manner by the quadrature and the mass of cell e is assigned to the set of particles \mathbf{x}_j and weighted by the associated weighting functions $z_k(\mathbf{x}_j, t_{n-1}^+)$ naturally. Algorithmically, we would evolve each particle \mathbf{x}_j at time step t_{n-1} to $\tilde{\mathbf{x}}_j$ at time step t_n along the streamline. Note that the streamlines are also computed from Eq. (3.3) in the context of single-phase flow and transport. In other words, we evolve each particle forward by solving the differential equation (3.3) and evaluate $z_k(\mathbf{x}, t_{n-1}^+)$ by the relation $z_k(\mathbf{x}, t_{n-1}^+) = z_k(\tilde{\mathbf{x}}, t_n)$ as in the case of the Eulerian-Lagrangian method (3.2).

The advantages of the proposed local streamline method can be summarized as follows: (1) Because the tracking is used only to evaluate the right-hand side of the scheme, it has no effect on the solution grids or the data structure of the scheme. Both flow and mass transport equations are solved on the fixed mesh. Thus, no grid distortion or artificial mapping is needed. (2) The choice of quadrature points can vary from cell to cell and from time step to time step. This adaptive feature naturally avoids the formation of clusters of points or missing cells. (3) It has been shown that the underlying Eulerian-Lagrangian formulation conserves mass in a systematic manner [20, 21, 19].

4. An Eulerian-Lagrangian method and a local streamline method for compositional flow and transport. We present an Eulerian-Lagrangian method for two-phase multicomponent flow and transport. We conduct preliminary numerical example runs in section 5 to show the potential of the formulation, compared to standard explicit and implicit upwind methods. Then we propose to integrate the streamline method with the Eulerian-Lagrangian method to develop a mass-conservative local streamline method for compositional flow and transport.

4.1. An Eulerian-Lagrangian method. The material balance equations (2.1) are expressed as a weighted sum of mole fractions c_i^l and c_i^v for $1 \leq i \leq n_c$. Choosing c_i^l or c_i^v as a primary variable could introduce extra numerical difficulties as the

corresponding phase vanishes. Thus, we choose the overall mole fraction c_i as a primary variable and rewrite the material balance equations (2.1) as

$$\{s4a:e1\} \quad (4.1) \quad \frac{\partial}{\partial t}(\phi \rho c_i) + \nabla \cdot \sum_{\alpha=l,v} (\mathbf{u}^\alpha \rho^\alpha c_i^\alpha) - \nabla \cdot \sum_{\alpha=l,v} (\rho^\alpha \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla c_i^\alpha) = \sum_{\alpha=l,v} \bar{c}_i^\alpha \bar{\rho}^\alpha q^\alpha.$$

The accumulation term in Eq. (4.1) is written in terms of c_i , but the advective and diffusive fluxes are expressed as a weighted sum of c_i^α for $\alpha = l, v$. In an IMPEC (implicit pressure and explicit composition) time-stepping procedure [1, 2], the advective and diffusive fluxes are discretized at the previous iterative or time step where c_i^α were already known from flash. Thus, the equations in (4.1) are decoupled naturally and solved independently for c_i at next iterative or time step. Upwind method often requires fine spatial and temporal partition to maintain stability and reasonable accuracy and to reduce excessive numerical dispersion and spurious effects due to grid orientation [2, 3].

To design an Eulerian-Lagrangian method for compositional flow and transport, we need to rewrite the mass transport equations (4.1) in a similar form to Eq. (3.1). Thus, we have to express the advective and diffusive fluxes in terms of the overall mole fraction c_i . We apply the chain rule to rewrite the diffusive flux as

$$\{s4a:e2\} \quad (4.2) \quad \begin{aligned} \nabla \cdot \sum_{\alpha=l,v} (\rho^\alpha \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla c_i^\alpha) &= \sum_{j=1}^{n_c} \nabla \cdot \sum_{\alpha=l,v} \left(\rho^\alpha \frac{\partial c_i^\alpha}{\partial c_j} \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla c_j \right) \\ &+ \nabla \cdot \sum_{\alpha=l,v} \left(\rho^\alpha \frac{\partial c_i^\alpha}{\partial p^\alpha} \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla p^\alpha \right). \end{aligned}$$

To derive an Eulerian-Lagrangian formulation, we have to define an overall component velocity \mathbf{u}_i for each component i so that Eq. (4.1) can be reformulated into a similar form to single-phase flow [8, 10]. We utilize momentum balance to define a barycentric component velocity \mathbf{u}_i for component i , based upon phase velocity \mathbf{u}^α and the relative presence c_i^α of component i in each phase $\alpha = l, v$

$$\{s4a:e3\} \quad (4.3) \quad \mathbf{u}_i = \frac{1}{\rho c_i} \sum_{\alpha=l,v} \rho^\alpha c_i^\alpha \mathbf{u}^\alpha.$$

With all these preparations, we can now rewrite the mass transport equation (2.1) as

$$\{s4a:e4\} \quad (4.4) \quad \begin{aligned} \frac{\partial}{\partial t}(\phi \rho c_i) + \nabla \cdot (\rho \mathbf{u}_i c_i) - \sum_{j=1}^{n_c-1} \nabla \cdot \left[\left(\sum_{\alpha=l,v} \rho^\alpha \frac{\partial c_i^\alpha}{\partial c_j} \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \right) \nabla c_j \right] \\ - \nabla \cdot \left[\left(\sum_{\alpha=l,v} \rho^\alpha \frac{\partial c_i^\alpha}{\partial p^\alpha} \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \right) \nabla p^\alpha \right] = \sum_{\alpha=l,v} \bar{\rho}^\alpha \bar{c}_i^\alpha q^\alpha. \end{aligned}$$

Eq. (4.4) is expressed in a similar form to the single-phase mass transport equation (3.1). Thus, we can write an Eulerian-Lagrangian scheme for compositional flow and transport, which is similar to the scheme (3.2). One important issue is we now need to carry out the characteristic tracking of (3.3) with the single-phase fluid velocity \mathbf{u} being replaced by the component velocity \mathbf{u}_i for each component i ($i = 1, \dots, n_c$).

The Eulerian-Lagrangian method for compositional flow and transport holds no matter the diffusion-dispersion tensor is included or not. When this term is included, different iterative techniques can be used to solve the mass balance equations (4.4).

For example, a Jacobi (or Gauss-Seidel) iterative technique would lag all the off-diagonal (or upper diagonal) terms in the diffusive flux to the previous time step or inner iterative step, and iterate between the equations in (4.4). Other options include solving these equations simultaneously by a Picard- or Newton-type of iterative techniques.

4.2. An integrated local streamline method. In the streamline method for compositional flow and transport [5], effects of gravity, capillary pressure, external source and sink, and the diffusion-dispersion tensor are neglected. Thus, the mass transport equation (2.1) can be written as

$$(4.5) \quad \frac{\partial}{\partial t}(\phi \rho c_i) + \mathbf{u} \cdot \nabla F_i = 0. \quad \{\text{s4b:e1}\}$$

Here \mathbf{u} is the total velocity of the fluid mixture and $F_i = f^l \rho^l c_i^l + f^v \rho^v c_i^v$ is the flux of component i . Let $\mathbf{r}(\xi; \mathbf{x}, t)$ be the streamline defined by the initial-value problem (3.3) with the temporal parameter θ replaced by ξ that parameterizes the streamline. Then, Eq. (4.5) is written as a one-dimensional conservation law in the streamline

$$(4.6) \quad \frac{\partial}{\partial t}(\phi \rho c_i) + \frac{\partial F_i}{\partial \xi} = 0. \quad \{\text{s4b:e2}\}$$

Semi-analytical methods [22, 23] or high resolution methods [24, 25, 26] are used to solve the one-dimensional conservation law (4.6) for the overall mole fraction c_i along each streamline.

The streamline method is implemented in an IMPEC framework. First, the pressure and velocity are computed on a fixed three-dimensional grid. Streamlines are traced throughout the computational domain. Next, compositions are mapped to streamlines, and are advected along the streamlines using local time-stepping methods until the next pressure update. The new compositions are mapped back to the pressure grid in the pressure update. Local time steps are used to advect the compositions along each individual streamline. The streamline solves are fully independent and parallelized. This makes streamline methods very efficient. There might be some potential limitations to this approach. First, streamline cross-flow is ignored during a global pressure step. This needs to be corrected for when the pressure is updated. When the impact of gravity segregation or capillary forces is important, many corrections may be required that could potentially reduce the efficiency of the method. Second, if the streamline density is insufficient, the mappings from streamlines to the pressure grid and back may cause smoothing and mass balance errors. Streamline adaptivity and grid adaptivity are introduced to control these mapping errors in recent works [27, 28].

In the integrated local streamline method, we decompose the overall mass balance equation (2.1) in terms of Eq. (4.5) plus external source and sink as well as residual terms. We rewrite the Eulerian-Lagrangian scheme accordingly to obtain a local

streamline formulation

$$\begin{aligned}
& \int_{\Omega} \phi \rho c_i(\mathbf{x}, t_n) z(\mathbf{x}, t_n) d\mathbf{x} \\
& + \Delta t_n \sum_j \sum_{\alpha=l,v} \int_{\Omega} \rho^\alpha \frac{\partial c_i^\alpha}{\partial c_j} \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla c_j(\mathbf{x}, t_n) \cdot \nabla z(\mathbf{x}, t_n) d\mathbf{x} \\
& + \Delta t_n \sum_{\alpha=l,v} \int_{\Omega} \rho^\alpha \frac{\partial c_i^\alpha}{\partial p^\alpha} \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla p^\alpha(\mathbf{x}, t_n) \cdot \nabla z(\mathbf{x}, t_n) d\mathbf{x} \\
(4.7) \quad & = \int_{\Omega} \phi \rho c_i(\mathbf{x}, t_{n-1}) z(\mathbf{x}, t_{n-1}^+) d\mathbf{x} \\
& + \Delta t_n \sum_{\alpha=l,v} \int_{\Omega} \bar{c}_i^\alpha(\mathbf{x}, t_n) \bar{\rho}^\alpha q^\alpha(\mathbf{x}, t_n) z(\mathbf{x}, t_n) d\mathbf{x} \\
& - \Delta t_n \int_{\Omega} \mathbf{F}_i^r \cdot \nabla z(\mathbf{x}, t_n) d\mathbf{x} - \Delta t_n \int_{\Omega} (\nabla \cdot \mathbf{F}_i) z(\mathbf{x}, t_n) d\mathbf{x}.
\end{aligned} \tag{s4b:e3}$$

Here $\mathbf{F}_i^r = \sum_{\alpha=l,v} (\mathbf{u}^\alpha \rho^\alpha c_i^\alpha) - \mathbf{u} F_i$ is the residual flux due to capillary pressure and gravity. The proposed integrated local streamline method possesses the advantages of the local streamline method in the context of single-phase flow and transport, which were summarized in section 3.2. Furthermore, we track streamlines (instead of characteristics) from certain quadrature points in each cell during a time step, which avoids potential challenges associated with tracking characteristics for complex flow systems. Finally, effects of gravity, capillary pressure, source and sink, and the diffusion-dispersion tensor are naturally incorporated into the formulation.

5. Preliminary numerical experiments. We conduct preliminary numerical experiments to perform an initial assessment on the feasibility and potential of the Eulerian-Lagrangian method, which also provides an underlying framework for the proposed integrated local streamline method. We also compare it with an explicit upwind scheme and an implicit upwind method to gain a better understanding about the performance of the Eulerian-Lagrangian scheme.

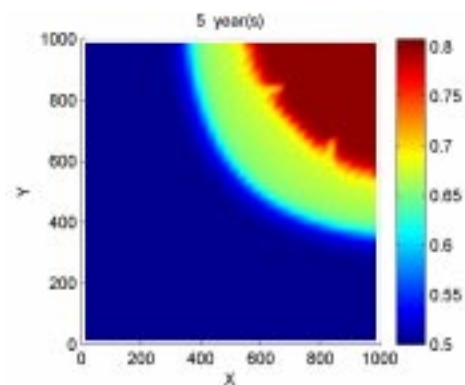
5.1. Single-phase flow and transport.

5.2. Compositional flow and transport. We simulate the transport of methane (CH_4), propane (C_3H_8), and n-hexane (C_6H_{14}) flowing in coexisting liquid and vapor phases in a horizontal reservoir $\Omega = (0, 1000) \times (0, 1000)$ ft² with a thickness of 1 ft over a time period of 15 years. The problem is for one quarter of a five-spot pattern with an injection well located at the upper-right corner of Ω with a volumetric injection rate of $Q = 15$ ft³/day. The production well is located at the lower-left corner with a production rate of $Q = -15$ ft³/day. The porosity $\phi = 0.1$ and the permeability $K = 60$ md. The relative permeability $k^{r,l} = (s^l)^2$ and $k^{r,v} = (1 - s^l)^2$. The effect of capillary pressure and the diffusion-dispersion tensor is neglected. The initial reservoir pressure is 2100 psia and the reservoir temperature is 350°K. The composition of the resident fluid is $c_{methane} = 0.5$, $c_{propane} = 0.2$, and $c_{n-hexane} = 0.3$, which is in liquid phase at the given temperature and pressure. The composition of the injected fluid is $\bar{c}_{methane} = 0.8$, $\bar{c}_{propane} = 0.15$, and $\bar{c}_{n-hexane} = 0.05$, which is in vapor phase.

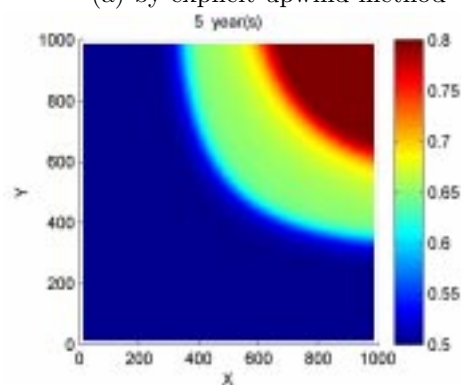
In the numerical example runs, we use a uniform coarse spatial grid of $\Delta x = \Delta y = 25$ ft. We use a time step of $\Delta t_{el} = 1$ year or 0.054 PVI (pore volume injected) for the Eulerian-Lagrangian method, a time step of $\Delta t_{ex} = 2$ days or 0.0003 PVI for the explicit upwind method that is the largest possible due to the CFL constraint,

Fig. 5.1: The overall mole fraction of methane at 5 years.

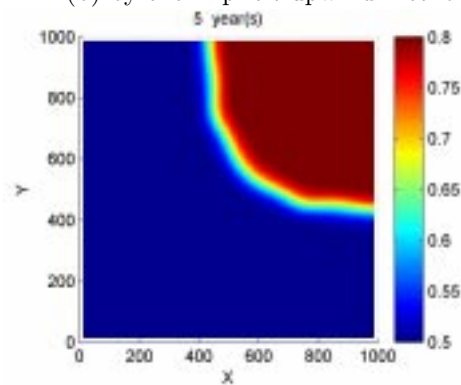
{Fig1}



(a) by explicit upwind method



(b) by the implicit upwind method

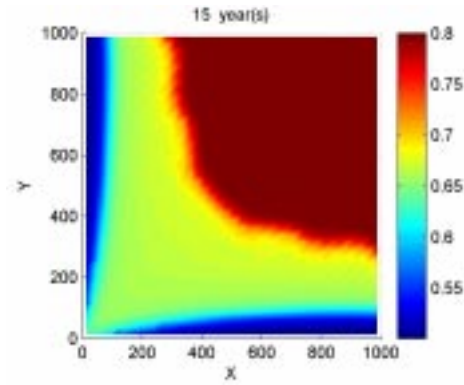


(c) by the Eulerian-Lagrangian scheme

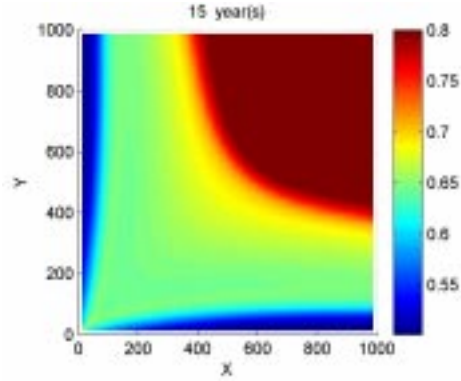
and a time step of $\Delta t_{im} = 1$ month or 0.0045 PVI for the implicit upwind method. We present the plots for the overall mole fraction c_1 of methane, which is computed by the explicit upwind method, by the implicit upwind method, and by the Eulerian-Lagrangian method at $t = 5$ years in Figure 5.1, and similar plots at $t = 15$ years in Figure 5.2. We can similarly present the plots for phase composition c_i^α , but these

Fig. 5.2: The overall mole fraction of methane at 5 years.

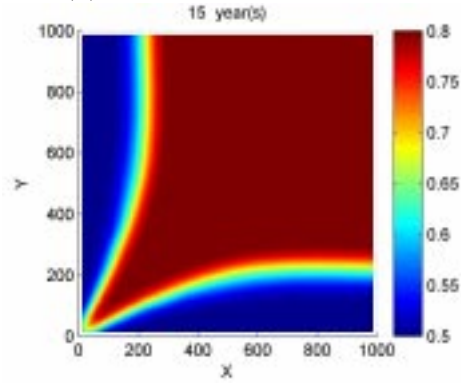
{Fig2}



(a) by explicit upwind method



(b) by the implicit upwind method



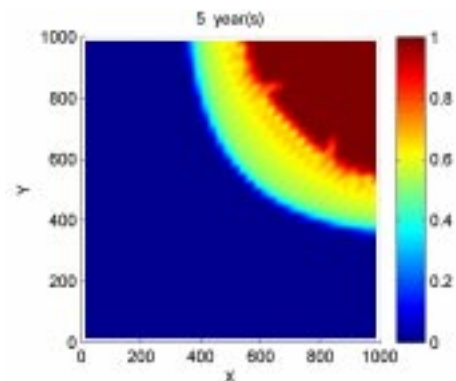
(c) by the Eulerian-Lagrangian scheme

plots could be misleading because c_i^α is an intensive variable and would keep constant as the corresponding phase vanishes. Thus, we introduce a normalized molar amount n_i^α

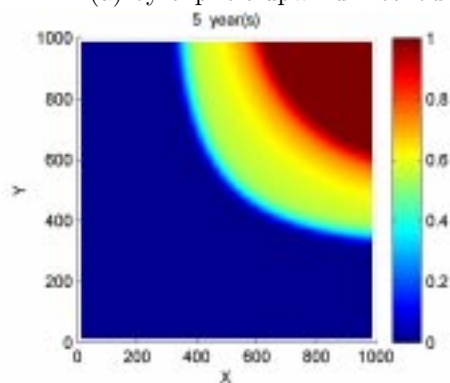
$$\{s5:e1\} \quad (5.1) \quad n_i^\alpha := \frac{\rho^\alpha s^\alpha c_i^\alpha}{\rho c_i}, \quad 1 \leq i \leq n_c, \quad \alpha = l, v.$$

Fig. 5.3: The molar amount of methane in vapor phase at 5 years.

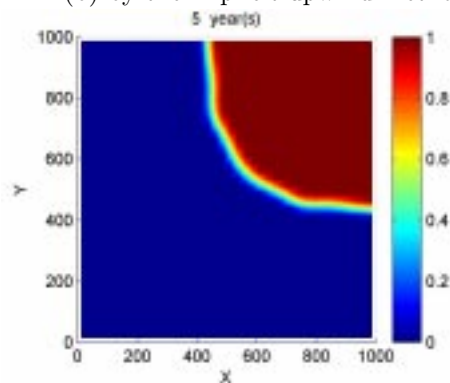
{Fig3}



(a) by explicit upwind method



(b) by the implicit upwind method

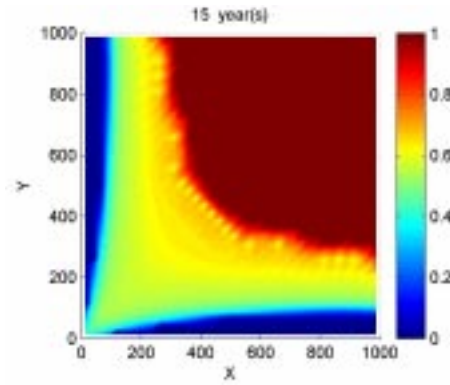


(c) by the Eulerian-Lagrangian scheme

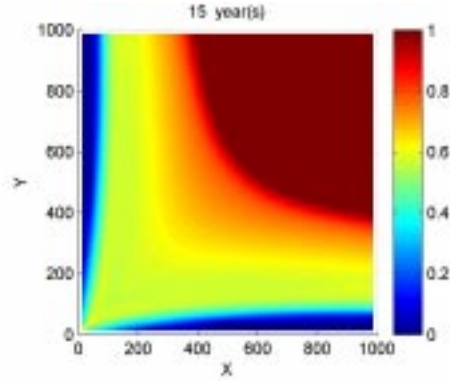
Note that n_i^α represents the molar amount of component i in phase α per unit amount of component i in the fluid mixture and ranges from 0 to 1. $n_i^\alpha = 1$ if all the component i is in phase α and $n_i^\alpha = 0$ if all the component i is in the other phase β . $0 < n_i^\alpha < 1$ if component i is present in both phases. We present the plots of the normalized molar amount $n_{methane}^v$ in vapor phase, which is computed by the explicit

Fig. 5.4: The molar amount of methane in vapor phase at 15 years.

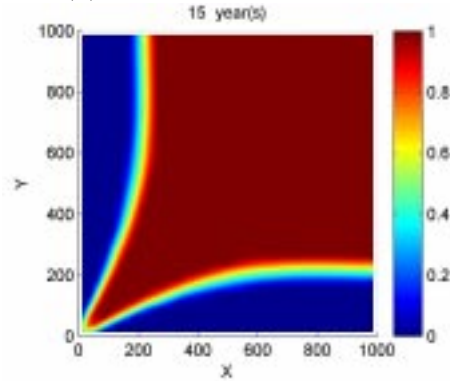
{Fig4}



(a) by explicit upwind method



(b) by the implicit upwind method



(c) by the Eulerian-Lagrangian scheme

upwind method, the implicit upwind method, and the Eulerian-Lagrangian method at $t = 5$ and 15 years in Figures 5.3 and 5.4.

These preliminary numerical experiments seem to suggest that the Eulerian-Lagrangian method generates stable and accurate numerical solutions that have preserved physically reasonable propagation fronts, even if a large time step of $\Delta t_{el} = 1$

year and a coarse spatial grid are used. In this example run, the largest possible time step for the explicit upwind method is $\Delta t_{up} = 2$ days. With a very fine time step and the same spatial grid, the explicit upwind method generates qualitatively similar overall mole fractions as the Eulerian-Lagrangian method but with a much wider propagation front. The front in the diagonal direction from the injection well to the production well is smeared out due to the transverse numerical diffusion. When we refine the spatial grid and time step in the upwind method, we obtain numerical solutions that are of similar qualitative behavior and are closer to the solutions by the Eulerian-Lagrangian method. The implicit upwind method allows the use of a time step of 1 month. However, it generates numerical solutions with even more numerical diffusion than the explicit upwind method.

Finally, it is instructive to compare the computational efficiency of the explicit upwind method, the implicit upwind method, and the Eulerian-Lagrangian method. In the context of multiphase component flow and transport processes, it is observed that all the three methods consume comparable CPU time per time step, because all these methods have to solve the same pressure equation and to conduct the same flash calculations that uses a large portion of CPU time. These results demonstrate that the Eulerian-Lagrangian approach not only represents the solutions properly, but also has obvious computational benefits compared to traditional methods.

REFERENCES

- [1] Aziz, H. and A. Settari (1979). *Petroleum Reservoir Simulation*. Applied Science Publishers, New York.
- [2] Ewing, R.E., editor (1984). *The Mathematics of Reservoir Simulation*. Research Frontiers in Applied Mathematics, 1, SIAM, Philadelphia.
- [3] Yanosik, J., McCracken, T.: A nine-point, finite difference reservoir simulator for realistic prediction of adverse mobility ratio displacements. *Soc. Pet. Eng. J.* 19:253–262 (1978)
- [4] M.J. King and A. Datta-Gupta, Streamline simulation: A current perspective, *In Site*, 22 (1998) 91–140.
- [5] B.T. Mallison, M.G. Gerritsen, K. Jessen, and F.M. Orr, Jr., High order upwind schemes for two-phase multicomponent flow, *SPE 79691*, 2003.
- [6] Ewing, R.E., T.F. Russell, and M.F. Wheeler (1983). Simulation of miscible displacement using mixed methods and a modified method of characteristics. *SPE*, 12241:71–81.
- [7] Russell, T.F. and M.F. Wheeler (1984). Finite element and finite difference methods for continuous flows in porous media. In R.E. Ewing, editor, *The Mathematics of Reservoir Simulation*, Research Frontiers in Applied Mathematics, 1, SIAM, Philadelphia.
- [8] Wang, H., Liang, D., Ewing, R.E., Lyons, S.L., Gin, G.: An approximation to miscible fluid flows in porous media with point sources and sinks by an Eulerian-Lagrangian localized adjoint method and mixed finite element methods. *SIAM J. Sci. Comput.* 22:561–581(2000)
- [9] Wang, H., Liang, D., Ewing, R.E., Lyons, S.L., Gin, G.: An ELLAM-MFEM solution technique for compressible fluid flows in porous media with point sources and sinks, *J. Comput. Phys.* 159:344-376 (2000)
- [10] H. Wang, D. Liang, R.E. Ewing, S.L. Lyons, and G. Qin, An ELLAM approximation for highly compressible multicomponent flows in porous media, *Computational Geosciences*, 6 (2002), 227–251.
- [11] M.S. Espedal and R.E. Ewing, Characteristic Petrov-Galerkin sub-domain methods for two-phase immiscible flow, *Comput. Meth. Appl. Mech. Engrg.*, 64, (1987) 113–135.
- [12] Douglas, J. Jr., Furtado, F., Pereira, F.: On the numerical simulation of waterflooding of heterogeneous petroleum reservoirs. *Computational Geoscience* 1:155–190 (1997)
- [13] Bear, J. (1972). *Dynamics of Fluids in Porous Materials*. American Elsevier, New York.
- [14] Chavent, G. and J. Jaffré (1986). *Mathematical Models and Finite Elements for Reservoir Simulation*. North-Holland, Amsterdam.
- [15] Michelsen, M.L. and J.M. Mollerup (2004). *Thermodynamic Models: Fundamentals & Computational Aspects*. Tie-Line Publications, Denmark.
- [16] Peng, D.Y. and D.B. Robinson (1976). A new two-constant equation of state. *Ind. Engr. Chem.*

- Fundam.*, 15:59–64.
- [17] Celia, M.A., T.F. Russell, I. Herrera, and R.E. Ewing (1990). An Eulerian-Lagrangian localized adjoint method for the advection-diffusion equation. *Advances in Water Resources*, 13:187–206.
 - [18] Wang, H. R.E. Ewing, G. Qin, S.L. Lyons, M. Al-Lawatia, and S. Man (1999). A family of Eulerian-Lagrangian localized adjoint methods for multi-dimensional advection-reaction equations. *J. Comput. Phys.*, 152:120–163.
 - [19] T.F. Russell and M.A. Celia, An overview of research on Eulerian-Lagrangian localized adjoint methods (ELLAM), *Adv. Water Resources*, 25, (2002), 1215–1231.
 - [20] T.F. Russell and R.V. Trujillo, *Eulerian-Lagrangian localized adjoint methods with variable coefficients in multiple dimensions*, Gambolati, *et al.* (eds.), Computational Methods in Surface Hydrology, Springer-Verlag, Berlin, 1990, pp. 357–363.
 - [21] Wang, H., H.K. Dahle, R.E. Ewing, M.S. Espedal, R.C. Sharpley, and S. Man (1999). An ELLAM Scheme for advection-diffusion equations in two dimensions. *SIAM J. Sci. Comput.*, 20:2160–2194.
 - [22] C.M. Dafermos, *Hyperbolic Conservation Laws in Continuum Physics*, Springer-Verlag, Berlin and New York 2000.
 - [23] H. Holden and N.H. Risebro, *Front Tracking for Hyperbolic Conservation Laws*, Springer-Verlag, New York 2002.
 - [24] A. Harten, B. Engquist, S. Osher, and S. Chakravarthy, Uniformly high order accurate essentially nonoscillatory schemes, III, *J. Comput. Phys.*, 71, (1987) 231–241.
 - [25] A. Harten and S. Osher, Uniformly high-order accurate non-oscillatory schemes, I, *SIAM J. Numer. Anal.*, 24, (1987), 279–309.
 - [26] R.J. LeVeque, *Finite volume methods for hyperbolic problems*, Cambridge Texts in Applied Mathematics, Cambridge University Press, Cambridge, 2002.
 - [27] Gerritsen, M.G. and Lambers, J., Integrating Grid Adaptivity with Local-Global Upscaling: An Attractive Approach for Accurate Solution of Flow in Heterogeneous Formations, *submitted to Advances in Water Resources*, 2005.
 - [28] Gerritsen, M. G., Jessen, K., Mallison, B.T. and Lambers, J.: A fully adaptive streamline framework for the challenging simulation fo gas-injection processes, *SPE ATC*, 2005, SPE 97270.