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On the development of component- or phase-based Eulerian-Lagrangian formulation for compositional flow and transport in porous media

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1. Introduction

Compositional models describe the simultaneous flow and transport processes of multiple components flowing in coexisting phases in porous media [1, 2]. Because each component can transfer between different phases, the mass of each phase or a component within a particular phase is no longer conserved. Instead, the total mass of each component among all the phases must be conserved, leading to strongly coupled systems of transient nonlinear partial differential equations of convection-diffusion type. These equations are closely coupled to a set of constraining equations, which are strongly nonlinear, implicit functions of phase pressure, temperature, and composition. These equations need to be solved in all spatial cells within the two-phase region at each iterative step of each time step via thermodynamic flash calculation. In industrial applications, upwind methods have commonly been used to stabilize the numerical approximations [1, 2]. However, these methods often generate excessive numerical dispersion and serious spurious effects due to grid orientation.

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 successfully applied in single-phase flow [4, 5, 6, 7] and in immiscible two-phase flow [8, 9].

In this paper we are concerned with the development of an Eulerian-Lagrangian formulation for two-phase multicomponent flow and transport processes in porous media. Such a formulation retains the numerical advantages of earlier Eulerian-Lagrangian methods for single or two-phase flow and transport. The accurate solution of the mass transport equations provides an accurate initial guess for flash calculation and, thus, speeds up the flash. Conversely, 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. Because of the complexities and strong nonlinearity and coupling of these processes, different Eulerian-Lagrangian formulations could be proposed based on different considerations of the physical and mathematical properties of compositional flow and transport. In this paper, we explore both component-based approach and phase-based approach.

Preliminary numerical experiments of two-phase multicomponent compositional flow and transport in a two-dimensional reservoir reveals the following observations: (1) on the same spatial partition, using a timestep > 100 times larger than that of the upwind method, the Eulerian-Lagrangian method generates more accurate solutions with steeper fronts than the upwind method; (2) both the Eulerian-Lagrangian method and upwind methods use comparable CPU time per time step.

2. Mathematical model

We consider the simultaneous transport of multiple hydrocarbon components indexed as $i = 1, 2, \ldots, n_c$, 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. Let et c_i^α be mole fraction of component i in phase α and r_i^α denote molar mass transfer of component i into phase α. A mass balance equation for component i in phase α is [1, 10, 2]

$$\frac{\partial}{\partial t}(\phi s^\alpha \rho^\alpha c_i^\alpha) + \nabla \cdot (\mathbf{u}^\alpha \rho^\alpha c_i^\alpha) - \nabla \cdot (\rho^\alpha \mathbf{D}(\mathbf{u}^\alpha, s^\alpha) \nabla c_i^\alpha) = r_i^\alpha. \tag{1}$$

The hydrodynamic dispersion tensor $\mathbf{D}(\mathbf{u}^\alpha, s^\alpha)$ is of the expression [1, 10]

$$\mathbf{D}(\mathbf{u}^\alpha, s^\alpha) = s^\alpha d_m \phi \, \mathbf{I} + d_t |\mathbf{u}^\alpha| \, \mathbf{I} + \frac{d_l - d_t}{|\mathbf{u}^\alpha|}(u_i^\alpha u_j^\alpha). \tag{2}$$

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.

Darcy's law establishes a relationship between Darcy velocity $\mathbf{u}^\alpha$ and the pressure gradient ∇p^α of phase α [1, 10]

$$\mathbf{u}^\alpha = -\frac{k^{r,\alpha}}{\mu^\alpha} \mathbf{K}(\nabla p^\alpha - \tilde{\rho}^\alpha \mathbf{g}). \tag{3}$$

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 $\tilde{\rho}^\alpha = \left(\sum_{i=1}^{n_c} MW_i c_i^\alpha\right) \rho^\alpha$ where MW_i is molecular weight of component i for $i = 1, 2, \ldots, n_c$.

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 [12]

$$\rho^\alpha = \frac{p^\alpha}{Z^\alpha RT}. \tag{4}$$

Here R is the universal gas constant. $Z^\alpha = Z^\alpha(c_1^\alpha, \ldots, c_{n_c}^\alpha, p^\alpha, T)$ 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 [13]

$$Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0. \tag{5}$$

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 $i = 1, \ldots, n_c$ [12, 13].

Given the fluid composition $c_1, c_2, \ldots, c_{n_c}$ of a fluid mixture, pressure p^α, and temperature T, the goal of flash is to compute phase mole fraction Y^α and phase composition $c_1^\alpha, c_2^\alpha, \ldots, c_{n_c}^\alpha$ 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 [12]

$$f_i^l(c_1^l, \ldots, c_{n_c}^l, p^l, T) \;=\; f_i^v(c_1^v, \ldots, c_{n_c}^v, p^v, T), \qquad 1 \le i \le n_c. \tag{6}$$

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

$$\begin{aligned} f_i^\alpha &= \frac{c_i^\alpha p^\alpha}{Z^\alpha - B^\alpha} \exp\left[\frac{b_i}{b^\alpha}(Z^\alpha - 1)\right] \left[\frac{Z^\alpha + (\sqrt{2}+1)B^\alpha}{Z^\alpha - (\sqrt{2}-1)B^\alpha}\right]^{-l_i^\alpha}, \\ l_i^\alpha &= \frac{A^\alpha}{2\sqrt{2}B^\alpha} \left[\frac{2}{a^\alpha} \sum_{j=1}^{n_c} \sqrt{a_i a_j}\; c_j^\alpha (1 - \kappa_{ij}) - \frac{b_i}{b^\alpha}\right]. \end{aligned} \tag{7}$$

3. A component-based Eulerian-Lagrangian formulation

A mathematical model for compositional flow involves a large number of unknown variables. Different sets of primary variables can be selected based on the physical, mathematical, and numerical properties of the problem. Due to mass transfer between different phases, mass of each component within a particular phase or of each phase is not conserved. Thus, r_i^α in (1) accounts for impact of the external sources and sinks as well as mass transfer of component i into phase α from the other phase. Nevertheless, overall mass of each component in the fluid mixture is conserved, leading to the system

$$\frac{\partial}{\partial t}\sum_{\alpha=l,v}(\phi s^\alpha \rho^\alpha c_i^\alpha) + \nabla\cdot\sum_{\alpha=l,v}(\mathbf{u}^\alpha \rho^\alpha c_i^\alpha) - \nabla\cdot\sum_{\alpha=l,v}(\rho^\alpha \mathbf{D}(\mathbf{u}^\alpha, s^\alpha)\nabla c_i^\alpha) = \sum_{\alpha=l,v} r_i^\alpha. \tag{8}$$

Since we assume an isothermal flow with no intraphase reaction present, the only change of the overall mass of each component i is from the external supplies of the component. Namely,

$$r_i^l + r_i^v = \bar{c}_i^l \bar{\rho}_i^l s^l + \bar{c}_i^v \bar{\rho}_i^v s^v. \tag{9}$$

Here $\bar{c}_i^\alpha$ is prescribed at sources and $\bar{c}_i^\alpha = c_i^\alpha$ at sinks. $\bar{\rho}^\alpha$ is determined from thermodynamic flash calculation at sources and $\bar{\rho}^\alpha = \rho^\alpha$ at sinks.

Equation (8) is expressed as a weighted sum of mole fractions c_i^l and c_i^v for $1 \le i \le n_c$. 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 overall mole fraction c_i as a primary variable

$$c_i = \frac{1}{\rho}(s^l \rho^l c_i^l + s^v \rho^v c_i^v l) \quad \text{with} \quad \rho = s^l \rho^l + s^v \rho^v \tag{10}$$

being the bulk molar density of the fluid mixture. We rewrite Eq. (1) as

$$\frac{\partial}{\partial t}(\phi \rho c_i) + \nabla\cdot\sum_{\alpha=l,v}(\mathbf{u}^\alpha \rho^\alpha c_i^\alpha) - \nabla\cdot\sum_{\alpha=l,v}(\rho^\alpha \mathbf{D}(\mathbf{u}^\alpha, s^\alpha)\nabla c_i^\alpha) = \sum_{\alpha=l,v} \bar{c}_i^\alpha \bar{\rho}^\alpha q^\alpha. \tag{11}$$

The accumulation term in Eq. (11) is written in terms of c_i, but the advective and diffusive fluxes are expressed as a weighted sum of c_i^l and c_i^v. To handle the coupling of Eq. (11) due to the advective and diffusive fluxes, we utilize momentum balance to define a barycentric overall component velocity $\mathbf{u}_i = \frac{1}{\rho c_i}(\rho^l c_i^l \mathbf{u}^l + \rho^v c_i^v \mathbf{u}^v)$. $\mathbf{u}_i$ naturally takes into account for the effect of gravity segregation since $\mathbf{u}^\alpha$ includes gravitational effect. This is another important feature of $\mathbf{u}_i$. The introduction of $\mathbf{u}_i$ also enables us to rewrite Eq. (11) in a similar form to a single-phase flow [5, 6, 7]

$$\begin{aligned}\frac{\partial}{\partial t}(\phi \rho c_i) + \nabla\cdot(\rho \mathbf{u}_i c_i) - \sum_j \nabla\cdot\Big[\Big(\sum_{\alpha=l,v}\rho^\alpha \frac{\partial c_i^\alpha}{\partial c_j}\mathbf{D}(\mathbf{u}^\alpha, s^\alpha)\Big)\nabla c_j\Big] \\ -\nabla\cdot\Big[\Big(\sum_{\alpha=l,v}\rho^\alpha \frac{\partial c_i^\alpha}{\partial p^\alpha}\mathbf{D}(\mathbf{u}^\alpha, s^\alpha)\Big)\nabla p^\alpha\Big] = \sum_{\alpha=l,v}\bar{\rho}^\alpha \bar{c}_i^\alpha q^\alpha.\end{aligned} \tag{12}$$

For simplicity of exposition, we assume a noflow boundary condition. Since many Eulerian-Lagrangian methods use a time-stepping procedure, we only need to focus on the current time interval $[t_{n-1}, t_n]$. Let $w_i(\mathbf{x}, t)$ be space-time test functions with certain regularity (e.g, continuous and piecewise smooth, depending on each individual method). We require w_i to vanish outside the space-time strip $\Omega \times (t_{n-1}, t_n]$ and to be discontinuous in time at time t_{n-1}.

In the ELLAM framework [14], an operator-splitting analysis concludes that the test functions $w_i(\mathbf{y}, \theta)$ should satisfy the hyperbolic part of the adjoint equation of Eq. (12)

$$\phi\frac{\partial w_i(\mathbf{y}, \theta)}{\partial \theta} + \mathbf{u}_i(\mathbf{y}, \theta)\cdot\nabla w_i(\mathbf{y}, \theta) = 0, \qquad \mathbf{y} \in \Omega, \quad \theta \in [t_{n-1}, t_n]. \tag{13}$$

Thus, the test functions $w_i(\mathbf{y},\theta)$ should be constant along the component-based characteristic curve $\mathbf{y}=\mathbf{r}_i(\theta;\mathbf{x},t_n)$ defined by the initial-value problem of the ordinary differential equation

$$\frac{d\mathbf{r}_i}{d\theta}=\frac{\mathbf{u}_i}{\phi},\qquad \mathbf{r}_i(\theta;\mathbf{x},t)\Big|_{\theta=t}=\mathbf{x},\qquad \theta\in[t_{n-1},t_n]. \tag{14}$$

Therefore, once the test functions $w_i(\mathbf{x},t_n)$ are defined in $\overline{\Omega}$ at time step t_n, they are determined completely in the space-time strip $\overline{\Omega}\times(t_{n-1},t_n]$ by a constant extension of $w_i(\mathbf{x},t_n)$ along the characteristic curves $\mathbf{r}_i(\theta;\mathbf{x},t_n)$ from time step t_n to time step t_{n-1}.

Incorporating the test functions into a space-time weak formulation and applying an Euler quadrature to evaluate the temporal integral yields an Eulerian-Lagrangian formulation

$$\begin{aligned}&\int_\Omega \phi\rho c_i(\mathbf{x},t_n)w_i(\mathbf{x},t_n)d\mathbf{x}+\Delta t_n\sum_j\sum_{\alpha=l,v}\int_\Omega \rho^\alpha\frac{\partial c_i^\alpha}{\partial c_j}\mathbf{D}(\mathbf{u}^\alpha,s^\alpha)\nabla c_j(\mathbf{x},t_n)\cdot\nabla w_i(\mathbf{x},t_n)d\mathbf{x}\\ &\quad+\Delta t_n\sum_{\alpha=l,v}\int_\Omega \rho^\alpha\frac{\partial c_i^\alpha}{\partial p^\alpha}\mathbf{D}(\mathbf{u}^\alpha,s^\alpha)\nabla p^\alpha(\mathbf{x},t_n)\cdot\nabla w_i(\mathbf{x},t_n)d\mathbf{x}\\ &=\int_\Omega \phi\rho c_i(\mathbf{x},t_{n-1})w_i(\mathbf{x},t_{n-1}^+)d\mathbf{x}+\Delta t_n\sum_{\alpha=l,v}\int_\Omega \bar{c}_i^\alpha(\mathbf{x},t_n)\bar{\rho}^\alpha q^\alpha(\mathbf{x},t_n)w_i(\mathbf{x},t_n)d\mathbf{x}.\end{aligned} \tag{15}$$

Here $w_i(\mathbf{x},t_{n-1}^+)=\lim_{t\to t_{n-1},t>t_{n-1}}w_i(\mathbf{x},t)$ takes into account that $w_i(\mathbf{x},t)$ might exhibit discontinuity in time at time t_{n-1}. The Eulerian-Lagrangian formulation generate a symmetric and positive-definite coefficient matrix and stabilize the numerical approximation. Except for the first term on the right-hand side, all other terms in Eq. (15) are defined on a fixed grid. A characteristic tracking of (14) is carried out only in the evaluation of the test function $w_i(\mathbf{x},t_{n-1}^+)$, which does not distort the solution grid that in turn requires mapping the solution back to the fixed pressure grid as encountered in some particle methods. Numerically, the test functions $w(\mathbf{x},t_n)$ are often chosen to be the same at time step t_n for all the components i. Since the overall component velocity $\mathbf{u}_i$ is component dependent, $w_i(\mathbf{x},t_{n-1}^+)$ differs from each other for different i.

4. A phase-based Eulerian-Lagrangian formulation

In a multiphase, multicomponent flow and transport process, there are two coexisting and closely coupled dynamic processes. One is the mass transfer of each component i between the liquid phase l and the vapor phase v. The other is the transport process of each fluid phase. In this section we present an alternative phase-based Eulerian-Lagrangian formulation by using the mass balance equation (1).

Let $w^\alpha(\mathbf{x},t)$ be space-time test functions defined for phase α. We write a space-time weak formulation. A similar temporal discretization to (15) yields a phase-based Eulerian-Lagrangian formulation

$$\begin{aligned}&\int_\Omega \phi s^\alpha\rho^\alpha c_i^\alpha(\mathbf{x},t_n)w^\alpha(\mathbf{x},t_n)d\mathbf{x}+\Delta t_n\int_\Omega \rho^\alpha\mathbf{D}(\mathbf{u}^\alpha,s^\alpha)\nabla c_i^\alpha(\mathbf{x},t_n)\cdot\nabla w^\alpha(\mathbf{x},t_n)d\mathbf{x}\\ &=\int_\Omega \phi s^\alpha\rho^\alpha c_i^\alpha(\mathbf{x},t_{n-1})w^\alpha(\mathbf{x},t_{n-1}^+)d\mathbf{x}+\Delta t_n\int_\Omega r_i^\alpha(\mathbf{x},t_n)w^\alpha(\mathbf{x},t_n)d\mathbf{x}.\end{aligned} \tag{16}$$

This phase-based formulation has similar properties to the component-based formulation (15), but is defined for the primary variable c_i^α not c_i. The evaluation of $w^\alpha(\mathbf{x},t_{n-1}^+)$ requires tracking a phase-based characteristic curve $\mathbf{r}^\alpha(\theta;\mathbf{x},t_{n-1})$ forward from time step t_{n-1} to time step t_n, where $\mathbf{r}^\alpha(\theta;\mathbf{x},t_{n-1})$ is defined by the initial-value problem (14) with the right-hand side of the differential equation being replaced by $\mathbf{u}^\alpha/(\phi\ s^\alpha)$. A phase-based Eulerian-Lagrangian method was developed in [15] for immiscible two-phase flow, aiming at eventually developing a phase-based Eulerian-Lagrangian method for compositional flow. Other Eulerian-Lagrangian methods

developed for immiscible two-phase flow (e.g., [8, 9, 16]) can also be viewed as phase-based Eulerian-Lagrangian methods. In the context of compositional flow, a crucial issue encountered in a phase-based formulation is how to evaluate the source term r_i^α in Eq. (16), which accounts for impact of the external sources and sinks as well as intraphase mass transfer of component i. Unless this issue is resolved, a phase-based Eulerian-Lagrangian formulation cannot be used to simulate compositional flow and transport process.

We propose a novel approach to circumvent this difficulty by taking the advantages of both the component-based approach (15) and the phase-based approach (16). We choose the same test functions $w(\mathbf{x}, t_n)$ in (16) for both phases at time step t_n. We then use the relations (9) and (10) to sum (16) for $\alpha = l$ and v to obtain a phase-based Eulerian-Lagrangian formulation

$$\begin{aligned}
&\int_\Omega \phi\rho c_i(\mathbf{x}, t_n)w(\mathbf{x}, t_n)d\mathbf{x} + \Delta t_n \sum_j \sum_{\alpha=l,v} \int_\Omega \rho^\alpha \frac{\partial c_i^\alpha}{\partial c_j}\mathbf{D}(\mathbf{u}^\alpha, s^\alpha)\nabla c_j(\mathbf{x}, t_n)\cdot\nabla w(\mathbf{x}, t_n)d\mathbf{x} \\
&\quad + \Delta t_n \sum_{\alpha=l,v} \int_\Omega \rho^\alpha \frac{\partial c_i^\alpha}{\partial p^\alpha}\mathbf{D}(\mathbf{u}^\alpha, s^\alpha)\nabla p^\alpha(\mathbf{x}, t_n)\cdot\nabla w(\mathbf{x}, t_n)d\mathbf{x} \\
&= \sum_{\alpha=l,v} \int_\Omega \phi s^\alpha \rho^\alpha c_i^\alpha(\mathbf{x}, t_{n-1})w^\alpha(\mathbf{x}, t_{n-1}^+)d\mathbf{x} + \Delta t_n \sum_{\alpha=l,v} \int_\Omega \bar{c}_i^\alpha \bar{\rho}^\alpha q^\alpha(\mathbf{x}, t_n)w(\mathbf{x}, t_n)d\mathbf{x}.
\end{aligned} \tag{17}$$

We observe that the phase-based Eulerian-Lagrangian formulation (17) naturally eliminates r_i^α, and differs from the component-based formulation (15) only in the first term on the right-hand side. Nevertheless, this difference may be substantial, especially in the context of complex flow patterns such as countercurrent flows. In this case, the first term on the right-hand side of the phase-based formulation (17) propagates the phase composition c_i^α forward from time step t_{n-1} to time step t_n, and requires tracking the base-phased characteristic curves $\mathbf{r}^l(\theta; \mathbf{x}, t_{n-1})$ and $\mathbf{r}^v(\theta; \mathbf{x}, t_{n-1})$ that could move in opposite directions. So the two integrals in this term are generally evaluated on different domains for $\alpha = l$ and v. In contrast, the first-term on the right-hand side of the component-based formulation (15) propagates the composition c_i of the fluid mixture from time step t_{n-1} to t_n with the barycentric component velocity $\mathbf{u}_i$, and requires tracking the component-based characteristic curve $\mathbf{r}_i(\theta; \mathbf{x}, t_{n-1})$. Further research will be carried out to study the physical, mathematical, and numerical properties of the component-based and phase-based Eulerian-Lagrangian formulations as well as their comparisons and relations.

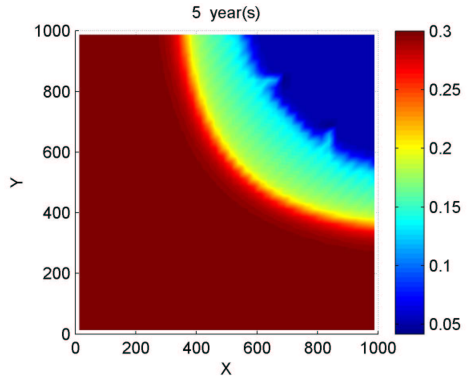
5. Numerical experiments

We conduct preliminary numerical experiments to perform an initial assessment on the feasibility and potential of the Eulerian-Lagrangian formulation. 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.

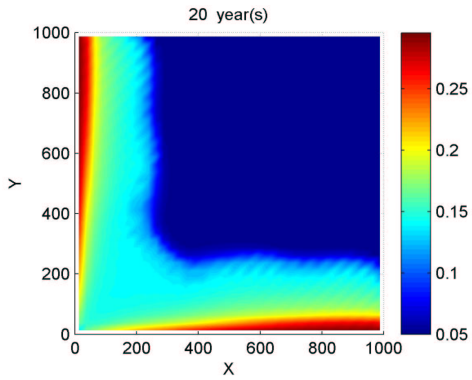
We simulate the transport of methane (CH_4), propane (C_3H_8), and n-hexane (C_6H_{14}) flowing in coexisting liquid and vapor phases in a horizontal reservoir $\Omega = (0, 1000) \times (0, 1000)$ ft^2 with a thickness of 1 ft over a time period of 20 years. The problem is for one quarter of a five-spot pattern with an injection well located at the upper-right corner of Ω with a volumetric injection rate of $Q = 15$ ft^3/day. The production well is located at the lower-left corner with a production rate of $Q = -15$ ft^3/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^{o}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 for the Eulerian-Lagrangian method, a time step of $\Delta t_{ex} = 2$

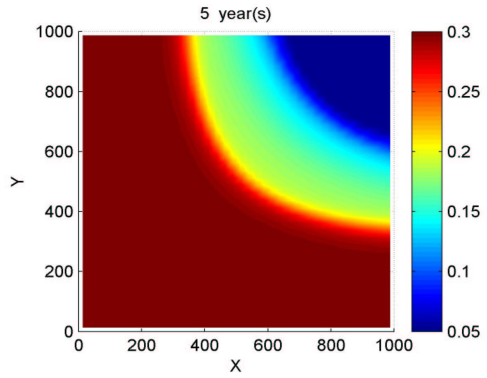
Figure 1: The mole fraction of n-Hexane at 5 and 20 years



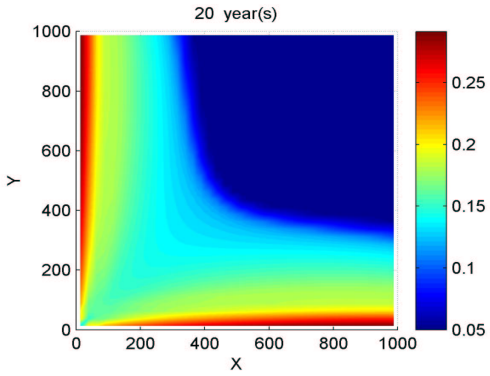
(a) by Upwind at Year 5



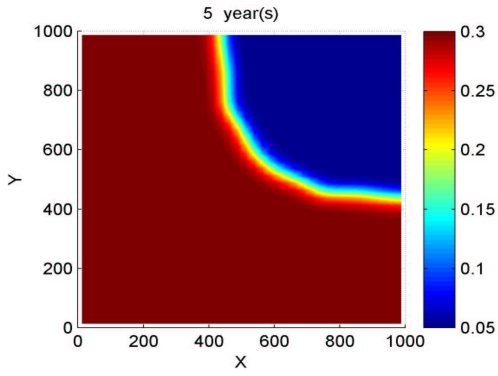
(b) by ELLAM at Year 5



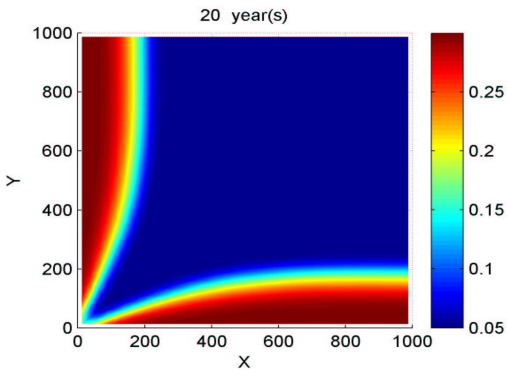
(c) by Upwind at Year 10



(d) by ELLAM at Year 10



(e) by Upwind at Year 20



(f) by ELLAM at Year 20

days for the explicit upwind method that is the largest possible due to the CFL constraint, and a time step of $\Delta t_{im} = 1$ month for the implicit upwind method. To gain a better understanding, we convert the time steps to a dimensionless form, the pore volume injected (PVI). This is defined to be the ratio of the volume of fluid injected during one time step over the overall void space in the porous medium reservoir. The PVI_{el} for the Eulerian-Lagrangian method is 0.054. Namely, within 19 time steps the injected fluid will fill in the entire reservoir. In contrast, the PVI_{ex} for the explicit upwind method is 0.0003. That is, the explicit upwind simulator needs to use 3300 time steps for the injected fluid to fill the entire reservoir. The PVI_{im} for implicit upwind method is 0.0045. That is, the implicit upwind method needs 220 time steps for the injected fluid to fill the entire reservoir. 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 $t = 5$ and 20 years in Figure 1.

These preliminary numerical experiments suggest that the Eulerian-Lagrangian formulation 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.

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