A FULLY MASS-CONSERVATIVE ITERATIVE IMPEC METHOD FOR MULTICOMPONENT COMPRESSIBLE FLOW IN POROUS MEDIA

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ABSTRACT. In this paper we consider efficient and fully mass-conservative numerical methods for the multi-component compressible single-phase Darcy flow in porous media. Compared with the classical Implicit Pressure Explicit Concentration (IMPEC) scheme by which one of the components may be not mass-conservative, the new scheme enjoys an appealing feature that the conservation of mass is retained for each of the components. The pressure-velocity system is obtained by the summation of the discrete conservation equation for each component multiplying an unknown parameter which is nonlinearly dependent of the molar concentrations. This approach is quite different from the conventional method which is used in the classical IMPEC scheme. We utilize a fully mass-conservative iterative IMPEC method to solve the nonlinear system for molar concentration, pressure and velocity fields. The upwind mixed finite element methods are used to solve the pressure-velocity system. Although the Peng-Robinson equation of state (EOS) is utilized to describe the pressure as a function of the molar concentrations, our method is suitable for any type of EOS. Under some reasonable conditions, the iterative scheme can be proved to be convergent, and the molar concentration of each component is positivity-preserving. Several interesting examples of multicomponent compressible flow in porous media are presented to demonstrate the robustness of the new algorithm.

1. INTRODUCTION

Modeling and simulation of compositional flow in subsurface media are prevalent and of interest in hydrogeology and hydrocarbon reservoirs (cf. [8, 28, 29, 20, 37, 36, 18, 26, 27, 40, 31, 32, 33, 34] and references therein). Mathematical model of multicomponent compressible flow in porous media includes the Darcy's law, the conservation of mass and the equation of state, which is a coupled nonlinear system. Most of the reservoir simulators solve the main governing equations of flow and transport equations in porous media by the Darcy's law, the conservation of mass and a pressure relation. The fully implicit methods can be directly applied to solve the coupled equations, and one can also use the improved sequential implicit technique [19, 7] and the adaptive implicit methods [30, 23]. It is known that the implicit methods exhibit greater numerical dispersion than explicit methods on the same grid [38], although the implicit methods deserve better stability than the explicit methods. The simultaneous global solution of all independent variables in implicit methods requires lots of computational resources per time step, particularly when the solution system is large. Thus, compared with the fully implicit methods, the IMPEC scheme has become a popular choice to simulate the multicomponent compressible flow in porous media (cf. [10, 6, 11, 7, 41, 23] and the references therein).

For the classical IMPEC schemes for the multicomponent compressible flow with n_c components, the pressure equation is firstly implicitly solved, then $n_c - 1$ transport equations are explicitly solved. For the molar concentration of the n_c -th component, it is derived from the difference based on the molar concentration of the $n_c - 1$ components and the total molar concentration of all components from the equation of state. Obviously, the conservation of mass holds for the $n_c - 1$ components which are computed from the associated transport equation. However, for the last n_c -th component, the conservation of mass does not always hold

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true due to the approach of solution. Recently, Kou and Sun [13] proposed an improved IMplicit Pressure Explicit Saturation (IMPES) method for the incompressible two-phase flow in porous media. Different from the conventional IMPES methods [12, 11, 6, 7], the pressure equation in [13] was obtained by summing the discretized conservation equations of two phases. This treatment yields a merit that the conservation of mass holds for both phases instead of only one phase in the conventional IMPES methods. Inspired by the technique in [13], our objective is to propose an improved IMPEC method for the multicomponent compressible flow with conservation of mass for all components. Fully mass-conservation of multicomponent systems at discrete level should be taken into account when developing some numerical algorithms even at pore-scale simulation (see [9, 14, 15, 16] and references therein).

We first recall the conventional iterative IMPEC method which is to use the IMPEC method as an iterative step of the fully implicit method and can be coupled within each Newton iteration loop [7]. The pressure equation used in the iterative IMPEC method is obtained by the equation of state at the continuous level, and we strictly derive this pressure relation. For the conventional iterative IMPEC method, the conservation of mass also holds only for the $n_c - 1$ components. At both the time-discrete and space-discrete level, we multiply the discretized conservation equation for each component with an unknown parameter which is nonlinearly dependent on the molar concentrations and make a summation to obtain the discrete pressure equation. The Peng-Robinson EOS is utilized to describe the pressure as a function of all components' molar concentration at constant temperature. Then we implicitly solve the pressure-velocity system and explicitly solve the transport equation for each component. Since the unknown parameters are nonlinear and dependent on the molar concentrations, we utilize the iterative approach to update the parameters based on the Peng-Robinson EOS. Similar to the improved IMPES method in [13], the new approach enjoys an appealing feature that the conservation of mass can be obtained for all the components. We call this new improved approach as a fully mass-conservative iterative IMPEC method.

Various numerical methods have been developed to solve the pressure equation and the transport equation, such as mixed finite element methods, discontinuous Galerkin methods (cf. e.g. [3, 21, 22] and the references therein). We will use the mixed finite element method with the upwind scheme in the fully mass-conservative iterative IMPEC method. Under the assumption that the time step size is small enough, we can derive the convergence of the fully mass-conservative iterative IMPEC method and the positivity-preserving property of the molar concentration which is important for the property of conservation of mass.

The rest of the paper is organized as follows. In Section 2, we introduce the mathematical model for the multicomponent compressible flow and the pressure equation which can be derived strictly from the equation of state. In Section 3, we propose the fully mass-conservative iterative IMPEC method and give the proof of local mass balance of each component. The convergence of the fully mass-conservative iterative IMPEC method and the positivity-preserving property of the molar concentration are derived in Section 4 and Section 5 respectively. In Section 6, we give some numerical results to verify the robustness of the proposed new method. Finally we provide a conclusion in Section 7.

2. MATHEMATICAL MODEL

In this section we recall the governing equations for the multicomponent compressible single-phase Darcy flow and strictly derive the explicit equation for the pressure and velocity fields which has been used in the literature (cf. [1, 35, 41]). We start with the mass balance of component i in a miscible and compressible flow which is given by the following continuity equation

$$(2.1) \quad \frac{\partial(\phi c_i)}{\partial t} + \nabla \cdot (c_i \mathbf{u}) = f_i, \quad \text{in } \Omega \times (0, \tau), \quad i = 1, \dots, n_c,$$

where $\Omega \subset \mathbb{R}^d$ is the domain of computation, ϕ is porosity of the rock, c_i is the molar concentration of component i , f_i is the source or sink term for component i , and n_c is the number of components. Here $\mathbf{u}$ is the velocity field described by the Darcy's law:

$$(2.2) \quad \mathbf{u} = -\frac{\mathbf{K}}{\mu} (\nabla p - \rho \mathbf{g}), \quad \text{in } \Omega \times (0, \tau),$$

where $\mathbf{K} \in [L^\infty(\Omega)]^{d \times d}$ is the intrinsic permeability tensor of the porous media which is assumed to be symmetric and positive definite, μ the viscosity of the fluid, which is a function of c_i ($i = 1, \dots, n_c$) and is evaluated based on Lee-Gonzalez correction [17], p the pressure, ρ the mass density of the fluid, and $\mathbf{g}$

the gravitational acceleration. We impose the boundary and initial conditions to the equations (2.1-2.2) as follows:

$$\begin{aligned}
(2.3) \quad & p(\mathbf{x}, t) = p_D(\mathbf{x}, t), & \text{on } \Gamma_D \times (0, \tau), \\
(2.4) \quad & c_i(\mathbf{x}, t) = c_i^B(\mathbf{x}, t), \quad i = 1, \dots, n_c, & \text{on } \Gamma_-(\mathbf{x}, t) \times (0, \tau), \\
(2.5) \quad & \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{n}(\mathbf{x}) = g^N(\mathbf{x}, t), & \text{on } \Gamma_N \times (0, \tau), \\
(2.6) \quad & c_i(\mathbf{x}, 0) = c_i^0(\mathbf{x}), & i = 1, \dots, n_c, \text{ in } \Omega,
\end{aligned}$$

where $\Gamma_-(\mathbf{x}, t) = \{\mathbf{x} \in \partial\Omega | \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{n}(\mathbf{x}) < 0\}$ is the inflow boundary, $\mathbf{n}(\mathbf{x})$ is the unit outward normal vector to the boundary $\partial\Omega$, Γ_N is the Neumann part of boundary, and Γ_D is the Dirichlet boundary. Let $\Gamma = \partial\Omega$ be composed of Γ_D and Γ_N such that $\Gamma = \Gamma_D \cup \Gamma_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$. Throughout this work, we use the Peng-Robinson EOS (A.1) to describe the pressure as a function of the molar concentrations of all components, temperature, and the details are shown in the appendix.

Clearly, the equations (2.1-2.2) coupling with the Peng-Robinson EOS (A.1) and the boundary and initial conditions build up a fully nonlinear system. The classical IMPEC or iterative IMPEC scheme (cf. [6, 7, 41]) is an efficient approach to decouple the nonlinear system and obtain the pressure and the molar concentration of the components respectively. The volume balance approach (cf. [1, 35, 41]) is used to obtain the pressure field for the compositional compressible flow, and in the following we write down the pressure equation based on the volume balance approach.

Let the partial molar volume of component i at constant temperature be defined as

$$\bar{V}_i = \bar{V}_i(p, \mathbf{N}) = \left(\frac{\partial V_f(p, \mathbf{N})}{\partial N_i} \right)_{p, \mathbf{N}_{\neq i}}, \quad i = 1, \dots, n_c$$

where V_f is the total fluid volume, $\mathbf{N} = (N_1, \dots, N_{n_c})$ the mole amounts vector, and $\mathbf{N}_{\neq i}$ denotes the vector $(N_1, N_2, \dots, N_{i-1}, N_{i+1}, \dots, N_{n_c})$. We denote the molar concentrations by

$$\mathbf{c} = (c_1, \dots, c_{n_c}) = \frac{\mathbf{N}}{V_f(p, \mathbf{N})} = \left(\frac{N_1}{V_f(p, \mathbf{N})}, \dots, \frac{N_{n_c}}{V_f(p, \mathbf{N})} \right)$$

and the total fluid compressibility by $C_f = -\frac{1}{V_f} \frac{\partial V_f}{\partial p}$. The volume balance approach yields that

$$(2.7) \quad \phi C_f \frac{\partial p}{\partial t} + \sum_{i=1}^{n_c} \bar{V}_i (\nabla \cdot (c_i \mathbf{u}) - f_i) = 0.$$

Then the classical IMPEC or iterative IMPEC scheme can be applied to solve the pressure field from the above equation (2.7) and (2.7) becomes

$$(2.8) \quad \phi \frac{\partial p}{\partial t} + \sum_{i=1}^{n_c} \beta_i (\nabla \cdot (c_i \mathbf{u}) - f_i) = 0,$$

where $\beta_i = \frac{\bar{V}_i}{C_f}$. Note that $p = p(c_1, \dots, c_{n_c})$, we have

$$(2.9) \quad \frac{\partial p}{\partial t} = \sum_{i=1}^{n_c} \frac{\partial p}{\partial c_i} \frac{\partial c_i}{\partial t}.$$

For the total fluid volume $V_f = V_f(p, \mathbf{N})$ at constant temperature, we can derive that

$$\begin{aligned}
dV_f &= \left(\frac{\partial V_f}{\partial p} \right)_{\mathbf{N}} dp + \sum_{i=1}^{n_c} \left(\frac{\partial V_f}{\partial N_i} \right)_{p, \mathbf{N}_{\neq i}} dN_i = -V_f C_f dp + \sum_{i=1}^{n_c} \bar{V}_i dN_i \\
&= -V_f C_f dp + \sum_{i=1}^{n_c} \bar{V}_i d(c_i V_f) = -V_f C_f dp + dV_f + \sum_{i=1}^{n_c} \bar{V}_i V_f dc_i,
\end{aligned}$$

where the last equality is derived based on a thermodynamic identity of summation $\sum_{i=1}^{n_c} \bar{V}_i c_i = 1$, which can be directly derived by the definition of $\bar{V}_i$ and the identity $\sum_{i=1}^{n_c} N_i \bar{V}_i = V$. Thus, it directly follows

that $\beta_i = \frac{\bar{V}_i}{C_f} = \left(\frac{\partial p}{\partial c_i} \right)_{\mathbf{c}_{\neq i}}$, where $\mathbf{c}_{\neq i}$ denotes the vector $(c_1, c_2, \dots, c_{i-1}, c_{i+1}, \dots, c_{n_c})$, and

$$(2.10) \quad \sum_{i=1}^{n_c} \beta_i c_i = 1/C_f.$$

Note that the equation (2.8) is uniquely determined. Since β_i is a nonlinear parameter which depends on the molar concentration of each component, we will present a fully mass-conservative iterative IMPEC method to solve the nonlinear system for molar concentrations, pressure and velocity based on (2.1), (2.2), (2.8) and the Peng-Robinson EOS (A.1).

3. FULLY MASS-CONSERVATIVE ITERATIVE IMPEC METHOD

In this section we present a fully mass-conservative iterative IMPEC method for the nonlinear system (2.1), (2.2) and the Peng-Robinson EOS (A.1) coupling with the boundary and initial conditions (2.3-2.6).

3.1. The time-discrete space-continuous schemes. Let Δt be the time step size. Note that the pressure p depends only on the molar concentrations $\mathbf{c}$ at constant temperature, the time-discrete space-continuous scheme for $\frac{\partial p}{\partial t}$ can be written as

$$\begin{aligned} \frac{p^{n+1} - p^n}{\Delta t} &= \frac{p(c_1^{n+1}, \dots, c_{n_c}^{n+1}) - p(c_1^n, \dots, c_{n_c}^n)}{\Delta t} \\ &= \frac{p(c_1^{n+1}, \dots, c_{n_c}^{n+1}) - p(c_1^{n+1}, \dots, c_{n_c-1}^{n+1}, c_{n_c}^n)}{\Delta t} \\ &\quad + \frac{p(c_1^{n+1}, \dots, c_{n_c-2}^{n+1}, c_{n_c-1}^{n+1}, c_{n_c}^n) - p(c_1^{n+1}, \dots, c_{n_c-2}^{n+1}, c_{n_c-1}^n, c_{n_c}^n)}{\Delta t} \\ &\quad + \dots + \frac{p(c_1^{n+1}, c_2^n, \dots, c_{n_c}^n) - p(c_1^n, \dots, c_{n_c}^n)}{\Delta t}, \end{aligned}$$

where n is the time step at the time t_n . Let

$$(3.1) \quad \beta_i^{n+1} = \frac{p(c_1^{n+1}, \dots, c_i^{n+1}, c_{i+1}^n, \dots, c_{n_c}^n) - p(c_1^{n+1}, \dots, c_{i-1}^{n+1}, c_i^n, c_{i+1}^n, \dots, c_{n_c}^n)}{c_i^{n+1} - c_i^n}.$$

Here the functions $p(c_1^{n+1}, \dots, c_i^{n+1}, c_{i+1}^n, \dots, c_{n_c}^n)$ with $i = 1, \dots, n_c$ are computed based on the Peng-Robinson EOS (A.1). Obviously, $\beta_i^{n+1} = RT$ if the ideal gas law EOS is considered, where R is the gas constant and T is the temperature.

We can obtain the time-discrete space-continuous scheme for the equation (2.9) as follows:

$$(3.2) \quad \frac{p^{n+1} - p^n}{\Delta t} = \sum_{i=1}^{n_c} \beta_i^{n+1} \frac{c_i^{n+1} - c_i^n}{\Delta t}.$$

Thus, we can easily see that the original time-discrete space-continuous scheme for the nonlinear system (2.1) with $i = 1, \dots, n_c$, (2.2) and $p^{n+1} = p(\mathbf{c}^{n+1})$ based on the Peng-Robinson EOS (A.1) is equivalent to the following system:

$$(3.3) \quad \phi \frac{p^{n+1} - p^n}{\Delta t} + \sum_{i=1}^{n_c} \beta_i^{n+1} (\nabla \cdot (\mathbf{u}^{n+1} c_i^{n+1}) - f_i^{n+1}) = 0,$$

$$(3.4) \quad \mathbf{u}^{n+1} = -\frac{\mathbf{K}}{\mu^{n+1}} (\nabla p^{n+1} - \rho^{n+1} \mathbf{g}),$$

$$(3.5) \quad \phi \frac{c_i^{n+1} - c_i^n}{\Delta t} + \nabla \cdot (\mathbf{u}^{n+1} c_i^{n+1}) = f_i^{n+1}, \quad i = 1, \dots, n_c.$$

Now we present the time-discrete space-continuous iterative IMPEC scheme for the nonlinear system (3.3-3.5) coupled with (3.1), the boundary and initial conditions (2.3-2.6).

Algorithm 3.1. Given p^n and $c_i^n|_{i=1}^{n_c}$, the pressure, velocity and molar concentration at the time step $n+1$ can be iteratively obtained as follows:

Step 1. Set $l = 0$. For $i = 1, \dots, n_c$, let the initial value of the density of fluid $\rho^{n+1,0}$ be $\rho^{n+1,0} = \rho^n$, the initial value of c_i^{n+1} be $c_i^{n+1,0} = c_i^n$ in $\bar{\Omega} \setminus \Gamma_-^{n+1}$, $c_i^{B,n+1} = c_i^B(\mathbf{x}, t_{n+1})$, $\Gamma_-^{n+1} = \Gamma_-(\mathbf{x}, t_{n+1})$, $g^{N,n+1} = g^N(\mathbf{x}, t_{n+1})$.

We use (A.2) to compute the initial value of β_i^{n+1} as $\beta_i^{n+1,0} = \left(\frac{\partial p}{\partial c_i}\right)_{c_{\neq i}}^n$ based on $c_i^n|_{i=1}^{n_c}$ by the Peng-Robinson EOS.

Step 2. Set $l := l + 1$. We find $p^{n+1,l}$ and $\mathbf{u}^{n+1,l}$ such that

$$(3.6a) \quad \phi \frac{p^{n+1,l} - p^n}{\Delta t} + \sum_{i=1}^{n_c} \beta_i^{n+1,l-1} \left(\nabla \cdot \left(\mathbf{u}^{n+1,l} c_i^{n+1,l-1} \right) - f_i^{n+1} \right) = 0,$$

$$(3.6b) \quad \mathbf{u}^{n+1,l} = -\frac{\mathbf{K}}{\mu^{n+1,l-1}} (\nabla p^{n+1,l} - \rho^{n+1,l-1} \mathbf{g}),$$

with the boundary conditions (2.3,2.4), where we assume the viscosity $\mu^{n+1,l-1}$ of the fluid depends on $\mathbf{c}^{n+1,l-1} = (c_1^{n+1,l-1}, \dots, c_{n_c}^{n+1,l-1})$, i.e., $\mu^{n+1,l-1} = \mu(\mathbf{c}^{n+1,l-1})$.

Step 3. For $i = 1, \dots, n_c$, we find $c_i^{n+1,l}$ such that

$$(3.7) \quad \phi \frac{c_i^{n+1,l} - c_i^n}{\Delta t} + \nabla \cdot \left(\mathbf{u}^{n+1,l} c_i^{n+1,l-1} \right) = f_i^{n+1}$$

with the inflow boundary condition (2.4). Then for $i = 1, \dots, n_c$, we update the parameter $\beta_i^{n+1,l}$ by

$$(3.8) \quad \beta_i^{n+1,l} = \frac{p(c_1^{n+1,l}, \dots, c_i^{n+1,l}, c_{i+1}^n, \dots, c_{n_c}^n) - p(c_1^{n+1,l}, \dots, c_{i-1}^{n+1,l}, c_i^n, c_{i+1}^n, \dots, c_{n_c}^n)}{c_i^{n+1,l} - c_i^n}.$$

If $|c_i^{n+1,l} - c_i^n|/|c_i^{n+1,l}| < \epsilon$, where ϵ is the square root of machine precision, we use $c_i^{n+1,l} := c_i^n + \epsilon c_i^{n+1,l}$.

Step 4. The iteration stops when

$$\max \left\{ \frac{\|p^{n+1,l} - p^{n+1,l-1}\|_{0,\Omega}^2}{\|p^{n+1,l}\|_{0,\Omega}^2}, \sum_{i=1}^{n_c} \frac{\|c_i^{n+1,l} - c_i^{n+1,l-1}\|_{0,\Omega}^2}{\|c_i^{n+1,l}\|_{0,\Omega}^2}, \sum_{i=1}^{n_c} \frac{\|\beta_i^{n+1,l} - \beta_i^{n+1,l-1}\|_{0,\Omega}^2}{\|\beta_i^{n+1,l}\|_{0,\Omega}^2} \right\} < tol,$$

where tol is an optional precision. Then we set $p^{n+1} = p^{n+1,l}$, $\mathbf{u}^{n+1} = \mathbf{u}^{n+1,l}$, $c_i^{n+1} = c_i^{n+1,l}$ for $i = 1, \dots, n_c$. Otherwise, we repeat step 2 – step 4.

3.2. The fully mass-conservative iterative IMPEC discrete schemes. We begin with some notations. We use the standard notations and definitions for Sobolev spaces (cf. [2]) throughout the paper. For any $D \subset \bar{\Omega}$, any scalar functions ψ and ϕ , or vector functions $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$, we define $(\psi, \phi)_D = \int_D \psi \phi$ and $(\boldsymbol{\psi}, \boldsymbol{\phi})_D = \int_D \boldsymbol{\psi} \cdot \boldsymbol{\phi}$. When $D = \Omega$, we use the notation $\|\cdot\|_{0,D}$ to denote the L^2 -norm on D . We denote by $\mathcal{T}_h$ the quasi-uniform grid on Ω , $\mathcal{E}_h$ the set of all faces ($d = 3$) or edges ($d = 2$) of $\mathcal{T}_h$, h_K the diameter of any element $K \in \mathcal{T}_h$, $h = \min_{K \in \mathcal{T}_h} h_K$, $\mathcal{E}_h^\partial(D_F)$ the set of boundary faces or edges on $D_F \subset \partial\Omega$, and P_{D_F} the L^2 -projection operator of $L^2(\mathcal{E}_h^\partial(D_F))$ into $P_0(\mathcal{E}_h^\partial(D_F))$. Let $K, K' \in \mathcal{T}_h$ and $F = \partial K \cap \partial K'$ with the outward unit normal vector $\mathbf{n}_F$ exterior to K . We denote $[[\psi]] = (\psi|_K)|_F - (\psi|_{K'})|_F$ the jump of scalar function ψ across F . We denote by C with or without subscript a positive constant depending on the shape regularity of the meshes. These constants can take on different values in different occurrences.

Next, we introduce the upwind Raviart-Thomas mixed finite element approximation in the fully discrete schemes. Let RT_0 be the well-known lowest order of Raviart-Thomas finite element space. For instance, on the simplicial mesh, $RT_0 = [P_0]^d + \mathbf{x}P_0$, where P_0 is the constant function space. We define

$$\begin{aligned} \mathbf{U}_h &= \{\mathbf{v}_h \in H(\text{div}, \Omega) : v_h|_K \in RT_0(K), \forall K \in \mathcal{T}_h\}, \\ Q_h &= \{q_h \in L^2(\Omega) : q_h|_K \in P_0(K), \forall K \in \mathcal{T}_h\}. \end{aligned}$$

Let $\mathbf{U}_h^0 = \{\mathbf{v} \in \mathbf{U}_h : \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \Gamma_- \cup \Gamma_+\}$. In the following we focus on the fully discrete schemes for (3.6) and (3.7) with the boundary conditions (2.3,2.4). The molar concentration $c_i^{n+1,l}$ of each component, the parameter $\beta_i^{n+1,l}$ and the viscosity $\mu^{n+1,l-1}$ are all approximated in the piecewise constant space Q_h , and are denoted as $c_{i,h}^{n+1,l}$, $\beta_{i,h}^{n+1,l}$, $\mu_h^{n+1,l-1}$. Particularly, $\mu_h^{n+1,l-1} = P_Q \mu(\mathbf{c}_h^{n+1,l})$, where P_Q is the L^2 -projection operator from $L^2(\Omega)$ into Q_h .

Based on Algorithm 3.1, now we present the fully mass-conservative iterative IMPEC discrete schemes. The key idea to construct the fully mass-conservative iterative IMPEC schemes is that we obtain the discretized pressure-velocity system by the summation of the discretized conservation equation for each component multiplying β_i in discrete value which is updated by iterative schemes. We mainly show the fully

discrete schemes for Steps 2 and 3 in Algorithm 3.1. For Step 2, given p_h^n and $c_{i,h}^n|_{i=1}^{n_c}$, for (3.6) with the boundary conditions (2.3,2.4), we find $(\mathbf{u}_h^{n+1,l}, p_h^{n+1,l}) \in \mathbf{U}_h \times Q_h$ such that

$$(3.9) \quad \left(\phi \frac{p_h^{n+1,l} - p_h^n}{\Delta t}, q \right)_\Omega + \sum_{i=1}^{n_c} \left(\beta_{i,h}^{n+1,l-1} \nabla \cdot (\mathbf{u}_h^{n+1,l} c_{i,h}^{n+1,l-1}), q \right)_\Omega \\ - \sum_{i=1}^{n_c} \sum_{K \in \mathcal{T}_h} \int_{\partial K_-^{n+1,l-1} \setminus \Gamma} \beta_{i,h}^{n+1,l-1} \llbracket c_{i,h}^{n+1,l-1} \rrbracket \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} q = \sum_{i=1}^{n_c} \left(\beta_{i,h}^{n+1,l-1} f_i^{n+1}, q \right)_\Omega, \\ (3.10) \quad \left(\mu_h^{n+1,l-1} \mathbf{K}^{-1} \mathbf{u}_h^{n+1,l}, \mathbf{v} \right)_\Omega - \left(p_h^{n+1,l}, \nabla \cdot \mathbf{v} \right)_\Omega = - \int_{\Gamma_D} p_D^{n+1} \mathbf{v} \cdot \mathbf{n} + \left(\rho^{n+1,l-1} \mathbf{g}, \mathbf{v} \right)_\Omega,$$

for any $(\mathbf{v}, q) \in \mathbf{U}_h^0 \times Q_h$, where $\partial K_-^{n+1,l-1} = \{F \subset \partial K : \mathbf{u}_h^{n+1,l-1} \cdot \mathbf{n}|_F < 0\}$ is the inflow boundary of any element $K \in \mathcal{T}_h$.

For Step 3, in order to solve the equation (3.7) with the inflow boundary condition (2.4), we find $c_{i,h}^{n+1,l} \in Q_h, i = 1, \dots, n_c$, such that

$$(3.11) \quad \left(\phi \frac{c_{i,h}^{n+1,l} - c_{i,h}^n}{\Delta t}, q \right)_\Omega + \left(\nabla \cdot (\mathbf{u}_h^{n+1,l} c_{i,h}^{n+1,l-1}), q \right)_\Omega \\ - \sum_{K \in \mathcal{T}_h} \int_{\partial K_-^{n+1,l-1} \setminus \Gamma} \llbracket c_{i,h}^{n+1,l-1} \rrbracket \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} q = (f_i^{n+1}, q)_\Omega,$$

for any $q \in Q_h$. Then $\beta_{i,h}^{n+1,l}$ is updated by (3.8) based on $c_{i,h}^{n+1,l}$ and $c_{i,h}^n$ with $i = 1, \dots, n_c$.

We note that $c_{i,h}^{n+1,l}$ is explicitly updated element-wise. We can also easily see that (3.9) can be obtained by (3.2) and adding all the discrete equations (3.11) for $i = 1, \dots, n_c$ with $q = \beta_{i,h}^{n+1,l-1} \tilde{q}$ for any $\tilde{q} \in Q_h$. For the discretization of the convection term in (3.11) on the local element $K \in \mathcal{T}_h$, we have

$$(3.12) \quad \left(\nabla \cdot (\mathbf{u}_h^{n+1,l} c_{i,h}^{n+1,l-1}), q \right)_K - \int_{\partial K_-^{n+1,l-1} \setminus \Gamma} \llbracket c_{i,h}^{n+1,l-1} \rrbracket \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} q \\ = \int_{\partial K} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} (c_{i,h}^{n+1,l-1})^* q,$$

where the upwind value of the molar concentration $(c_{i,h}^{n+1,l-1})^*|_F$ on any $F \subset \partial K \setminus \Gamma_-^{n+1}$ is defined as

$$(c_{i,h}^{n+1,l-1})^*|_F = \begin{cases} c_{i,h}^{n+1,l-1}|_K, & \text{if } \mathbf{u}_h^{n+1,l-1} \cdot \mathbf{n}_F \geq 0, \\ c_{i,h}^{n+1,l-1}|_{K'}, & \text{if } \mathbf{u}_h^{n+1,l-1} \cdot \mathbf{n}_F < 0, \end{cases}$$

and we let $(c_{i,h}^{n+1,l-1})^*|_F = P_F c_i^{B,n+1}$ on any $F \subset \partial K \cap \Gamma_-^{n+1}$, and $(\mathbf{u}_h^{n+1,l} \cdot \mathbf{n})|_F = P_F g^{N,n+1}$ on any $F \subset \partial K \cap \Gamma^{N,n+1}$, where P_F is the L^2 -projection operator from $L^2(F)$ into $P_0(F)$. Thus we actually use the upwind values of molar concentration in (3.9-3.11), i.e., we use the upwind mixed finite element method to solve the pressure-velocity system (3.9-3.10) which is well-posed based on the theory of mixed finite element method (cf. [4, 5]).

Theorem 3.1. (Local mass balance of each component). *The approximation of each component $c_{i,h}^{n+1,l}$ in the iterative scheme (3.11) for $i = 1, \dots, n_c$ satisfies the mass conservative property on each element $K \in \mathcal{T}_h$ such that*

$$\left(\phi \frac{c_{i,h}^{n+1,l} - c_{i,h}^n}{\Delta t}, 1 \right)_K + \left(\nabla \cdot (\mathbf{u}_h^{n+1,l} c_{i,h}^{n+1,l-1}), 1 \right)_K - \int_{\partial K_-^{n+1,l-1} \setminus \Gamma} \llbracket c_{i,h}^{n+1,l-1} \rrbracket \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} = (f_i^{n+1}, 1)_K.$$

Proof. The desired result can be easily obtained by taking $q = 1$ in $\bar{K}$ and $q = 0$ in $\mathcal{T}_h \setminus K$ in (3.11). $\square$

Compared with the classical IMPEC scheme, the proposed fully mass-conservative iterative IMPEC scheme enjoys an appealing feature of mass conservation for all components in the solution of multicomponent compressible flow. When the iterative scheme converges at each time step, the conservation of mass property of each component holds true.

Remark 3.1. When the iterative scheme in Algorithm 3.1 converges at each time step, we easily have $p^{n+1} = p(\mathbf{c}^{n+1})$. The conservation of mass for each component can be easily obtained (cf. Theorem 3.1), and the total molar concentration c_{EOS}^{n+1} which is computed through the equation of state by the pressure p^{n+1} deserves that $c_{EOS}^{n+1} = \sum_{i=1}^{n_c} c_i^{n+1}$. In the computation, we use a tolerance to control the errors in the iterative process. When the iterative solutions converge, our scheme can guarantee the error at each time step between c_{EOS}^{n+1} and $\sum_{i=1}^{n_c} c_i$ in the magnitude of machine error.

Remark 3.2. In the conventional IMPEC-based schemes, the molar concentrations of the first $(n_c - 1)$ components are computed from the transport equations and are mass conservative, however, the molar concentration of n_c -th species $c_{n_c}^{n+1,l} = c_{EOS}^{n+1,l} - \sum_{i=1}^{n_c-1} c_i^{n+1,l}$, where $c_{EOS}^{n+1,l} = p^{n+1,l} / (Z^{n+1,l-1} RT)$. Hence the mass conservation law for n_c -th species is not satisfied in the conventional IMPEC-based schemes. And the compressibility factor Z is computed, which may be difficult to determine which one is the most appropriate among the three roots when they are all real and their values are very close to each other. These two issues are avoided in our scheme.

4. CONVERGENCE OF THE FULLY MASS-CONSERVATIVE ITERATIVE IMPEC SCHEME

In this section we present the convergence of (3.9-3.11) at any time step. Obviously, if the iterative schemes (3.9-3.11) converge, it will converge to a fully nonlinear discrete system as follows:

Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}, c_{1,h}^{n+1}, \dots, c_{n_c,h}^{n+1}) \in \mathbf{U}_h \times Q_h \times Q_h \times \dots \times Q_h$ such that

$$(4.1) \quad \left(\phi \frac{p_h^{n+1} - p_h^n}{\Delta t}, q \right)_\Omega + \sum_{i=1}^{n_c} \left(\beta_{i,h}^{n+1} \nabla \cdot (\mathbf{u}_h^{n+1} c_{i,h}^{n+1}), q \right)_\Omega - \sum_{i=1}^{n_c} \sum_{K \in \mathcal{T}_h} \int_{\partial K_-^{n+1} \setminus \Gamma} \beta_{i,h}^{n+1} \llbracket c_{i,h}^{n+1} \rrbracket \mathbf{u}_h^{n+1} \cdot \mathbf{n} q = \sum_{i=1}^{n_c} \left(\beta_{i,h}^{n+1} f_i^{n+1}, q \right)_\Omega,$$

$$(4.2) \quad (\mu_h^{n+1} \mathbf{K}^{-1} \mathbf{u}_h^{n+1}, \mathbf{v})_\Omega - (p_h^{n+1}, \nabla \cdot \mathbf{v})_\Omega = - \int_{\Gamma_D} p_D^{n+1} \mathbf{v} \cdot \mathbf{n} + (\rho^{n+1} \mathbf{g}, \mathbf{v})_\Omega,$$

$$(4.3) \quad \left(\phi \frac{c_{i,h}^{n+1} - c_{i,h}^n}{\Delta t}, q \right)_\Omega + \left(\nabla \cdot (\mathbf{u}_h^{n+1} c_{i,h}^{n+1}), q \right)_\Omega - \sum_{K \in \mathcal{T}_h} \int_{\partial K_-^{n+1} \setminus \Gamma} \llbracket c_{i,h}^{n+1} \rrbracket \mathbf{u}_h^{n+1} \cdot \mathbf{n} q = (f_i^{n+1}, q)_\Omega,$$

for any $(\mathbf{v}, q) \in \mathbf{U}_h^0 \times Q_h$. Here $\partial K_-^{n+1} = \{F \subset \partial K : \mathbf{u}_h^{n+1} \cdot \mathbf{n}|_F < 0\}$ and

$$\beta_{i,h}^{n+1} = P_Q \frac{p(c_{1,h}^{n+1}, \dots, c_{i,h}^{n+1}, c_{i+1,h}^n, \dots, c_{n_c,h}^n) - p(c_{1,h}^{n+1}, \dots, c_{i-1,h}^{n+1}, c_{i,h}^n, c_{i+1,h}^n, \dots, c_{n_c,h}^n)}{c_{i,h}^{n+1} - c_{i,h}^n}.$$

We assume the above nonlinear system (4.1-4.3) is well-posed.

Theorem 4.1. *For the iterative schemes (3.9-3.11) at the time step $n+1$, if $\frac{\Delta t}{h}$ is sufficiently small, the iterative scheme (3.11) for the molar concentration converges, i.e., $\lim_{l \rightarrow +\infty} c_{i,h}^{n+1,l} = c_{i,h}^{n+1}, i = 1, \dots, n_c$, there exists $0 < \gamma < 1$ such that*

$$(4.4) \quad \sum_{i=1}^{n_c} \|c_{i,h}^{n+1} - c_{i,h}^{n+1,l}\|_{0,\mathcal{T}_h} \leq \gamma \sum_{i=1}^{n_c} \|c_{i,h}^{n+1} - c_{i,h}^{n+1,l-1}\|_{0,\mathcal{T}_h},$$

and the iterative solutions of pressure and velocity from (3.9-3.10) also converge which depend on the molar concentrations.

Proof. For any $K \in \mathcal{T}_h$, similar to the notations ∂K_-^{n+1} and $\partial K_-^{n+1,l}$, we denote by $\partial K_+^{n+1} = \{F \subset \partial K : \mathbf{u}_h^{n+1} \cdot \mathbf{n}|_F \geq 0\}$, $\partial K_+^{n+1,l} = \{F \subset \partial K : \mathbf{u}_h^{n+1,l} \cdot \mathbf{n}|_F \geq 0\}$. Let $\widehat{\partial K_+}^{n+1} = \partial K_+^{n+1} \cap \partial K_+^{n+1,l-1}$ and

$\widehat{\partial K_-}^{n+1} = \partial K_-^{n+1} \cap \partial K_-^{n+1,l-1}$. By (3.11,4.3) and (3.12), we can easily derive that

$$\left(\phi \frac{c_{i,h}^{n+1} - c_{i,h}^{n+1,l}}{\Delta t}, q \right)_{\Omega} + T_1 + T_2 + T_R = 0,$$

where

$$\begin{aligned} T_1 &= \sum_{K \in \mathcal{T}_h} \int_{\widehat{\partial K_+}^{n+1}} \left(\mathbf{u}_h^{n+1} \cdot \mathbf{n} c_{i,h}^{n+1} - \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} c_{i,h}^{n+1,l-1} \right) q, \\ T_2 &= \sum_{K \in \mathcal{T}_h} \int_{\widehat{\partial K_-}^{n+1}} \left(\mathbf{u}_h^{n+1} \cdot \mathbf{n} (c_{i,h}^{n+1})^* - \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} (c_{i,h}^{n+1,l-1})^* \right) q, \\ T_R &= \sum_{K \in \mathcal{T}_h} \left(\int_{\partial K_+^{n+1} \setminus \widehat{\partial K_+}^{n+1}} \mathbf{u}_h^{n+1} \cdot \mathbf{n} c_{i,h}^{n+1} q - \int_{\partial K_+^{n+1,l-1} \setminus \widehat{\partial K_+}^{n+1}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} c_{i,h}^{n+1,l-1} q \right) \\ &\quad + \sum_{K \in \mathcal{T}_h} \left(\int_{\partial K_-^{n+1} \setminus \widehat{\partial K_-}^{n+1}} \mathbf{u}_h^{n+1} \cdot \mathbf{n} (c_{i,h}^{n+1})^* q - \int_{\partial K_-^{n+1,l-1} \setminus \widehat{\partial K_-}^{n+1}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} (c_{i,h}^{n+1,l-1})^* q \right). \end{aligned}$$

Note that the velocity changes the direction on the boundaries of elements in each term of T_R , thus in each term of T_R we assume that there exists sufficiently small $\epsilon_{\mathbf{u}}$ such that $|\mathbf{u}_h^{n+1,l} \cdot \mathbf{n}| < \epsilon_{\mathbf{u}}$. Then we have

$$T_R \leq C \epsilon_{\mathbf{u}} h^{-1} \left(\|c_{i,h}^{n+1}\|_{0,\mathcal{T}_h} + \|c_{i,h}^{n+1,l-1}\|_{0,\mathcal{T}_h} \right) \|q\|_{0,\mathcal{T}_h}.$$

Since the pressure is dependent on the molar concentrations by the equation of state and the Darcy's law is considered, we have that the discrete velocity $\mathbf{u}_h$ is dependent of the molar concentrations, i.e., $\mathbf{u}_h^{n+1} = \mathbf{u}_h(c_h^{n+1})$, $\mathbf{u}_h^{n+1,l} = \mathbf{u}_h(c_h^{n+1,l-1})$. We may further assume that $\mathbf{u}_h$ is Lipschitz continuous for partial derivatives on the molar concentrations, then we have

$$(4.5) \quad \left| (\mathbf{u}_h^{n+1} - \mathbf{u}_h^{n+1,l}) \cdot \mathbf{n} \right|_F \leq \sum_{i=1}^{n_c} C_j \sum_{K \subset \omega_F} \left| (c_{j,h}^{n+1} - c_{j,h}^{n+1,l-1})|_K \right|, \quad \forall F \in \mathcal{E}_h,$$

where $\omega_F = \{K \in \mathcal{T}_h : \partial K \cap F \neq \emptyset\}$. By the trace inequality, the Hölder's inequality and (4.5), we have

$$\begin{aligned} T_1 &= \sum_{K \in \mathcal{T}_h} \int_{\widehat{\partial K_+}^{n+1}} \left(\mathbf{u}_h^{n+1} \cdot \mathbf{n} (c_{i,h}^{n+1} - c_{i,h}^{n+1,l-1}) + (\mathbf{u}_h^{n+1} - \mathbf{u}_h^{n+1,l}) \cdot \mathbf{n} c_{i,h}^{n+1,l-1} \right) q \\ &\leq Ch^{-1} \sum_{K \in \mathcal{T}_h} \|\mathbf{u}_h^{n+1} \cdot \mathbf{n}\|_{0,\widehat{\partial K_+}^{n+1}} \|c_{i,h}^{n+1} - c_{i,h}^{n+1,l-1}\|_{0,K} \|q\|_{0,K} \\ &\quad + Ch^{-1} \sum_{K \in \mathcal{T}_h} \|c_{i,h}^{n+1,l-1}\|_{0,K} \|q\|_{0,K} \sum_{j=1}^{n_c} C_j \sum_{K' \subset \omega_F, F \subset \widehat{\partial K_+}^{n+1}} \|c_{j,h}^{n+1} - c_{j,h}^{n+1,l-1}\|_{0,K'}. \end{aligned}$$

We denote $\mathcal{N}(\widehat{\partial K_-}^{n+1}) = \{\tilde{K} \in \mathcal{T}_h : \tilde{K} \neq K, \partial \tilde{K} \cap \widehat{\partial K_-}^{n+1} \neq \emptyset\}$. Similarly, T_2 can be estimated as follows:

$$\begin{aligned} T_2 &\leq Ch^{-1} \sum_{K \in \mathcal{T}_h} \|\mathbf{u}_h^{n+1} \cdot \mathbf{n}\|_{0,\widehat{\partial K_-}^{n+1}} \|q\|_{0,K} \sum_{\tilde{K} \in \mathcal{N}(\widehat{\partial K_-}^{n+1})} \|c_{i,h}^{n+1} - c_{i,h}^{n+1,l-1}\|_{0,\tilde{K}} \\ &\quad + Ch^{-1} \sum_{K \in \mathcal{T}_h} \|q\|_{0,K} \sum_{\tilde{K} \in \mathcal{N}(\widehat{\partial K_-}^{n+1})} \|c_{i,h}^{n+1,l-1}\|_{0,\tilde{K}} \sum_{j=1}^{n_c} C_j \sum_{K' \subset \omega_F, F \subset \widehat{\partial K_-}^{n+1}} \|c_{j,h}^{n+1} - c_{j,h}^{n+1,l-1}\|_{0,K'}. \end{aligned}$$

Let $q = c_{i,h}^{n+1} - c_{i,h}^{n+1,l}$. By the above estimates for T_1, T_2 and T_R , one can find that if $\frac{\Delta t}{h}$ is small enough, there exists $0 < \gamma < 1$ such that

$$\begin{aligned} \sum_{i=1}^{n_c} \|c_{i,h}^{n+1} - c_{i,h}^{n+1,l}\|_{0,\mathcal{T}_h} &\leq C \frac{\Delta t}{h} \sum_{i=1}^{n_c} \|c_{i,h}^{n+1} - c_{i,h}^{n+1,l-1}\|_{0,\mathcal{T}_h} + C\epsilon_u \frac{\Delta t}{h} \sum_{i=1}^{n_c} \left(\|c_{i,h}^{n+1}\|_{0,\mathcal{T}_h} + \|c_{i,h}^{n+1,l-1}\|_{0,\mathcal{T}_h} \right) \\ &\leq \gamma \sum_{i=1}^{n_c} \|c_{i,h}^{n+1} - c_{i,h}^{n+1,l-1}\|_{0,\mathcal{T}_h}, \end{aligned}$$

which yields the desired estimate (4.4). The above second estimate is due to the fact that ϵ_u is sufficiently small.

Now we have the convergence result $\lim_{l \rightarrow +\infty} c_{i,h}^{n+1,l} = c_{i,h}^{n+1}, i = 1, \dots, n_c$ at each time step which indicates the convergence of $\beta_{i,h}^{n+1,l}$, i.e., $\lim_{l \rightarrow +\infty} \beta_{i,h}^{n+1,l} = \beta_{i,h}^{n+1}, i = 1, \dots, n_c$. By the pressure-velocity system (3.9-3.10), we further have $\lim_{l \rightarrow +\infty} \mathbf{u}_h^{n+1,l} = \mathbf{u}_h^{n+1}$ and $\lim_{l \rightarrow +\infty} p_h^{n+1,l} = p_h^{n+1}$. Now we conclude the proof. $\square$

5. POSITIVITY-PRESERVING PROPERTY OF THE MOLAR CONCENTRATION

The positivity-preserving property of the molar concentration is important for the conservation of mass of each component. In this section, we will show that under the condition of sufficiently small time step size, the positivity-preserving property of molar concentration of each component holds true at every iterative step in (3.11) for the molar concentration.

Theorem 5.1. *For the iterative scheme (3.11), we assume $c_{i,h}^{n+1,l-1} > 0$ and $c_{i,h}^n > 0$ with tolerance concentration $c_i^t, i = 1, \dots, n_c$. If $\frac{\Delta t}{h}$ is sufficiently small, we have*

$$c_{i,h}^{n+1,l} > 0, \quad i = 1, \dots, n_c.$$

Proof. For any $K \in \mathcal{T}_h$ and $\partial K \cap \Gamma_-^{n+1} = \emptyset$, by (3.11), we have

$$(5.1) \quad \phi \frac{c_{i,h}^{n+1,l} - c_{i,h}^n}{\Delta t} |K| + \int_{\partial K} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n}(c_{i,h}^{n+1,l-1})^* = P_K f_i^{n+1} |K|, \quad i = 1, \dots, n_c,$$

where P_K is the L^2 -projection operator of $L^2(K)$ into $P_0(K)$. Let $\widetilde{\partial K_+^{n+1,l}} = \partial K_+^{n+1,l} \cap \partial K_+^{n+1,l-1}$. Then the left-hand side of (5.1) becomes

$$\phi \frac{c_{i,h}^{n+1,l} - c_{i,h}^n}{\Delta t} |K| + \sum_{F \subset \partial K_+^{n+1,l}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n}(c_{i,h}^{n+1,l-1})^* |F| + \sum_{F \subset \partial K_-^{n+1,l}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n}(c_{i,h}^{n+1,l-1})^* |F|.$$

Particularly, we have

$$\begin{aligned} \sum_{F \subset \partial K_+^{n+1,l}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n}(c_{i,h}^{n+1,l-1})^* |F| &= \sum_{F \subset \partial K_+^{n+1,l}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} c_{i,h}^{n+1,l-1} |F| \\ &\quad + \sum_{F \subset \partial K_+^{n+1,l} \setminus \widetilde{\partial K_+^{n+1,l}}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} \left((c_{i,h}^{n+1,l-1})^* - c_{i,h}^{n+1,l-1} \right) |F|. \end{aligned}$$

Obviously from the iterative step $l-1$ to l in (3.11), the velocity changes the direction on any $F \subset \partial K_+^{n+1,l} \setminus \widetilde{\partial K_+^{n+1,l}}$, thus we can assume there exists ϵ_u which is sufficiently small such that $|\mathbf{u}_h^{n+1,l} \cdot \mathbf{n}| < \epsilon_u$ on F . Then by (5.1) and the above equalities, we have

$$\begin{aligned} (5.2) \quad \phi c_{i,h}^{n+1,l} &= \phi c_{i,h}^n - \frac{\Delta t}{Ch_K} \sum_{F \subset \partial K_+^{n+1,l}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} c_{i,h}^{n+1,l-1} \\ &\quad - \frac{\Delta t}{Ch_K} \sum_{F \subset \partial K_+^{n+1,l} \setminus \widetilde{\partial K_+^{n+1,l}}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} \left((c_{i,h}^{n+1,l-1})^* - c_{i,h}^{n+1,l-1} \right) \\ &\quad - \frac{\Delta t}{Ch_K} \sum_{F \subset \partial K_-^{n+1,l}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} (c_{i,h}^{n+1,l-1})^* + \Delta t P_K f_i^{n+1}. \end{aligned}$$

If there is injection source or no source on K , we have $f_i^{n+1} \geq 0$. Otherwise, $f_i^{n+1} < 0$ is production term, and we can assume $f_i^{n+1} = q_{i,c}^{n+1,l} c_{i,h}^{n+1,l}$ with $q_{i,c}^{n+1,l} < 0$. Moreover, for the third term of the right-hand side of (5.2), we have

$$\frac{\Delta t}{Ch_K} \sum_{F \subset \partial K_+^{n+1,l} \setminus \widetilde{\partial K_+^{n+1,l}}} \mathbf{u}_h^{n+1,l} \cdot \mathbf{n} \left((c_{i,h}^{n+1,l-1})^* - c_{i,h}^{n+1,l-1} \right) \leq C \epsilon_u \frac{\Delta t}{h_K} |(c_{i,h}^{n+1,l-1})^* - c_{i,h}^{n+1,l-1}|.$$

Then combining the above estimates and noting the tolerance concentration assumption for c_i^t , we can observe that if $\frac{\Delta t}{h}$ and ϵ_u are small enough, we have $c_{i,h}^{n+1,l} \geq C c_i^t > 0$ on K . When $\partial K \cap \Gamma_-^{n+1} \neq \emptyset$, $c_{i,h}^{n+1,l} > 0$ can be similarly derived. Now we conclude the proof. $\square$

6. NUMERICAL EXPERIMENTS

In this section, we demonstrate some numerical experiments to verify the proposed schemes. In all these examples, the porous medium is isotropic. In the first example we check the convergence rate of our proposed scheme. An analytic solution is given for a simplified problem and the numerical solutions computed by our proposed scheme are shown and compared with the analytic solution. In the second example, we simulate the gas mixture with the ideal gas law EOS. It is designed to verify that when the true value of β_i^{n+1} can be analytically given (or $\beta_i^{n+1,l}$ converges to the true value β_i^{n+1}) then our scheme can guarantee the error at each time step between the total molar concentration computed from EOS and $\sum_{i=1}^{n_c} c_i$ in the magnitude of machine error. In the third example, we consider a three-component gas mixture flow in homogeneous porous media. In the fourth example, we simulate the gas mixture flow in a heterogeneous media. We show, in the fifth example, some results of gas mixture flow in a porous medium with two channels. In the sixth example, we simulate a thirteen-component gas mixture flow in a heterogeneous porous medium. For all the six examples, we simulate the problem in two-dimensional domain and the gravity is at the direction perpendicular to this domain and therefore we ignore the gravity effect. The Peng-Robinson EOS is applied in the last fourth experiments for its more accuracy in the hydrocarbon systems. In all the numerical experiments, the convergence tolerance tol is taken identically as 10^{-8} . We will show the molar concentration of each species. The mass residuals for each component at every time step are calculated.

Example 6.1. In this example, the convergence of the proposed methods is verified. Setting $n_c = 1$, $f = 0$, $\mathbf{g} = 0$, $\mathbf{K} = I$, $\mu = 1$, and $p = c$, we have a simplified model

$$(6.1) \quad \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) = 0,$$

$$(6.2) \quad \mathbf{u} = -\nabla c,$$

with initial conditions and boundary conditions as follows:

$$(6.3) \quad c(\mathbf{x}, t_0) = B_2(\mathbf{x}, t_0), \quad \mathbf{x} \in \Omega,$$

$$(6.4) \quad p(\mathbf{x}, t_0) = B_2(\mathbf{x}, t), \quad \mathbf{x} \in \Gamma_D, t \in (t_0, \tau),$$

$$(6.5) \quad \mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{x} \in \Gamma_N, t \in (t_0, \tau).$$

Here $B_2(\mathbf{x}, t)$ is the Barenblatt solution (see [39] and references therein) of (6.1) and (6.2) as follows:

$$(6.6) \quad B_m(\mathbf{x}, t) = \max \left\{ 0, t^{-\alpha} \left(1 - \frac{\alpha(m-1)}{2m} \frac{|\mathbf{x}|^2}{t^{2\alpha}} \right)^{\frac{1}{m-1}} \right\},$$

where $\alpha = (m+1)^{-1}$, $m = 2$. We apply the numerical scheme developed in Section 3 to solve (6.1) and (6.2) in a rectangular domain of $64 \text{ m} \times 32 \text{ m}$, where $\Gamma_D = \{0, 64\} \times [0, 32]$ and $\Gamma_N = \partial\Omega \setminus \Gamma_D$. The initial time $t_0 = 10 \text{ s}$ and the final time $t = 2 \times 10^3 \text{ s}$. As the convergence analysis in [25], we have computed the errors of concentration $E_h = c - c_h$ in L^1, L^2 and L^∞ norms respectively (where c is exact solution and c_h is computed by the proposed numerical scheme) and their corresponding convergence rates γ on five uniform meshes with $2n_x \times n_y$ elements. Time step for the computations on the five grids is taken as $\Delta t = 20\text{s}, 13\text{s}, 9\text{s}, 6\text{s}, 2\text{s}$, respectively, which is almost linear with the mesh size h . The results are listed in Table 1. We can observe that the convergence rate γ at $t = 2 \times 10^3 \text{ s}$ is almost $O(h)$ in three different error norms.

TABLE 1. Convergence rates γ and errors of concentration at $t = 2 \times 10^3 s$ compared with analytical solution. The time step size is $\Delta t = Ch$, where h is mesh size.

Grids	$\ E_h\ _{L^1(\Omega)}$	γ	$\ E_h\ _{L^2(\Omega)}$	γ	$\ E_h\ _{L^\infty(\Omega)}$	γ
32×16	2.2358×10^{-2}		9.3211×10^{-4}		5.6471×10^{-5}	
		1.8925		1.7533		1.1244
64×32	6.0219×10^{-3}		2.7648×10^{-4}		2.5903×10^{-5}	
		1.4257		1.3520		1.1021
128×64	2.2416×10^{-3}		1.0831×10^{-4}		1.2067×10^{-5}	
		1.1734		1.0997		1.1369
256×128	9.9386×10^{-4}		5.054×10^{-5}		5.4871×10^{-6}	
		1.0522		1.0274		1.2881
512×256	4.7927×10^{-4}		2.4795×10^{-5}		2.2469×10^{-6}	

Example 6.2. This example shows the flow of a three-component gas mixture in homogeneous porous media with ideal gas law EOS. Some properties of the porous media are listed in Table 2. Initially, the porous medium is fully saturated with propane and the initial pressure is 1.5×10^5 Pa everywhere in the domain. Mixture of methane and ethane is constantly injected at rate of $3.17 \times 10^{-6} m^3/s$ on the bottom-left boundary of one mesh size. The gas mixture is produced on the top-right boundary of one mesh size with constant pressure 10^5 Pa. The rest of the boundary is impermeable. During the simulation, the temperature is assumed to be a constant.

TABLE 2. Porous media property parameters and other relevant data (for Examples 6.2 and 6.3)

Temperature [K]	554.8		
Porosity [-]	0.2		
Permeability [mD]	100		
Mole fraction of initial gas [-]	0.0 C1	0.0 C2	1.0 C3
Mole fraction of injected gas [-]	0.8 C1	0.2 C2	0.0 C3
Domain size ($L_x \times L_y \times L_z$) [m^3]	$50 \times 50 \times 1$		
Number of mesh grids ($n_x \times n_y \times n_z$) [-]	$40 \times 40 \times 1$		
time step size [seconds]	131.67

FIGURE 6.1. Molar concentration distribution after injection for 61 days. Left: methane; Middle: ethane; Right: propane.

We firstly utilize the conventional iterative IMPEC algorithm (cf. [7]) to solve this problem and check the mass conservation of each component. The results show that the residual of transport equation for the first two components (methane and ethane) is in magnitude of 10^{-14} , however, the residual of transport equation for the last species (propane) is in magnitude of 10^2 from the beginning step and keeps growing at every time step. Thus the conventional IMPEC scheme blows up quickly for this case.

FIGURE 6.2. Molar concentration distribution after injection for 305 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.3. Molar concentration distribution after injection for 1067 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.4. Error between the total molar concentration computed from EOS and the summation of all species from mass conservation equation at different time.

Then we start to apply the proposed fully mass-conservative iterative IMPEC scheme to solve the underlying problem and the following examples. We show the results of the molar concentration distribution and the quiver of velocity field in Figures 6.1-6.3 at different time steps. From these figures, we can see that the gas mixture flow from injection location towards the production location. Propane is displaced by the injected gas mixture (C1/C2). After 1481 days, 1% of initial propane mass is remained. We calculate the total mass error of each species at each time step, which is in magnitude of 10^{-14} for all species at each

time step. We also calculate the relative error at each time step $e_c^{n+1} = \frac{\|c_{EOS}^{n+1} - \sum_{i=1}^{n_c} c_i^{n+1}\|_2}{\|c_{EOS}^{n+1}\|_2}$, and the result is shown in Figure 6.4. From the result we can see that the error is in magnitude of machine error. Thus, we can see that the mass conservation is preserved for all species in this example based on the proposed scheme. We checked the iterations required for both the classical scheme and the proposed scheme. At the beginning time steps it takes around 10 iterations to get convergent results, but after 20 time steps it takes at most 3 iterations to converge.

Example 6.3. This example shows the flow of a three-component gas mixture in homogeneous porous media. The properties of the porous media and some relevant data are used as Example 6.2 (cf. Table 2). In the following experiments, the Peng-Robinson EOS is applied. Initially, the porous medium is fully saturated with propane and the initial pressure is 1.5×10^5 Pa everywhere in the domain. Mixture of methane and ethane is constantly injected at rate of $3.17 \times 10^{-6} m^3/s$ on the bottom-left boundary of one mesh size. The gas mixture is produced on the top-right boundary of one mesh size with constant pressure 10^5 Pa. The rest part of boundary is no-flow. During the simulation, the temperature is assumed to be a constant.

FIGURE 6.5. Molar concentration distribution after injection for 74 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.6. Molar concentration distribution after injection for 370 days. Left: methane; Middle: ethane; Right: propane.

We show the results of the molar concentration distribution and quiver of velocity field in Figures 6.5-6.7 at different time. From these figures, we can see that the gas mixture flow from injection location towards the production location. Propane is displaced by the injected gas mixture (C1/C2). After 1481 days, 99% of initial propane mass is produced. We calculate the total mass error of each species at each time step, which is in magnitude of 10^{-14} for all species at each time step. This illustrates that the mass conservation is preserved for all species based on the proposed scheme. In this example, at the beginning time steps it takes about 10 iterations to converge, but after about 50 time steps it takes at most 3 iterations to converge.

FIGURE 6.7. Molar concentration distribution after injection for 1481 days. Left: methane; Middle: ethane; Right: propane.

Example 6.4. In this example we consider a three-component compressible flow in heterogeneous porous media. Some properties of the porous media are listed in Table 3. We plot the permeability distribution in Figure 6.8. Initially, the propane is fully saturated in the porous media and the initial pressure is 1.5×10^5 Pa everywhere in the domain. Mixture of methane and ethane is constantly injected at a rate of $3.17 \times 10^{-6} m^3/s$ on the whole west boundary. The gas mixture is produced on the whole east boundary with constant pressure 10^5 Pa. No-flow conditions are imposed for the rest of the boundary. The temperature is assumed to be a constant.

TABLE 3. Media property parameters and other relevant data (for Example 6.4)

Temperature [K]	554.8		
Porosity [-]	0.2		
Permeability [mD]	shown in Figure 6.8		
Mole fraction of initial gas [-]	0.0 C1	0.0 C2	1.0 C3
Mole fraction of injected gas [-]	0.8 C1	0.2 C2	0.0 C3
Domain size ($L_x \times L_y \times L_z$) [m^3]	$50 \times 50 \times 1$		
Number of mesh grids ($n_x \times n_y \times n_z$) [-]	$40 \times 40 \times 1$		
time step size [seconds]	16.5

FIGURE 6.8. Permeability distribution (in minidarcy).

We show the results of the molar concentration distribution and quiver of velocity field in Figures 6.9-6.11 at different time. From these figures, we can see that the gas mixture flow from west towards east. The larger permeability area attracts the injected gas and propane is more quickly displaced in this area. After 80 days, almost all the initial propane mass is produced. We calculate the total mass error of each species at each time step, which is in magnitude of 10^{-14} for all species at each time step. This again indicates the

FIGURE 6.9. Molar concentration distribution after injection for 20 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.10. Molar concentration distribution after injection for 40 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.11. Molar concentration distribution after injection for 80 days. Left: methane; Middle: ethane; Right: propane.

fully mass-conservative property of the proposed scheme. In this experiment, at the beginning 50 time steps it takes about 20 iterations to converge, but after that it takes at most 4 iterations to obtain the convergent results.

Example 6.5. In this example we consider a three-component compressible flow in porous media with two channels. Here the width of channels is the width of one grid. Some properties of the porous media are listed in Table 4. The permeability of channels is 200 times of that in matrix domain, and the permeability

of matrix domain is 10 minidarcy. We plot the permeability distribution in Figure 6.12. Initially, the porous medium is fully saturated with propane and the initial pressure is 1.5×10^5 Pa everywhere in the domain. Mixture of methane and ethane is constantly injected at rate of $3.17 \times 10^{-6} m^3/s$ on the whole west boundary. The gas mixture is produced on the whole east boundary with constant pressure 10^5 Pa. We impose no-flow conditions on the rest boundary. During the simulation, the temperature is assumed to be a constant.

TABLE 4. Media property parameters and other relevant data (for Example 6.5)

Temperature [K]	554.8		
Porosity [-]	0.2		
Permeability [mD]	shown in Figure 6.12		
Mole fraction of initial gas [-]	0.0 C1	0.0 C2	1.0 C3
Mole fraction of injected gas [-]	0.8 C1	0.2 C2	0.0 C3
Domain size ($L_x \times L_y \times L_z$) [m^3]	$50 \times 50 \times 1$		
Number of mesh grids ($n_x \times n_y \times n_z$) [-]	$40 \times 40 \times 1$		
time step size [seconds]	16.5

FIGURE 6.12. Permeability distribution (in minidarcy).

FIGURE 6.13. Molar concentration distribution after injection for 40 days. Left: methane; Middle: ethane; Right: propane.

We show the results of the molar concentration distribution and quiver of velocity field in Figures 6.13-6.15 at different time. From these figures, we can see that the gas mixture flow from west towards east. The injected gas flows into the channels much more quickly than that into the matrix domain and propane is faster displaced by injected gas mixture. After 1000 days, 99% of initial propane mass is produced. We calculate the total mass error of each species at each time step, which is in magnitude of 10^{-14} for all species at each time step. Thus this shows that the mass conservation is preserved for all species based on the

FIGURE 6.14. Molar concentration distribution after injection for 200 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.15. Molar concentration distribution after injection for 1000 days. Left: methane; Middle: ethane; Right: propane.

proposed scheme. In this case, at the beginning of 65 time steps it takes about 23 iterations to converge, but after that it takes at most 4 iterations to obtain the convergent results.

Example 6.6. All the previous examples consist of three species. In this example, we illustrate an example consisting of thirteen components. These thirteen species are major ingredients of natural gas. Relevant parameters and data are shown in Table 5. The permeability distribution is plotted in Figure 6.16. A mixture gas of nitrogen and carbon dioxide is injected on the whole west boundary with injection rate of $5.71 \times 10^{-6} m^3/s$ and on the east boundary a uniformly constant pressure of 1.5×10^5 Pa is fixed. No-flow conditions are set on the rest boundary.

Figures 6.17-6.28 demonstrate the evolution of the molar density of the species C1-C10, N2 and CO2 in the mixture. The evolution of the molar density of the species C11+ is similar with that of C1-C10 and is not plotted. We also compute the total mass error of each species at each time step, which is in magnitude of 10^{-14} for all species at each time step. Thus, the computational results show that the mass conservation is also preserved for all species in this example, which once again verifies the property of our proposed scheme. In this situation, at the beginning 50 time steps it takes about 20 iterations to converge, but after that it takes at most 4 iterations to obtain the convergent results.

TABLE 5. Media property parameters and other relevant data (for Example 6.6)

FIGURE 6.16. Permeability distribution (in minidarcy).

Temperature [K]	1039.7		
Porosity [-]	0.2		
Permeability [mD]	shown in Figure 6.16		
Mole fraction of initial gas [-]	0.0064 C1	0.0287 C2	0.6314 C3
0.0962 C4	0.0592 C5	0.0286 C6	
0.0166 C7	0.0201 C8	0.0199 C9	0.0158 C10
0.0094 C11+	0.0063 N2	0.0613 CO2	
Mole fraction of injected gas [-]	0.1 N2	0.9 CO2	
Domain size ($L_x \times L_y \times L_z$) [m^3]	$50 \times 50 \times 1$		
Number of mesh grids ($n_x \times n_y \times n_z$) [-]	$40 \times 40 \times 1$		
time step size [seconds]	16.5

FIGURE 6.17. Molar concentration distribution after injection for 10 days. Left: methane; Middle: ethane; Right: propane.

7. CONCLUSION

We have designed the mass-conservative numerical methods for the multicomponent compressible single-phase Darcy flow in porous media. The key idea is to obtain the totally discretized conservation equation from the discretized conservation equation of each component multiplying a parameter which is defined in a Gauss-Seidel type. Then we use the fully mass-conservative iterative IMPEC scheme to solve the nonlinear system for molar concentration, pressure and velocity fields, and the upwind mixed finite element methods are used to solve the pressure-velocity system. The Peng-Robinson EOS is used to describe the pressure as a function of the molar concentrations of all components at constant temperature. When the time step is small enough on a fixed mesh, we have proved that the fully mass-conservative iterative IMPEC scheme is

FIGURE 6.18. Molar concentration distribution after injection for 10 days. Left: butane; Middle: pentane; Right: hexane.

FIGURE 6.19. Molar concentration distribution after injection for 10 days. Left: heptane; Middle: octane; Right: nonane.

FIGURE 6.20. Molar concentration distribution after injection for 10 days. Left: alkane; Middle: nitrogen; Right: carbon dioxide.

convergent and the molar concentration of each component is positivity-preserving. The appealing feature of the new scheme that guarantees the mass conservation of all components is well verified by the numerical results. For the multicomponent compressible flow in fractured porous media, we will further consider the fully mass-conservative scheme in our future work.

FIGURE 6.21. Molar concentration distribution after injection for 20 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.22. Molar concentration distribution after injection for 20 days. Left: butane; Middle: pentane; Right: hexane.

FIGURE 6.23. Molar concentration distribution after injection for 20 days. Left: heptane; Middle: octane; Right: nonane.

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FIGURE 6.24. Molar concentration distribution after injection for 20 days. Left: alkane; Middle: nitrogen; Right: carbon dioxide.

FIGURE 6.25. Molar concentration distribution after injection for 30 days. Left: methane; Middle: ethane; Right: propane.

FIGURE 6.26. Molar concentration distribution after injection for 30 days. Left: butane; Middle: pentane; Right: hexane.

APPENDIX. PENG-ROBINSON EOS

Since the Peng-Robinson EOS was developed in 1976 [24], it has become the most popular EOS for natural gas systems in the petroleum industry. For a multicomponent fluid system comprised of M components in a container of invariant volume occupying a domain $\Omega \subset \mathbb{R}^d$. The Peng-Robinson EOS can be written as

FIGURE 6.27. Molar concentration distribution after injection for 30 days. Left: heptane; Middle: octane; Right: nonane.

FIGURE 6.28. Molar concentration distribution after injection for 30 days. Left: alkane; Middle: nitrogen; Right: carbon dioxide.

follows:

$$(A.1) \quad p = \frac{nRT}{1 - bn} - \frac{a(T)n^2}{1 + 2bn - b^2n^2},$$

where R is the gas constant, T the temperature, $n = \sum_{i=1}^M n_i$ the total molar concentration, and $n_i = c_i$ the molar concentration of component i . For pure component, the parameters $a = a(T)$ and b are given by

$$a = a(T) = 0.45724 \frac{R^2 T_c^2}{P_c} \left(1 + m \left(1 - \sqrt{T_r} \right) \right)^2, \quad b = 0.07780 \frac{RT_c}{P_c},$$

where T_c and P_c are the critical temperature and critical pressure respectively, T_r is the reduced temperature defined as T/T_c , and the parameter m is a fitting formula of the acentric factor ω of the substance:

$$m = \begin{cases} 0.37464 + 1.5422\omega - 0.26992\omega^2, & \omega \leq 0.49, \\ 0.379462 + 1.485030\omega - 0.164423\omega^2 + 0.016666\omega^3, & \omega > 0.49. \end{cases}$$

The acentric factor can be calculated by the critical pressure P_c , critical temperature T_c , and the normal boiling point temperature T_b in the following formula:

$$\omega = \frac{3}{7} \left(\frac{\log_{10} \left(\frac{P_c}{1 \text{ atm}} \right)}{\frac{T_c}{T_b} - 1} \right) - 1.$$

For mixtures, the two parameters a and b are given by the mixing rules associating with the pure component in the fluids:

$$a = \sum_{i=1}^M \sum_{j=1}^M x_i x_j (a_i a_j)^{\frac{1}{2}} (1 - k_{ij}) = \sum_{i=1}^M \sum_{j=1}^M \frac{n_i}{n} \frac{n_j}{n} (a_i a_j)^{\frac{1}{2}} (1 - k_{ij}),$$

$$b = \sum_{i=1}^M x_i b_i = \sum_{i=1}^M \frac{n_i}{n} b_i,$$

where a_i and b_i stand for the pure-component Peng-Robinson parameters and x_i is mole ratio of component i defined by $x_i = \frac{n_i}{n}$. Here k_{ij} is the binary interaction coefficient of Peng-Robinson EOS, and it is given by experimental correlation and is frequently assumed to be constant for a given binary.

Moreover, we can rewrite the Peng-Robinson EOS as follows:

$$p = \frac{nRT}{1 - bn} - \frac{a(T)n^2}{1 + 2bn - b^2n^2} = \frac{nRT}{1 - \sum_{i=1}^M b_i n_i} - \frac{\sum_{i=1}^M \sum_{j=1}^M (a_i a_j)^{\frac{1}{2}} (1 - k_{ij}) n_i n_j}{1 + 2 \sum_{i=1}^M b_i n_i - \left(\sum_{i=1}^M b_i n_i \right)^2}.$$

Clearly, we can directly have

$$(A.2) \quad \frac{\partial p}{\partial n_i} = \frac{RT}{1 - \sum_{k=1}^M b_k n_k} + \frac{RT b_i n}{\left(1 - \sum_{k=1}^M b_k n_k \right)^2}$$

$$- \frac{2 \sum_{k=1}^M (a_i a_k)^{\frac{1}{2}} (1 - k_{ik}) n_k \left(1 + 2 \sum_{k=1}^M b_k n_k - \left(\sum_{k=1}^M b_k n_k \right)^2 \right)}{\left(1 + 2 \sum_{k=1}^M b_k n_k - \left(\sum_{k=1}^M b_k n_k \right)^2 \right)^2}$$

$$+ \frac{2 b_i \left(1 - \sum_{k=1}^M b_k n_k \right) \sum_{j=1}^M \sum_{k=1}^M (a_j a_k)^{\frac{1}{2}} (1 - k_{jk}) n_j n_k}{\left(1 + 2 \sum_{k=1}^M b_k n_k - \left(\sum_{k=1}^M b_k n_k \right)^2 \right)^2}$$

$$= \frac{RT}{1 - \sum_{k=1}^M b_k n_k} + \frac{RT b_i n}{\left(1 - \sum_{k=1}^M b_k n_k \right)^2} - \frac{2 \sum_{k=1}^M (a_i a_k)^{\frac{1}{2}} (1 - k_{ik}) n_k}{1 + 2 \sum_{k=1}^M b_k n_k - \left(\sum_{k=1}^M b_k n_k \right)^2}$$

$$+ \frac{2 b_i \left(1 - \sum_{k=1}^M b_k n_k \right) \sum_{j=1}^M \sum_{k=1}^M (a_j a_k)^{\frac{1}{2}} (1 - k_{jk}) n_j n_k}{\left(1 + 2 \sum_{k=1}^M b_k n_k - \left(\sum_{k=1}^M b_k n_k \right)^2 \right)^2}.$$

The above equality for $\frac{\partial p}{\partial n_i}$ is utilized in our proposed algorithm as an initial guess of β_i^{n+1} .

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