

The Single-Cell Transport Problem for Two-Phase Flow with Polymer

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Abstract Polymer injection is a widespread strategy in enhanced oil recovery. Polymer increases the water viscosity and creates a more favorable mobility ratio between the injected water and the displaced oil. The computational cost of simulating polymer injection can be significantly reduced if one splits the governing system of two-phase equations into a pressure equation and a set of saturation/component equations and use a Gauss–Seidel algorithm with optimal cell ordering to solve the nonlinear systems arising from an implicit discretization of the saturation/component equations. This approach relies on a robust single-cell solver that computes the saturation and polymer concentration of a cell, given the total flux and the saturation and polymer concentration of the neighboring cells. In this paper, we consider a relatively comprehensive polymer model used in an industry-standard simulator, and show that, in the case of a discretization using a two-point flux approximation, the single-cell problem always admits a solution that is also unique.

1 Introduction

In reservoirs with highly viscous oil, fingering effects lead to water penetrating easily the most permeable parts of the reservoir. To avoid a situation in which early water breakthrough leaves large fractions of the reservoir unswept, polymer is used to increase the water viscosity and establish a more favorable mobility ratio between the two phases. In this paper, we consider a two-phase flow problem with a polymer component. Polymer is miscible in water, but in realistic reservoir models the coarseness of the grid does not allow for a detailed computation of the mixing zone. Instead, we have to resort to averaging models (see [1, 6]) and consider the Todd–Longstaff mixing model [12], which is commonly used in commercial simulators. We also include the effects of permeability reduction and polymer adsorption in the model.

The governing equations are the mass-conservation equations for water, oil, and polymer. Fully-implicit solvers are usually preferred for their robustness, but are computationally expensive since one needs to solve a large, coupled system of nonlinear equations. To reduce the computational cost, the equations can be split into a pressure equation and two transport equations, one for water saturation and the other for polymer concentration. The pressure and transport equations are then solved sequentially. In the transport step, one can in certain cases reorder the cells following the direction of the flow, so that the system of discrete transport equations takes a triangular form and can be solved iteratively cell-by-cell in a very efficient and robust manner; see [11] for the two-phase case without polymer. In particular, in the absence of gravity and when using a two-point flux-approximation scheme to discretize the pressure equation, such an ordering can be obtained by sorting the cell pressures in descending order, from injection to production wells. This property can also be utilized in the presence of gravity if one splits the transport equation into a Darcy component, which can be ordered into a triangular system, and a gravity component, in which cells are only coupled in the vertical direction. Such a splitting is particularly attractive for heavy-oil reservoirs, where the effect of gravity segregation is weak because of small density differences between injected water and the heavy oil.

In the general case, the system of discrete transport equations can be permuted to a block-triangular form, in which each block contains a set of cells that are made interdependent by the orientation of the flux. When setting up such a permutation, we try to minimize the size of the blocks. In the case when the cells can be completely reordered, each block will contain only one cell. Once the ordering of blocks has been computed, we can use a nonlinear Gauss–Seidel algorithm to solve the transport equations on each block, see [10] for a detailed description of the algorithm in this context. In the case of a two-phase flow problem without polymer, it is shown in [7] that a nonlinear Gauss–Seidel algorithm for the transport equation is globally convergent, that is, converges from any given starting point. They prove the convergence of the nonlinear Gauss–Seidel algorithm using monotonicity arguments. Monotonicity arguments can do an excellent job for scalar equations, but are usually difficult to adapt to systems, as we have herein with two unknowns, the saturation and the polymer concentration. In this paper, we do not formally prove convergence of the nonlinear Gauss–Seidel algorithm. Instead we give a compelling argument for its utility by proving that each of the nonlinear sub-problems that are required in the algorithm admits a unique solution. This, to back up the numerical experiments in [10], which show the good scalability properties and computational efficiency of this method.

The single-cell problem consists of computing the saturation and concentration in a given cell, knowing the total flux in and out of neighboring cells as well as the saturation and concentration values in these cells. The total flux is obtained by solving the pressure equation in the pressure step. Mathematically, the single-cell equations are a set of two nonlinear equations whose particular form depends on the time step, the local cell geometry, the fluid and rock properties, the saturation and concentration values of the neighboring cells, and the total flux across the cell faces. The main achievement in this paper is to show that the single-cell problem is always well-posed for any time-step length. By well-posed, we mean that there exists a solution and that this solution is unique. For the Darcy component of the transport equation, we extend the results obtained in [10] with equal fluid com-

compressibilities to the case with different compressibilities, assuming that one of the two phases is always more compressible than the other. This assumption is not too restrictive as oil is typically always more compressible than water. Our result relies on some properties of the pressure equation, which have to be chosen with care. For the gravity component, we use a standard phase upstreaming for saturation, whereas for the polymer concentration it turns out that phase upstreaming is not appropriate and we present a numerical flux that guarantees well-posedness.

2 Mathematical Model for Polymer Flooding

Our starting point is the mass-conservation equations for oil, water, and polymer

$$\frac{\partial}{\partial t}(\rho_\alpha \phi S_\alpha) + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha) = 0, \quad \alpha \in \{w, o\}, \quad (1)$$

$$\frac{\partial}{\partial t}(\rho_w \phi S_w c) + \nabla \cdot (c \rho_w \mathbf{v}_{wp}) = 0. \quad (2)$$

Here, ρ_α , \mathbf{v}_α , and S_α denote the density, flux, and saturation of the phase α . The porosity is denoted by ϕ and is assumed to be a function $\phi(p)$ of pressure only, c is the polymer concentration, and \mathbf{v}_{wp} is the velocity of water containing diluted polymer. Fluid sources and sinks may be included in a manner equivalent to boundary conditions, and are left out of the above equations. The capillary pressure $p_c(S) = p_o - p_w$ is a decreasing function of the water saturation S (subscript w is dropped henceforth). To model the viscosity change of the mixture, we use the Todd–Longstaff model [12]. This model introduces a mixing parameter $\omega \in [0, 1]$ that takes into account the degree of mixing of polymer into water. The viscosity μ_m of a fully mixed polymer solution is a given function of the concentration. The effective polymer viscosity is defined as

$$\mu_{p,\text{eff}} = \mu_m(c)^\omega \mu_p^{1-\omega} \quad \text{with} \quad \mu_p = \mu_m(c_{\max}), \quad (3)$$

where c_{\max} is the polymer concentration of a saturated solution. The viscosity of the partially mixed water is given in a similar way by

$$\mu_{w,e} = \mu_m(c)^\omega \mu_w^{1-\omega}. \quad (4)$$

The effective water viscosity $\mu_{w,\text{eff}}$ is defined by interpolating linearly between the inverse of the effective polymer viscosity and the partially mixed water viscosity

$$\frac{1}{\mu_{w,\text{eff}}} = \frac{1 - c/c_{\max}}{\mu_{w,e}} + \frac{c/c_{\max}}{\mu_{p,\text{eff}}}. \quad (5)$$

For the polymer flux term \mathbf{v}_{wp} , the relative permeability is assumed to be equal to the relative permeability of water, k_{rw} , and the viscosity is equal to $\mu_{p,\text{eff}}$. Darcy's law, written in terms of the oil pressure p , then gives us

$$\mathbf{v}_w = -\frac{k_{rw}}{\mu_{w,\text{eff}} R_k(c^a)} \mathbf{K}(\nabla p - \nabla p_c - \rho_w g \nabla z), \quad (6)$$

$$\mathbf{v}_{wp} = -\frac{k_{rw}}{\mu_{p,\text{eff}} R_k(c^a)} \mathbf{K}(\nabla p - \nabla p_c - \rho_w g \nabla z) = m(c) \mathbf{v}_w, \quad (7)$$

as we assume that the presence of polymer does not affect the pressure and the density. The polymer mobility factor $m(c)$ that enters (7) is defined as

$$m(c) = \frac{\mu_{w,\text{eff}}}{\mu_{p,\text{eff}}}$$

and, after some simplifications, we get

$$m(c) = \left[\left(1 - \frac{c}{c_{\text{max}}}\right) \left(\frac{\mu_p}{\mu_w}\right)^{1-\omega} + \frac{c}{c_{\text{max}}} \right]^{-1}. \quad (8)$$

Since we assume that the polymer viscosity is larger than the water viscosity, i.e., $\mu_w \leq \mu_p$, we have $m \leq 1$ for all $c \in [0, c_{\text{max}}]$. The function $R_k(c^a)$ denotes the actual resistance factor and is a non-decreasing function that models the reduction of the permeability of the rock to the water phase due to the presence of adsorbed polymer. The concentration of adsorbed polymer is denoted by c^a . We introduce the total flux as $\mathbf{v} = \mathbf{v}_w + \mathbf{v}_o$. We have

$$\mathbf{v} = -(\lambda_w + \lambda_o)\mathbf{K}\nabla p + \lambda_w\mathbf{K}\nabla p_c + g(\lambda_w\rho_w + \lambda_o\rho_o)\mathbf{K}\nabla z$$

and after some computation, we obtain the following expression for the phase velocities \mathbf{v}_α as functions of the total velocity \mathbf{v}

$$\mathbf{v}_w = f_w\mathbf{v} + \mathbf{v}_{\text{cap}} + \mathbf{v}_g \quad \text{and} \quad \mathbf{v}_o = f_o\mathbf{v} - \mathbf{v}_{\text{cap}} - \mathbf{v}_g \quad (9)$$

with

$$f_\alpha = \frac{\lambda_\alpha}{\lambda_w + \lambda_o}, \quad \mathbf{v}_{\text{cap}} = \frac{\lambda_w\lambda_o}{\lambda_w + \lambda_o}\mathbf{K}\nabla p_c, \quad (10)$$

and

$$\mathbf{v}_g = \frac{\lambda_w\lambda_o}{\lambda_w + \lambda_o}(\rho_w - \rho_o)g\mathbf{K}\nabla z. \quad (11)$$

Here, λ_α denotes the mobility of phase α , i.e.,

$$\lambda_w = \frac{k_{rw}}{\mu_{w,\text{eff}}R_k(c^a)} \quad \text{and} \quad \lambda_o = \frac{k_{ro}}{\mu_o}.$$

The timescale of adsorption is much smaller than that of mass transport. Thus, we assume that adsorption takes place instantaneously so that c^a is a function of c only. Let $\rho_{r,\text{ref}}$ denote the reference rock density and ϕ_{ref} the reference porosity. The adsorption of polymer is then taken into account by replacing (2) by

$$\frac{\partial}{\partial t}(\rho_w\phi S_w c) + \frac{\partial}{\partial t}(\rho_{r,\text{ref}}(1 - \phi_{\text{ref}})c^a) + \nabla \cdot (c\rho_w\mathbf{v}_{wp}) = 0. \quad (12)$$

It is natural to assume that c^a is an increasing function of c . Finally the modeling equations are

$$\frac{\partial}{\partial t}(\rho_\alpha\phi S_\alpha) + \nabla \cdot (\rho_\alpha\mathbf{v}_\alpha) = 0, \quad \alpha \in \{w, o\} \quad (13a)$$

$$\frac{\partial}{\partial t}(\rho_w\phi S_w c) + \frac{\partial}{\partial t}(\rho_{r,\text{ref}}(1 - \phi_{\text{ref}})c^a) + \nabla \cdot (c\rho_w\mathbf{v}_{wp}) = 0. \quad (13b)$$

where \mathbf{v}_α and \mathbf{v}_{wp} are defined in (6) and (7) using (3), (4), and (5).

3 Discretization and Splitting of the Equations

Simple PVT behavior is modeled through the formation-volume factors $b_\alpha = b_\alpha(p)$, defined by $\rho_\alpha = b_\alpha \rho_\alpha^S$, where ρ_α^S is the surface density of phase $\alpha \in \{w, o\}$. Inserting this into (13), the system can be simplified by dividing each equation with the appropriate surface density ρ_α^S ,

$$\frac{\partial}{\partial t}(b_\alpha \phi S_\alpha) + \nabla \cdot (b_\alpha \mathbf{v}_\alpha) = 0, \quad (14a)$$

$$\frac{\partial}{\partial t}(b_w \phi S_w c) + \frac{\partial}{\partial t}((1 - \phi_{\text{ref}}) \hat{c}^a) + \nabla \cdot (b_w c \mathbf{v}_{wp}) = 0, \quad (14b)$$

where we for convenience have introduced the short-hand $\hat{c}^a = c^a \rho_{r,\text{ref}} / \rho_w^S$. To discretize (14), we introduce a grid consisting of cells C_i with a bulk volume V_i , integrate over each cell in space, and apply a standard implicit method for the temporal derivative. This gives the following residual equations

$$0 = (b_{\alpha,i} \phi_i S_{\alpha,i})^{n+1} - (b_{\alpha,i} \phi_i S_{\alpha,i})^n + \frac{\Delta t}{V_i} \sum_j (b_{\alpha,ij} v_{\alpha,ij})^{n+1} = R_{\alpha,i}, \quad (15a)$$

for $\alpha \in \{w, o\}$ and

$$0 = \left(b_{w,i} \phi_i S_{w,i} c_i + (1 - \phi_{\text{ref},i}) \hat{c}_i^a \right)^{n+1} - \left(b_{w,i} \phi_i S_{w,i} c_i + (1 - \phi_{\text{ref},i}) \hat{c}_i^a \right)^n + \frac{\Delta t}{V_i} \sum_j (b_{w,ij} c_{ij} v_{wp,ij})^{n+1} = R_{c,i}. \quad (15b)$$

Here, subscripts i denote quantities associated with the cell C_i and subscripts ij denote quantities associated with the interface between the cells C_i and C_j . Superscripts denote time steps. To derive a discrete pressure equation, we sum the two phase equations (15a), using (9) and the condition $S_w + S_o = 1$ to obtain the pressure residual equation

$$0 = \phi_i^{n+1} - \phi_i^n \sum_{\alpha \in \{w, o\}} \left(\frac{b_{\alpha,i}^n}{b_{\alpha,i}^{n+1}} S_{\alpha,i}^n \right) + \frac{\Delta t}{V_i} \sum_j \sum_{\alpha \in \{w, o\}} \frac{b_{\alpha,ij}^{n+1}}{b_{\alpha,ij}^{n+1}} (f_{\alpha,ij}^n v_{ij}^{n+1} + g_{\alpha,ij}^n + \pi_{\alpha,ij}^n) = R_{p,i}. \quad (16)$$

Here, v_{ij} is a discretization of the total flux. We use a two-point flux approximation to obtain a relation of the form

$$v_{ij} = -T_{ij}(p_j - p_i) + g_{ij} + \pi_{ij}. \quad (17)$$

The transmissibility T_{ij} depends on saturation and concentration, g_{ij} is a discretization of the gravity term $\int_{C_i \cap C_j} g(\lambda_w \rho_w + \lambda_o \rho_o) \mathbf{K} \nabla z \cdot \mathbf{n} dA$, and π_{ij} is a discretization of the capillary term $\int_{C_i \cap C_j} \lambda_w \mathbf{K} \nabla p_c \cdot \mathbf{n} dA$. The exact forms of g_{ij} and π_{ij} do not matter for the results that are presented here as long as $g_{ij} = -g_{ji}$ and $\pi_{ij} = -\pi_{ji}$ to ensure mass conservation. Similarly, we require that $T_{ij} = T_{ji}$ for conservative reasons. The terms $g_{w,ij}$ and $g_{o,ij}$ correspond to discretizations of

$\int_{C_i \cap C_j} \mathbf{v}_g \cdot \mathbf{n} dA$ and they therefore depend on saturation and polymer concentration. For conservation reasons, we require that $g_{w,ij} = -g_{w,ji}$. We also impose that $g_{o,ij} = -g_{w,ij}$, which is the only property that is required for $g_{\alpha,ij}$ in Section 4. The terms $\pi_{w,ij}$ and $\pi_{o,ij}$ correspond to discretizations of $\int_{C_i \cap C_j} \mathbf{v}_{\text{cap}} \cdot \mathbf{n} dA$. Similarly, we require $\pi_{w,ij} = -\pi_{w,ji}$ and $\pi_{o,ij} = -\pi_{w,ji}$. When solving the pressure equation, the terms T_{ij} , $f_{\alpha,ij}$, g_{ij} , $g_{\alpha,ij}$, π_{ij} , and $\pi_{\alpha,ij}$ are evaluated using the saturation and concentration values of the previous step.

Our overall system consist of the pressure equation (16) and two transport equations: Equation (15a) with $\alpha = w$ for the water saturation and equation (15b) for the polymer concentration. To solve this coupled system, we use a standard sequential procedure in which the pressure and transport equations are solved in consecutive steps. We also split the transport equations (15) into a Darcy component and a component for the segregation and capillary pressure effects. The Darcy step consists of solving a discrete transport equation for the water phase

$$(b_{w,i}\phi_i S_{w,i}^*)^{n+1} - (b_{w,i}\phi_i S_{w,i})^n + \frac{\Delta t}{V_i} \sum_j (b_{w,ij} f_w v_{ij})^{n+1} = 0, \quad (18)$$

and a corresponding residual equation for the polymer (see (24)) to obtain saturation and concentration values $S_i^{*,n+1}$ and $c_i^{*,n+1}$. These intermediate values are then used in the segregation/capillary pressure step given by the water equation

$$(b_{w,i}\phi_i (S_{w,i} - S_{w,i}^*))^{n+1} + \frac{\Delta t}{V_i} \sum_j (b_{w,ij} (g_{w,ij} + \pi_{w,ij}))^{n+1} = 0, \quad (19)$$

and a similar residual equation for polymer (see (39)) to update S_w^{n+1} and c^{n+1} . Even though the terms $g_{\alpha,ij}$ and $\pi_{\alpha,ij}$ in (16) and (19) share the same notations, they are not the same. In particular, $g_{w,ij}$ and $\pi_{w,ij}$ in (19) depend on saturations and polymer concentrations at step $n+1$ so that (19) is indeed an implicit equation. The notations should not be confused and the definitions of $g_{w,ij}$ and $\pi_{w,ij}$ for equation (19) are given in Section 5, see (50), and (51). In the two following sections, we show that the single-cell problems for the Darcy component (18) and for the gravity/capillary component (19) are well-posed.

4 The Darcy Component

Henceforth, we will follow the convention that when a time superscript is omitted, the corresponding term is evaluated at the time step $n+1$ (for example p_i and ϕ_i stand for p_i^{n+1} and $\phi(p_i^{n+1})$, respectively). Also, S without the phase subscript will mean S_w , the water saturation. To decouple the pressure and transport equation, all properties that depend on S and c in (16) are evaluated using saturation and concentration taken at the previous time step n . With v_{ij} given by (17) and using an upstream evaluation of the fractional flow f_α , the pressure equation can be

rewritten as

$$\begin{aligned}
R_{p,i} = & \phi_i - \phi_i^n \sum_{\alpha \in \{w,o\}} \left(\frac{b_{\alpha,i}^n}{b_{\alpha,i}} S_{\alpha,i}^n \right) \\
& + \frac{\Delta t}{V_i} \sum_{\alpha \in \{w,o\}} \sum_{\{j|v_{ij}<0\}} \left(f_{\alpha}(S_j^n, c_j^n) \frac{b_{\alpha,ij}}{b_{\alpha,i}} v_{ij} \right) \\
& + \frac{\Delta t}{V_i} \sum_{\alpha \in \{w,o\}} \left(f_{\alpha}(S_i^n, c_i^n) \sum_{\{j|v_{ij}>0\}} \left(\frac{b_{\alpha,ij}}{b_{\alpha,i}} v_{ij} \right) \right) \\
& + \frac{\Delta t}{V_i} \sum_j (g_{o,ij} + \pi_{o,ij})^n \left(\frac{b_{o,ij}}{b_{o,i}} - \frac{b_{w,ij}}{b_{w,i}} \right) = 0. \tag{20}
\end{aligned}$$

Here, the values of the surface volume factors have to be evaluated at the interface. To do so, we could consider an approximation of the interface pressure, denoted p_{ij} , and set $b_{\alpha,ij} = b_{\alpha}(p_{ij})$. However, to be able to prove uniform stability of the Darcy component, we have to use a type of upwinding for the evaluation of $b_{\alpha,ij}$. That is, for $v_{ij} < 0$ we set

$$b_{\alpha,ij} = \begin{cases} b_{\alpha}(p_i), & \text{if } (f_o(S_i^n, c_i^n)v_{ij} + g_{o,ij}^n + \pi_{o,ij}^n)(p_i - p_j) \leq 0, \\ b_{\alpha}(p_j), & \text{if } (f_o(S_i^n, c_i^n)v_{ij} + g_{o,ij}^n + \pi_{o,ij}^n)(p_i - p_j) \geq 0, \end{cases} \tag{21a}$$

and similarly for $v_{ij} > 0$

$$b_{\alpha,ij} = \begin{cases} b_{\alpha}(p_i), & \text{if } (f_o(S_j^n, c_j^n)v_{ij} + g_{o,ij}^n + \pi_{o,ij}^n)(p_i - p_j) \leq 0, \\ b_{\alpha}(p_j), & \text{if } (f_o(S_j^n, c_j^n)v_{ij} + g_{o,ij}^n + \pi_{o,ij}^n)(p_i - p_j) \geq 0. \end{cases} \tag{21b}$$

Because $v_{ij} = -v_{ji}$, $g_{ij} = -g_{ji}$, and $\pi_{ij} = -\pi_{ji}$, one can check that $b_{\alpha,ij} = b_{\alpha,ji}$, a condition that is required for the scheme to be conservative. Note that $f_o v_{ij} + g_{o,ij} + \pi_{o,ij}$ is an approximation of the oil flux $\mathbf{v}_o \cdot \mathbf{n}$ so that, assuming that oil is always the most compressible phase, condition (21) can be rephrased as follows: If the flux of the most compressible phase is in the same direction as the inverse pressure gradient and the total flux, then we evaluate the densities by taking the pressure value downwind; otherwise, we use the upwind value. The motivation for definition (21) will appear in the proof. The definition of v_{ij} has been introduced (17) and is of the form

$$v_{ij} = -T_{ij}(S_i^n, c_i^n, S_j^n, c_j^n)(p_j - p_i) + g_{ij}(S_i^n, c_i^n, S_j^n, c_j^n) + \pi_{ij}(S_i^n, c_i^n, S_j^n, c_j^n). \tag{22}$$

The transmissibility coefficients T_{ij} are computed using harmonic means of the permeabilities weighted with the mobilities. Since the particular definition of T_{ij} is standard and has no incidence in the results that are presented, we do not detail it here. For the same reasons, we do not give explicit expressions for the discretization of the terms g_{ij} and π_{ij} . Once p_i and v_{ij} are obtained by solving (20), (21), and (22), we can proceed with the transport step. The Darcy component for the water residual equation is

$$\begin{aligned}
R_{w,i}(S, c) = & (b_{w,i}\phi_i S_i) - (b_{w,i}\phi_i S_i)^n \\
& + \frac{\Delta t}{V_i} \sum_{\{j|v_{ij}<0\}} (f_w(S_j, c_j)b_{w,ij}v_{ij}) + \frac{\Delta t}{V_i} f_w(S_i, c_i) \sum_{\{j|v_{ij}>0\}} (b_{w,ij}v_{ij}) = 0, \tag{23}
\end{aligned}$$

while, for the polymer residual equation, it is given by

$$\begin{aligned} R_{c,i}(S, c) = & \left[b_{w,i} \phi_i S_i c_i + \hat{c}^a(c_i)(1 - \phi_{\text{ref},i}) \right] - \left[b_{w,i} \phi_i S_i c_i + \hat{c}^a(c_i)(1 - \phi_{\text{ref},i}) \right]^n \\ & + \frac{\Delta t}{V_i} \sum_{\{j|v_{ij}<0\}} (m(c_j)c_j f_w(S_j, c_j) b_{w,ij} v_{ij}) \\ & + (m(c_i)c_i f_w(S_i, c_i)) \frac{\Delta t}{V_i} \sum_{\{j|v_{ij}>0\}} (b_{w,ij} v_{ij}) = 0. \end{aligned} \quad (24)$$

Note that the polymer concentrations are also evaluated upstream. The single-cell problem for cell C_i now consists of solving

$$R_{w,i}(S, c) = 0 \quad \text{and} \quad R_{c,i}(S, c) = 0, \quad (25)$$

where we by slightly abusing notation let (S, c) denote the unknown cell values (S_i, c_i) . The other values S_j , for $j \neq i$ are assumed to be known. The main result of this section is the following existence and uniqueness theorem.

Theorem 1 *Assume that oil is more compressible than water. Then, given the solutions p_i and v_{ij} to the pressure equation (20), (21), and (22), the solution to the single-cell problem (25) exists and is unique for any physical value of the other parameters and, in particular, for any time step size Δt .*

Proof We decompose the proof into two steps:

- Step 1: We prove that, for any $c \in [0, c_{\text{max}}]$, there exists a unique S , which we denote $S(c)$, such that $R_{w,i}(S(c), c) = 0$.
- Step 2: We prove that $R_{c,i}(S(c), c) = 0$ admits a unique solution $c \in [0, c_{\text{max}}]$.

The conclusion of Step 2 is equivalent to the conclusion of the theorem and therefore also concludes the proof.

Proof of Step 1: Given c , let us compute the values of the water residual at the endpoints, that is, for $S = 0$ and $S = 1$. For $S = 0$, we have

$$R_{w,i}(0, c) = -(b_{w,i} \phi_i S_i)^n + \frac{\Delta t}{V_i} \sum_{\{j|v_{ij}<0\}} (f_w(S_j, c_j) b_{w,ij} v_{ij}) \leq 0. \quad (26)$$

For $S = 1$, after using (20), we have

$$\frac{1}{b_{w,i}} R_{w,i}(1, c) = \frac{1}{b_{w,i}} R_{w,i}(1, c) - R_{p,i} = A + B + C + D,$$

where

$$\begin{aligned} A = & \left(\phi_i - \frac{b_{w,i}^n}{b_{w,i}} \phi_i^n S_{w,i}^n \right) - \left(\phi_i S_{w,i} - \frac{b_{w,i}^n}{b_{w,i}} \phi_i^n S_{w,i}^n \right) - \left(\phi_i S_{o,i} - \frac{b_{o,i}^n}{b_{o,i}} \phi_i^n S_{o,i}^n \right), \\ B = & \frac{\Delta t}{V_i} \sum_{\{v_{ij}<0\}} v_{ij} \left(f_w(S_j, c_j) \frac{b_{w,ij}}{b_{w,i}} - f_w(S_j^n, c_j^n) \frac{b_{w,ij}}{b_{w,i}} - f_o(S_j^n, c_j^n) \frac{b_{o,ij}}{b_{o,i}} \right), \\ C = & \frac{\Delta t}{V_i} \sum_{\{v_{ij}>0\}} v_{ij} \left(f_w(1, c) \frac{b_{w,ij}}{b_{w,i}} - f_w(S_i^n, c_i^n) \frac{b_{w,ij}}{b_{w,i}} - f_o(S_i^n, c_i^n) \frac{b_{o,ij}}{b_{o,i}} \right), \end{aligned}$$

and

$$D = \frac{\Delta t}{V_i} \sum_j (g_{o,ij} + \pi_{o,ij})^n \left(\frac{b_{w,ij}}{b_{w,i}} - \frac{b_{o,ij}}{b_{o,i}} \right).$$

These expressions simplify as follows. We have

$$A = \frac{b_{o,i}^n}{b_{o,i}} \phi_i^n S_{o,i}^n,$$

so that $A \geq 0$, and

$$B = \frac{\Delta t}{V_i} \sum_{\{v_{ij} < 0\}} v_{ij} \left(f_o(S_j^n, c_j^n) \left(\frac{b_{w,ij}}{b_{w,i}} - \frac{b_{o,ij}}{b_{o,i}} \right) - \frac{b_{w,ij}}{b_{w,i}} (1 - f_w(S_j, c_j)) \right),$$

$$C = \frac{\Delta t}{V_i} \sum_{\{v_{ij} > 0\}} v_{ij} f_o(S_i^n, c_i^n) \left(\frac{b_{w,ij}}{b_{w,i}} - \frac{b_{o,ij}}{b_{o,i}} \right).$$

In the case where oil and water compressibilities are equal so that $b_o = b_w$, we have $C = D = 0$ and $B \geq 0$. In the general case, a sufficient condition to ensure that $R_w(1, c) \geq 0$ is that the quantity E , defined as

$$E = \sum_{\{v_{ij} > 0\}} (f_o(S_i^n, c_i^n) v_{ij} + g_{o,ij}^n + \pi_{o,ij}^n) \left(\frac{b_{w,ij}}{b_{w,i}} - \frac{b_{o,ij}}{b_{o,i}} \right)$$

$$+ \sum_{\{v_{ij} < 0\}} (f_o(S_j^n, c_j^n) v_{ij} + g_{o,ij}^n + \pi_{o,ij}^n) \left(\frac{b_{w,ij}}{b_{w,i}} - \frac{b_{o,ij}}{b_{o,i}} \right)$$

is positive, because we have

$$B + C + D = \frac{\Delta t}{V_i} E + \frac{\Delta t}{V_i} \sum_{\{v_{ij} < 0\}} |v_{ij}| \frac{b_{w,ij}}{b_{w,i}} (1 - f_w(S_j, c_j)).$$

We assume that the water compressibility is smaller than the oil compressibility in the pressure range we are interested in, that is,

$$c_w(p) \leq c_o(p) \text{ for all } p \in [p_{\min}, p_{\max}]. \quad (27)$$

Let us prove that, for any $p_1, p_2 \in [p_{\min}, p_{\max}]$, if $p_1 \leq p_2$, then

$$\frac{b_o(p_2)}{b_o(p_1)} - \frac{b_w(p_2)}{b_w(p_1)} \geq 0. \quad (28)$$

By definition, we have $\frac{1}{b_\alpha} \frac{db_\alpha}{dp} = c_\alpha(p)$. Hence, $d(\ln(b_o)) = c_o(p) dp$. After integrating and using that $p_1 < p_2$, we obtain

$$\ln \left(\frac{b_w(p_2)}{b_w(p_1)} \right) = \int_{p_1}^{p_2} c_w(p) dp \leq \int_{p_1}^{p_2} c_o(p) dp = \ln \left(\frac{b_o(p_2)}{b_o(p_1)} \right)$$

so that (28) holds. The definition (21) of $b_{\alpha,ij}$ at the interface precisely guarantees that E remains positive in all cases. To prove that $R_w(S, c)$ admits a unique solution

in S for a given c , it remains to prove that the function $S \mapsto R_w(S, c)$ is strictly increasing. We simplify the notations and rewrite the residuals in cell C_i as

$$R_w(S, c) = \sigma_1 S + \sigma_2 f_w(S, c) - \sigma_3, \quad (29a)$$

$$R_c(S, c) = \sigma_1 S c + \sigma_4 \hat{c}^a(c) + \sigma_2 m(c) c f_w(S, c) - \sigma_5, \quad (29b)$$

where $\{\sigma_i\}_{i=1}^5$ are constants whose definition can be inferred from the definition of the residuals. These constants depend only on the values of S_j and c_j of previous time steps or other cells than C_i . Moreover, all these constants are non-negative and $\sigma_1 > 0$. We have

$$\frac{\partial R_w}{\partial S} = \sigma_1 + \sigma_2 \frac{\partial f_w}{\partial S}$$

As expected, the fractional flow is an increasing function of saturation. Indeed, we have

$$\frac{\partial f_w}{\partial S} = \left(\frac{\partial \lambda_w}{\partial S} \lambda_o - \lambda_w \frac{\partial \lambda_o}{\partial S} \right) (\lambda_w + \lambda_o)^{-2} \geq 0,$$

because $\frac{\partial \lambda_w}{\partial S} \geq 0$ and $\frac{\partial \lambda_o}{\partial S} \leq 0$. Since

$$R_w(0, c) \leq 0, \quad R_w(1, c) \geq 0 \quad \text{and} \quad \frac{\partial R_w}{\partial S} > 0,$$

there exists a unique solution $S(c)$ to $R_w(S(c), c) = 0$ for any given $c \in [0, c_{\max}]$. This concludes the proof of Step 1.

Proof of Step 2: As in Step 1, we start by checking the endpoints, which in this case are $c = 0$ and $c = c_{\max}$. We have

$$\begin{aligned} R_c(S(0), 0) &= -(b_i \phi_i S_i c_i + \hat{c}^a(c_i)(1 - \phi_{\text{ref}, i}))^n \\ &\quad + \frac{\Delta t}{V_i} \sum_{\{j|v_{ij}<0\}} (m(c_j)c_j f(S_j, c_j) b_{ij} v_{ij}), \end{aligned}$$

so that $R_c(S(0), 0) \leq 0$. For $c = c_{\max}$, using that $R_w(S(c_{\max}), c_{\max}) = 0$, we have

$$R_c(S(c_{\max}), c_{\max}) = R_c(S(c_{\max}), c_{\max}) - c_{\max} R_w(S(c_{\max}), c_{\max}) = A + B + C,$$

where

$$\begin{aligned} A &= (\hat{c}^a(c_{\max}) - \hat{c}^a(c_i^n))(1 - \phi_{\text{ref}, i}) + (c_{\max} - c_i^n) b_{w,i}^n \phi_i^n S_i^n \geq 0, \\ B &= \frac{\Delta t}{V_i} \sum_{\{j|v_{ij}<0\}} (m(c_j)c_j - c_{\max}) f_w(S_j, c_j) b_{ij} v_{ij} \\ C &= \frac{\Delta t}{V_i} (m(c_{\max})c_{\max} - c_{\max}) f_w(S(c_{\max}), c_{\max}) \sum_{\{j|v_{ij}>0\}} b_{ij} v_{ij}. \end{aligned}$$

Since $m(c_{\max}) = 1$, we have $C = 0$. The function $m(c)$ is non-decreasing because

$$\frac{d}{dc} \frac{1}{m} = \frac{1}{c_{\max}} \left(1 - \left(\frac{\mu_p}{\mu_w} \right)^{1-\omega} \right) \quad (30)$$

and $\mu_p > \mu_w$ by assumption. Hence, $m(c_j)c_j - c_{\max} \leq c_j - c_{\max} \leq 0$, so that $B \geq 0$ and it follows that $R_w(S(c_{\max}), c_{\max}) \geq 0$. Let us now prove that the function $c \mapsto R_c(S(c), c)$ is a non-decreasing function. We have

$$dR_c = \sigma_1(c dS + S dc) + \sigma_4 d\hat{c}^a + \sigma_2 f d(m(c)c) + \sigma_2 m(c)c df. \quad (31)$$

Since $S(c)$ is solution of $R_w(S(c), c) = 0$, we have

$$\sigma_1 dS + \sigma_2 df = 0 \quad (32)$$

from (29a). Plugging this result into (31), we get

$$dR_c = \sigma_1 c(1 - m(c)) dS + \sigma_1 S dc + \sigma_4 d\hat{c}^a + \sigma_2 f d(m(c)c). \quad (33)$$

From (32), we obtain that

$$(\sigma_1 + \sigma_2 \frac{\partial f}{\partial S}) dS = -\sigma_2 \frac{\partial f}{\partial c} dc,$$

which yields, by (33),

$$\begin{aligned} (\sigma_1 + \sigma_2 \frac{\partial f}{\partial S}) \frac{dR_c}{dc} &= \sigma_1^2 S + \sigma_2^2 \frac{\partial f}{\partial S} \kappa f m^2 + \sigma_4 (\sigma_1 + \sigma_2 \frac{\partial f}{\partial S}) \frac{d\hat{c}^a}{dc} \\ &\quad + \sigma_1 \sigma_2 (S \frac{\partial f}{\partial S} + f \frac{d}{dc}(mc) - c(1 - m) \frac{\partial f}{\partial c}). \end{aligned} \quad (34)$$

Let us prove that $\frac{\partial f}{\partial c} \leq 0$ so that (34) implies $\frac{dR_c}{dc} \geq 0$. Since $\lambda_w = k_{rw}/\mu_{w,\text{eff}} R_k$, we have

$$\frac{\partial f}{\partial c} = \frac{\partial \lambda_w}{\partial c} \frac{\lambda_o}{(\lambda_w + \lambda_o)^2} = -\frac{\partial}{\partial c} (\mu_{w,\text{eff}} R_k) \frac{k_{rw}}{\mu_{w,\text{eff}}^2 R_k^2} \frac{\lambda_o}{(\lambda_w + \lambda_o)^2} \leq 0. \quad (35)$$

Indeed, by assumption, $\frac{\partial R_k}{\partial c} \geq 0$ and we expect that $\frac{\partial \mu_{w,\text{eff}}}{\partial c} \geq 0$ because the effect of polymer is to increase the effective viscosity of water. Let us check this directly. Because $\mu_{w,\text{eff}} = m(c)\mu_{p,\text{eff}}$ and $\mu_{p,\text{eff}} = \mu_m(c)^\omega \mu_p^{1-\omega}$, we have

$$\frac{d}{dc} \ln(\mu_{w,\text{eff}}) = \frac{d}{dc} \ln(m) + \omega \frac{d}{dc} \ln(\mu_m).$$

Since m and, by assumption, μ_m are non-decreasing functions, we can conclude that $\mu_{w,\text{eff}}$ is non-decreasing. Thus we have

$$R_c(S(0), 0) \leq 0 \text{ and } R_c(S(c_{\max}), c_{\max}) \geq 0,$$

and there exists at least one solution c to $R_c(S(c), c) = 0$ in $[0, c_{\max}]$. If $S(c) > 0$ for this solution, then $\frac{dR_c}{dc} > 0$ because $\sigma_1 > 0$ and the solution is unique. Otherwise, if there exists a c_0 such that $S(c_0) = 0$ and $R_c(S(c_0), c_0) = 0$, then we have by (26) that $S_i^n = 0$ and $f_w(S_j, c_j) = 0$ for all j such that $v_{ij} < 0$. The polymer residual becomes

$$R_c(S, c) = \hat{c}^a(c) - \hat{c}^a(c_i^n).$$

In the absence of adsorption, this yields $R_c(S, c) = 0$ for all $c \in [0, c_{\max}]$. Thus, the solution is not unique. This property simply reflects the fact that concentration is not a well-defined quantity in the absence of water. Note that adsorption will have a stabilizing effect. Indeed, assuming that \hat{c}^a is a strictly increasing function, we recover uniqueness. This concludes the proof of Step 2.

5 The Segregation and Capillary-Pressure Component

To take the effects of gravity segregation and capillary pressure into account, we have introduced an additional operator splitting for the transport equations as described at the end of Section 3. This operator splitting method was first introduced within streamline simulation [4, 5, 2], but can also offer certain benefits for finite-volume methods, e.g., as discussed in [9]. In this section, we will first discuss the monotonicity properties in the scalar and then use this insight to formulate a suitable discretization and prove that this second segregation/capillary step is well-posed in the sense that it admits a unique solution.

5.1 Residual equations

The discrete residual equations for the segregation of water and polymer are given by

$$b_{w,i}\phi_i(S_i - S_i^*) + \frac{\Delta t}{V_i} \sum_j b_{w,ij} (g_{w,ij} + \pi_{w,ij}) = 0, \quad (36a)$$

$$\left(b_w \phi c (S - S^*) + (1 - \phi_{\text{ref}}) (c^a(c) - c^a(c^*)) \right)_i + \frac{\Delta t}{V_i} \sum_j b_{w,ij} (g_{c,ij} + \pi_{c,ij}) = 0. \quad (36b)$$

Here, the terms $g_{w,ij}$, $g_{c,ij}$, $\pi_{w,ij}$, and $\pi_{c,ij}$ that correspond to the following approximations

$$\begin{aligned} g_{w,ij} &\approx \int_{C_i \cap C_j} \mathbf{v}_g \cdot \mathbf{n} dA, & g_{c,ij} &\approx \int_{C_i \cap C_j} cm(c) \mathbf{v}_g \cdot \mathbf{n} dA, \\ \pi_{w,ij} &\approx \int_{C_i \cap C_j} \mathbf{v}_{\text{cap}} \cdot \mathbf{n} dA, & \pi_{c,ij} &\approx \int_{C_i \cap C_j} cm(c) \mathbf{v}_{\text{cap}} \cdot \mathbf{n} dA, \end{aligned}$$

respectively, remain to be defined precisely. We use a two-point flux-approximation scheme to discretize the terms $\int_{C_i \cap C_j} b_w (\rho_w - \rho_o) g \mathbf{K} \nabla z \cdot \mathbf{n} dA$ and $\int_{C_i \cap C_j} \mathbf{K} \nabla p_c \cdot \mathbf{n} dA$. For a face $C_i \cap C_j$, the flux of the gradient of a function ψ is approximated by

$$\int_{C_i \cap C_j} \mathbf{K} \nabla \psi \cdot \mathbf{n}_{ij} dA, \approx \hat{T}_{ij} (\psi_j - \psi_i),$$

where

$$\hat{T}_{ij} = \left(\frac{1}{t_{ij}} + \frac{1}{t_{ji}} \right)^{-1}. \quad (37)$$

Here, t_{ij} denotes the one-sided transmissibility coefficient of cell C_i with respect to face $C_i \cap C_j$, defined as

$$t_{ij} = \mathbf{n}_{ij} \cdot \mathbf{K} \mathbf{c}_{ij} / |\mathbf{c}_{ij}|^2,$$

where \mathbf{c}_{ij} denotes the vector from the cell centroid of C_i to the face centroid of $C_i \cap C_j$, see [8] for more details. Let us denote $T_{i,j}^g$ as

$$T_{i,j}^g = gb_{w,ij} (b_{w,ij} \rho_w^S - b_{o,ij} \rho_w^S) \hat{T}_{ij},$$

where \hat{T}_{ij} is defined by (37) and the face values of the formation-volume factors $b_{\alpha,ij}$ are given in (21). Similarly, we introduce

$$T_{i,j}^{\pi} = b_{w,ij} \hat{T}_{ij}.$$

We introduce the notation $\mathbf{u} = (S, c, z)$. The last variable z is included to make a unified presentation of the various definitions and concepts, but it is never going to be an unknown value as S or c . Then, we rewrite (36) as

$$b_{w,i} \phi_i (S_i - S_i^*) + \frac{\Delta t}{V_i} T_{ij}^g \sum_j F^g(\mathbf{u}_i, \mathbf{u}_j) + \frac{\Delta t}{V_i} T_{ij}^{\pi} \sum_j F^{\pi}(\mathbf{u}_i, \mathbf{u}_j) = 0 \quad (38)$$

and

$$b_{w,i} \phi_i (S_i c_i - S_i^* c_i^*) + (1 - \phi_{\text{ref}}) (c^a(c_i) - c^a(c_i^*)) + \frac{\Delta t}{V_i} T_{ij}^g \sum_j G^g(\mathbf{u}_i, \mathbf{u}_j) + \frac{\Delta t}{V_i} T_{ij}^{\pi} \sum_j G^{\pi}(\mathbf{u}_i, \mathbf{u}_j) = 0. \quad (39)$$

The functions $F^{\kappa}(\mathbf{u}_l, \mathbf{u}_r)$ and $G^{\kappa}(\mathbf{u}_l, \mathbf{u}_r)$, for $\kappa \in \{g, \pi\}$, will be defined below, after a short discussion of the scalar case. For the numerical flux F^g , we will use a phase-upwind mobility approximation,

$$F^g(\mathbf{u}_l, \mathbf{u}_r) = \frac{\lambda_w(S_l, c_l) \lambda_o(1 - S_r)}{\lambda_w(S_l, c_l) + \lambda_o(1 - S_r)} (z_r - z_l). \quad (40)$$

Note that the value of the polymer concentration in the mobility term λ_w is taken from the same cell as the water saturation (with value (S_l, c_l)); that is, we use upwinding from the water phase. For the numerical flux G^g , a similar phase upwinding argument would again lead us to take the value of the polymer concentration from the same cell as the water saturation, because polymer belongs to the water phase and we would consider the numerical flux

$$G^g(\mathbf{u}_l, \mathbf{u}_r) = m(c_l) c_l \frac{\lambda_w(S_l, c_l) \lambda_o(1 - S_r)}{\lambda_w(S_l, c_l) + \lambda_o(1 - S_r)} (z_r - z_l). \quad (41)$$

Unfortunately, this choice does not guarantee a well-posed scheme.

5.2 Monotonicity properties in the scalar case

Let us investigate in a scalar setting what are the requirements on the numerical flux function to obtain an unconditionally stable single-cell problem. We consider the scalar conservation law

$$u_t + f(u)_z = 0,$$

which we discretize using an implicit Euler scheme. That is, we write

$$u_i^{n+1} - u_i^n + \frac{\Delta t}{\Delta z} [F^g(u_i^{n+1}, u_{i+1}^{n+1}) - F^g(u_{i-1}^{n+1}, u_i^{n+1})] = 0,$$

where the function $F^g(u_l, u_r)$ is a discrete approximation of the flux between two cells. For compatibility reason, we require

$$F^g(u, u) = f(u).$$

The single-cell problem consists of finding the solution of $R(u) = 0$, where

$$R(u) = u - u_i^n + \frac{\Delta t}{\Delta z} [F^g(u, u_{i+1}) - F^g(u_{i-1}, u)]$$

and u_i^n , u_{i-1} , and u_{i+1} are known. Let us determine the conditions for which this scalar equation admits a unique solution for any given u_i^n , u_{i-1} , u_{i+1} and Δt . Since u_i^n is arbitrary, we must have that R is monotone. By taking Δt small, we obtain that if R is monotone, it can only be increasing. By taking Δt very large, we see that we must have $\frac{d}{du}(F(u, u_{i+1}) - F(u_{i-1}, u))$ positive. Since this must hold for any u_{i+1} and u_{i-1} , we end up with the following monotonicity conditions for F^g ,

$$\frac{\partial F^g}{\partial u_l} \geq 0 \quad \text{and} \quad \frac{\partial F^g}{\partial u_r} \leq 0. \quad (42)$$

The Engquist–Osher flux [3]

$$F^g(u_l, u_r) = \int_0^{u_l} \max(0, f'(u)) du + \int_0^{u_r} \min(0, f'(u)) du + f(0)$$

is an example of a flux function satisfying this condition. In the case of gravity segregation, it is common to use a numerical flux with phase-wise mobility upwinding,

$$F^g(S_l, S_r) = \frac{\lambda_w(S_l)\lambda_o(1 - S_r)}{\lambda_w(S_l) + \lambda_o(1 - S_r)}.$$

Since λ_w and λ_o are non-decreasing functions, we can check that this discrete flux satisfies the condition (42).

Let us now turn our attention to the capillary pressure term, which will change the nature of the transport equation from hyperbolic to parabolic. We consider a generic, nonlinear, scalar, parabolic equation of the form

$$u_t = a(u)_{xx} \quad (43)$$

where a is an increasing function. For stability reasons, it is well known that we have to use implicit schemes to discretize (43). A standard finite-difference approximation gives us

$$R^\pi(u_i^{n+1}) := u_i^{n+1} - u_i^n + \frac{\Delta t}{2\Delta x} [2a(u_i^{n+1}) - a(u_{i-1}^{n+1}) - a(u_{i+1}^{n+1})] = 0. \quad (44)$$

Then, we observe that R^π is an increasing function so that the solution to R^π is unique. Moreover, the discretization (44) implies the following maximum principle: If $u_i^{n+1} > u_i^n$ for some index i that does not correspond to a boundary cell and n , then we cannot have $u_i^{n+1} = \max_j u_j^{n+1}$. Indeed, $u_i^{n+1} = \max_j u_j^{n+1}$ and the monotonicity of a implies that $2a(u_i^{n+1}) - a(u_{i-1}^{n+1}) - a(u_{i+1}^{n+1}) \geq 0$, which is not compatible with (44) if $u_i^{n+1} > u_i^n$. Thus, the scheme enjoys good robustness properties. Our discretization of the capillary pressure term is closely related to (44), which becomes clear when we rewrite (44) in the following finite-volume form

$$u_i^{n+1} - u_i^n + \frac{\Delta t}{2\Delta x} \sum_j F^\pi(u, u_j) = 0$$

with $F^\pi(u_u, u_r) = a(u_u) - a(u_r)$ and the index j spans the values $\{i - 1, i + 1\}$.

5.3 Well-posedness of the single-cell problem

For the full polymer model, the residual $R_w(\mathbf{u})$ and $R_c(\mathbf{u})$ for water and polymer in cell C_i are given

$$R_w(\mathbf{u}) = b_{w,i}\phi_i(S - S_i^*) + \frac{\Delta t}{V_i}T_{ij}^g \sum_j F^g(\mathbf{u}, \mathbf{u}_j) + \frac{\Delta t}{V_i}T_{ij}^\pi \sum_j F^\pi(\mathbf{u}, \mathbf{u}_j) \quad (45)$$

and

$$\begin{aligned} R_c(\mathbf{u}) = & b_{w,i}\phi_i(Sc - S_i^*c_i^*) + (1 - \phi_{\text{ref}})(c^a(c) - c^a(c_i^*)) \\ & + \frac{\Delta t}{V_i}T_{ij}^g \sum_j G^g(\mathbf{u}, \mathbf{u}_j) + \frac{\Delta t}{V_i}T_{ij}^\pi \sum_j G^\pi(\mathbf{u}, \mathbf{u}_j) \end{aligned} \quad (46)$$

where the numerical fluxes are defined below. The single cell problem for the cell C_i consists of finding $\mathbf{u} = (S, c, z)$ such that

$$R_w(\mathbf{u}) = 0, \quad R_c(\mathbf{u}) = 0, \quad z = z_i.$$

For the numerical flux functions of the segregation term, we define, for $z_r > z_l$,

$$F^g(\mathbf{u}_l, \mathbf{u}_r) = \frac{\lambda_w(S_l, c_l)\lambda_o(1 - S_r)}{\lambda_w(S_l, c_l) + \lambda_o(1 - S_r)}(z_r - z_l), \quad (47a)$$

$$G^g(\mathbf{u}_l, \mathbf{u}_r) = m(c_l)c_l \frac{\lambda_w(S_l, c_r)\lambda_o(1 - S_r)}{\lambda_w(S_l, c_r) + \lambda_o(1 - S_r)}(z_r - z_l), \quad (47b)$$

$$(47c)$$

For the capillary pressure term, we define, for $S_l > S_r$,

$$F^\pi(\mathbf{u}_l, \mathbf{u}_r) = \frac{\lambda_w(S_l, c_l)\lambda_o(1 - S_r)}{\lambda_w(S_l, c_l) + \lambda_o(1 - S_r)}(p_c(S_r) - p_c(S_l)), \quad (47d)$$

$$G^\pi(\mathbf{u}_l, \mathbf{u}_r) = m(c_l)c_l \frac{\lambda_w(S_l, c_r)\lambda_o(1 - S_r)}{\lambda_w(S_l, c_r) + \lambda_o(1 - S_r)}(p_c(S_r) - p_c(S_l)). \quad (47e)$$

and we extend the definitions of F^κ and G^κ to all values of \mathbf{u}_l and \mathbf{u}_r by requiring that

$$F^\kappa(\mathbf{u}_r, \mathbf{u}_l) = -F^\kappa(\mathbf{u}_l, \mathbf{u}_r) \quad \text{and} \quad G^\kappa(\mathbf{u}_r, \mathbf{u}_l) = -G^\kappa(\mathbf{u}_l, \mathbf{u}_r), \quad (48)$$

for all \mathbf{u}_l and \mathbf{u}_r , which is a necessary condition for the method to be conservative. Note that G^κ for $\kappa \in \{g, \pi\}$ depends on both c_l and c_r . These functions have been chosen because they enjoy the following monotonicity properties

$$\frac{\partial F^\kappa}{\partial S_l} \geq 0, \quad \frac{\partial F^\kappa}{\partial c_l} \leq 0, \quad \frac{\partial G^\kappa}{\partial S_l} \geq 0, \quad \frac{\partial G^\kappa}{\partial c_l} \geq 0, \quad (49a)$$

$$\frac{\partial F^\kappa}{\partial S_r} \leq 0, \quad \frac{\partial F^\kappa}{\partial c_r} = 0 \geq 0, \quad \frac{\partial G^\kappa}{\partial S_r} \leq 0, \quad \frac{\partial G^\kappa}{\partial c_r} \leq 0 \quad (49b)$$

when $z_r > z_l$ for $\kappa = g$ and when $S_l > S_r$ for $\kappa = \pi$. The proofs of (49) follow from the chain rule and the fact that $\frac{d(mc)}{dc} \geq 0$ (as m is an increasing function, see (30)), $\frac{\partial p_c}{\partial S} < 0$ (by assumption), $\frac{\partial \lambda_w}{\partial c} \leq 0$ (see (35)), and $\frac{\partial \lambda_w}{\partial S_w} \geq 0$ and $\frac{\partial \lambda_o}{\partial S_o} \geq 0$

(by assumption). The notations that are necessary to define the terms $g_{w,ij}$, $g_{c,ij}$, $\pi_{w,ij}$ and $\pi_{c,ij}$ in (19) have now been introduced and we have

$$g_{w,ij} = \frac{T_{ij}^g}{b_{w,ij}} F^g(\mathbf{u}_i, \mathbf{u}_j), \quad g_{c,ij} = \frac{T_{ij}^g}{b_{w,ij}} G^g(\mathbf{u}_i, \mathbf{u}_j) \quad (50)$$

and

$$\pi_{w,ij} = \frac{T_{ij}^\pi}{b_{w,ij}} F^\pi(\mathbf{u}_i, \mathbf{u}_j), \quad \pi_{c,ij} = \frac{T_{ij}^\pi}{b_{w,ij}} G^\pi(\mathbf{u}_i, \mathbf{u}_j). \quad (51)$$

Our main result on well-posedness for the gravity/capillary step reads as follows:

Theorem 2 *For the numerical fluxes defined by (47) and (48), there exists a unique solution (S, c) to the single-cell problem*

$$R_w(S, c) = 0 \quad \text{and} \quad R_c(S, c) = 0,$$

for any value of the other parameters and, in particular, for any time-step size Δt .

Proof To simplify the notation, we rewrite (45) and (46) as

$$R_w(\mathbf{u}) = \alpha(S - S_i^*) + \sum_j \beta_j^g F^g(\mathbf{u}, \mathbf{u}_j) + \sum_j \beta_j^\pi F^\pi(\mathbf{u}, \mathbf{u}_j) \quad (52)$$

and

$$R_c(\mathbf{u}) = \alpha(Sc - S_i^* c_i^*) + \delta(c^a(c) - c^a(c_i^*)) \\ + \sum_j \beta_j^g G^g(\mathbf{u}, \mathbf{u}_j) + \sum_j \beta_j^\pi G^\pi(\mathbf{u}, \mathbf{u}_j). \quad (53)$$

The definitions of the constants α , β_j^k and δ follow from (45) and (46). All these constants are positive and $\alpha > 0$. We introduce the sets of indices I_+^g and I_-^g of the neighboring cells of C_i for which $z_j > z_i$ and $z_i < z_j$, respectively. Similarly, I_+^π and I_-^π denote the sets of indices of the neighboring cells of C_i for which $S_j < S_i$ and $S_j > S_i$, respectively. We can decompose the sums over neighboring cells in (52) and (53) as follows

$$\sum_j \beta_j^k F^k(\mathbf{u}, \mathbf{u}_j) = \sum_{j \in I_+^k} \beta_j^k F^k(\mathbf{u}, \mathbf{u}_j) - \sum_{j \in I_-^k} \beta_j^k F^k(\mathbf{u}_j, \mathbf{u}),$$

and

$$\sum_j \beta_j^k G^k(\mathbf{u}, \mathbf{u}_j) = \sum_{j \in I_+^k} \beta_j^k G^k(\mathbf{u}, \mathbf{u}_j) - \sum_{j \in I_-^k} \beta_j^k G^k(\mathbf{u}_j, \mathbf{u}),$$

These decompositions are convenient because, each of the F^k and G^k on the right-hand side of these expressions, are only evaluated where they take positive values and where the inequalities (49) hold. Again, we split the proof in two steps:

- Step 1: We prove that, for any $c \in [0, c_{\max}]$, there exists a unique S , which we will denote $S(c)$, such that $R_w^c(S(c), c) = 0$.
- Step 2: We prove that $R_c(S(c), c)$ admits a unique solution in $c \in [0, c_{\max}]$.

Proof of Step 1: We differentiate these expressions and obtain

$$dR_w = \left[\alpha + \sum_{\kappa=\{g,\pi\}} \left(\sum_{j \in I_+^\kappa} \beta_j^\kappa \frac{\partial F^\kappa}{\partial S_l} - \sum_{j \in I_-^\kappa} \beta_j^\kappa \frac{\partial F^\kappa}{\partial S_r} \right) \right] dS \\ + \left[\sum_{\kappa=\{g,\pi\}} \left(\sum_{j \in I_+^\kappa} \beta_j^\kappa \frac{\partial F^\kappa}{\partial c_l} - \sum_{j \in I_-^\kappa} \beta_j^\kappa \frac{\partial F^\kappa}{\partial c_r} \right) \right] dc \quad (54a)$$

and

$$dR_c = \left[\alpha c + \sum_{\kappa=\{g,\pi\}} \left(\sum_{j \in I_+^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial S_l} - \sum_{j \in I_-^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial S_r} \right) \right] dS \\ + \left[\alpha S + \delta \frac{dc^a}{dc} + \sum_{\kappa=\{g,\pi\}} \left(\sum_{j \in I_+^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial c_l} - \sum_{j \in I_-^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial c_r} \right) \right] dc. \quad (54b)$$

To simplify the notation in the previous expressions, we do not write the values at which the partial derivatives are evaluated and assume that they are evaluated at $(\mathbf{u}, \mathbf{u}_j)$ if the expression occurs in a sum over I_+^κ , and evaluated at $(\mathbf{u}_j, \mathbf{u})$ if in a sum over I_-^κ . We will follow this convention in the remainder of the section. Given $c \in [0, c_{\max}]$, for $\mathbf{u} = (0, c)$, we have

$$F^\kappa(\mathbf{u}, \mathbf{u}_j) = 0$$

so that

$$R_w(0, c) = -\alpha S_i^* - \sum_{j \in I_-^g} \beta_j^g F^g(\mathbf{u}_j, \mathbf{u}) - \sum_{j \in I_-^\pi} \beta_j^\pi F^\pi(\mathbf{u}_j, \mathbf{u}) \leq 0.$$

For $\mathbf{u} = (1, c)$, we have

$$F^\kappa(\mathbf{u}_j, \mathbf{u}) = 0$$

and it follows that

$$R_w(1, c) = \alpha(1 - S_i^*) + \sum_{j \in I_+^g} \beta_j^g F^g(\mathbf{u}, \mathbf{u}_j) + \sum_{j \in I_+^\pi} \beta_j^\pi F^\pi(\mathbf{u}, \mathbf{u}_j) \geq 0.$$

Moreover, we have

$$\frac{\partial R_w}{\partial S} = \alpha + \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_+^\kappa} \beta_j^\kappa \frac{\partial F^\kappa}{\partial S_l} - \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_-^\kappa} \beta_j^\kappa \frac{\partial F^\kappa}{\partial S_r} > 0$$

so that the function is $S \mapsto R_w(S, c)$ is strictly increasing for a given c . Therefore there exists a unique solution $S(c)$ in $[0, 1]$ to the equation $R_w(S, c) = 0$. This concludes the proof of Step 1.

Proof of Step 2: For $c = 0$, that is, $\mathbf{u} = (S(0), 0)$, we have $G^\kappa(\mathbf{u}, \mathbf{u}_j) = 0$ for all j so that

$$R_c(S(0), 0) = -\alpha S_i^* c_i^* + \delta(c^a(0) - c^a(c_i^*)) - \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_-^\kappa} \beta_j^\kappa G^\kappa(\mathbf{u}_j, \mathbf{u}) \leq 0.$$

Since $R_w(\mathbf{u}_{\max}) = 0$, for $\mathbf{u}_{\max} = (S(c_{\max}), c_{\max})$, we obtain from (53) that

$$\begin{aligned} R_c(\mathbf{u}_{\max}) &= R_c(\mathbf{u}_{\max}) - c_{\max}R_w(\mathbf{u}_{\max}) \\ &= \alpha S_i^*(c_{\max} - c_i^*) + \delta(c^a(c_{\max}) - c^a(c_i^*)) \\ &\quad + \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_+^\kappa} \beta_j^\kappa [G^\kappa(\mathbf{u}_{\max}, \mathbf{u}_j) - c_{\max}F^\kappa(\mathbf{u}_{\max}, \mathbf{u}_j)] \\ &\quad - \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_-^\kappa} \beta_j^\kappa [G^\kappa(\mathbf{u}_j, \mathbf{u}_{\max}) - c_{\max}F^\kappa(\mathbf{u}_j, \mathbf{u}_{\max})]. \end{aligned}$$

We have

$$\begin{aligned} G^g(\mathbf{u}_{\max}, \mathbf{u}_j) - c_{\max}F^g(\mathbf{u}_{\max}, \mathbf{u}_j) &= \\ c_{\max} \left(\frac{\lambda_w(S(c_{\max}), c_j)\lambda_o(1 - S_j)}{\lambda_w(S(c_{\max}), c_j) + \lambda_o(1 - S_j)} - \frac{\lambda_w(S(c_{\max}), c_{\max})\lambda_o(1 - S_j)}{\lambda_w(S(c_{\max}), c_{\max}) + \lambda_o(1 - S_j)} \right) &\geq 0 \end{aligned}$$

because the function

$$c \mapsto \frac{\lambda_w(S(c_{\max}), c)\lambda_o(1 - S_j)}{\lambda_w(S(c_{\max}), c) + \lambda_o(1 - S_j)}$$

is non-increasing as $\frac{\partial \lambda_w}{\partial c} \leq 0$. Similarly,

$$\begin{aligned} G^g(\mathbf{u}_j, \mathbf{u}_{\max}) - c_{\max}F^g(\mathbf{u}_j, \mathbf{u}_{\max}) &= \\ &= m(c_j)c_j \frac{\lambda_w(S_j, c_{\max})\lambda_o(1 - S(c_{\max}))}{\lambda_w(S_j, c_{\max}) + \lambda_o(1 - S(c_{\max}))} \\ &\quad - c_{\max} \frac{\lambda_w(S_j, c_j)\lambda_o(1 - S(c_{\max}))}{\lambda_w(S_j, c_j) + \lambda_o(1 - S(c_{\max}))} \\ &= c_{\max} \left(\frac{\lambda_w(S_j, c_{\max})\lambda_o(1 - S(c_{\max}))}{\lambda_w(S_j, c_{\max}) + \lambda_o(1 - S(c_{\max}))} \right. \\ &\quad \left. - \frac{\lambda_w(S_j, c_j)\lambda_o(1 - S(c_{\max}))}{\lambda_w(S_j, c_j) + \lambda_o(1 - S(c_{\max}))} \right) \\ &\quad + (m(c_j)c_j - c_{\max}) \frac{\lambda_w(S_j, c_{\max})\lambda_o(1 - S(c_{\max}))}{\lambda_w(S_j, c_{\max}) + \lambda_o(1 - S(c_{\max}))} \leq 0, \end{aligned}$$

because $m(c_j)c_j - c_{\max} \leq m(c_{\max})c_{\max} - c_{\max} = 0$. From the definitions, we can check that

$$\begin{aligned} G^\pi(\mathbf{u}_{\max}, \mathbf{u}_j) - c_{\max}F^\pi(\mathbf{u}_{\max}, \mathbf{u}_j) &= \\ &= \left(G^g(\mathbf{u}_{\max}, \mathbf{u}_j) - c_{\max}F^g(\mathbf{u}_{\max}, \mathbf{u}_j) \right) (p_c(S_j) - p_c(S(c_{\max}))) \end{aligned}$$

which is positive when $j \in I_+^\pi$, that is $S(c_{\max}) > S_j$, and

$$\begin{aligned} G^\pi(\mathbf{u}_j, \mathbf{u}_{\max}) - c_{\max}F^\pi(\mathbf{u}_j, \mathbf{u}_{\max}) &= \\ &= \left(G^g(\mathbf{u}_j, \mathbf{u}_{\max}) - c_{\max}F^g(\mathbf{u}_j, \mathbf{u}_{\max}) \right) (p_c(S(c_{\max})) - p_c(S_j)) \end{aligned}$$

which is negative when $j \in I_-^\pi$, that is $S(c_{\max}) < S_j$. Hence, $R_c(S(c_{\max}), c_{\max}) \geq 0$. From (54a) and (49), we have that

$$\frac{dS}{dc} \geq 0$$

so that, by (54b) and again (49), we get

$$\begin{aligned} \frac{d}{dc} R_c(S(c), c) &= \left[\alpha c + \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_+^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial S_l} - \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_-^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial S_r} \right] \frac{dS}{dc} \\ &+ \left[\alpha S + \delta \frac{dc^a}{dc} + \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_+^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial c_l} - \sum_{\kappa=\{g,\pi\}} \sum_{j \in I_-^\kappa} \beta_j^\kappa \frac{\partial G^\kappa}{\partial c_r} \right] \geq 0. \end{aligned} \quad (55)$$

Therefore the function $R_c(S(c), c)$ is non-decreasing and there exists a solution $c \in [0, c_{\max}]$. The solution (S, c) is unique if $S > 0$ because the function $R_c(S(c), c)$ is then strictly increasing at c . In the case where the equation has a solution (S, c) such that $S = 0$, the conclusion is the same as at the end of the previous section, that is, the solution is unique only if the adsorption function is strictly increasing. This concludes the proof of Step 2.

6 The Unsplit Transport Equations

In the previous section, we have seen that the well-posedness of the discrete system of transport equations for segregation and capillary pressure follows as a consequence of the monotonicity conditions (49) on the numerical fluxes. If we apply the same notations to the transport equations (23) and (24) for the Darcy component, we obtain

$$\begin{aligned} 0 &= (b_{w,i} \phi_i S) - (b_{w,i} \phi_i S_i)^n \\ &+ \frac{\Delta t}{V_i} \left[\sum_{\{j|v_{ij}>0\}} b_{w,ij} |v_{ij}| F^d(\mathbf{u}, \mathbf{u}_j) - \sum_{\{j|v_{ij}<0\}} b_{w,ij} |v_{ij}| F^d(\mathbf{u}_j, \mathbf{u}) \right] \end{aligned} \quad (56)$$

and

$$\begin{aligned} 0 &= [b_{w,i} \phi_i S c + \hat{c}^a(c)(1 - \phi_{\text{ref},i})] - [b_{w,i} \phi_i S_i c_i + \hat{c}^a(c_i)(1 - \phi_{\text{ref},i})]^n \\ &+ \frac{\Delta t}{V_i} \left[\sum_{\{j|v_{ij}>0\}} b_{w,ij} |v_{ij}| G^d(\mathbf{u}, \mathbf{u}_j) - \sum_{\{j|v_{ij}<0\}} b_{w,ij} |v_{ij}| G^d(\mathbf{u}_j, \mathbf{u}) \right], \end{aligned} \quad (57)$$

where

$$F^d(\mathbf{u}_l, \mathbf{u}_r) = \frac{\lambda_w(S_l, c_l)}{\lambda_w(S_l, c_l) + \lambda_o(1 - S_l)}, \quad (58a)$$

$$G^d(\mathbf{u}_l, \mathbf{u}_r) = c_l m(c_l) \frac{\lambda_w(S_l, c_l)}{\lambda_w(S_l, c_l) + \lambda_o(1 - S_l)}. \quad (58b)$$

We observe that the conditions (49) are not fulfilled because $\frac{\partial G^d}{\partial c_l}$ and $\frac{\partial F^d}{\partial c_l}$ do not in general have a given sign. In the case of the gravity segregation and capillary-pressure terms, we have been able to formulate fluxes that satisfy the monotonicity

conditions (49) by changing the dependence with respect to the concentration values in G^g and G^π . The same strategy can be used for the Darcy term and, after replacing c_l with c_r in the mobility terms of G^d , we obtain

$$F^d(\mathbf{u}_l, \mathbf{u}_r) = \frac{\lambda_w(S_l, c_l)}{\lambda_w(S_l, c_l) + \lambda_o(1 - S_l)}, \quad (59a)$$

$$G^d(\mathbf{u}_l, \mathbf{u}_r) = c_l m(c_l) \frac{\lambda_w(S_l, c_r)}{\lambda_w(S_l, c_r) + \lambda_o(1 - S_l)}, \quad (59b)$$

which indeed satisfy the monotonicity properties (49). However, the expressions in (59), as the ones in (47), depend on both u_l and u_r , which means in practice that the evaluation of a numerical flux at a given interface requires the cell values on both sides of the interface. This double dependence prohibits the use of any ordering scheme. In comparison, the expressions in (58) depend only on u_l and, as a result, ordering schemes can be used to significantly reduce the computation time. These considerations show that one of the major achievements in Section 4 was in fact to obtain well-posedness for numerical fluxes that do not fulfill the monotonicity conditions (49). They also provide us with the following discretization for the unsplit transport equations,

$$0 = (b_{w,i}\phi_i S) - (b_{w,i}\phi_i S_i)^n + \sum_{\kappa=\{d,g,\pi\}} \sum_{j \in I_+^\kappa} \beta_j^\kappa F^\kappa(\mathbf{u}, \mathbf{u}_j) - \sum_{\kappa=\{d,g,\pi\}} \sum_{j \in I_-^\kappa} \beta_j^\kappa F^\kappa(\mathbf{u}_j, \mathbf{u}) \quad (60a)$$

and

$$0 = [b_{w,i}\phi_i S c + \hat{c}^a(c)(1 - \phi_{\text{ref},i})] - [b_{w,i}\phi_i S_i c_i + \hat{c}^a(c_i)(1 - \phi_{\text{ref},i})]^n + \sum_{\kappa=\{d,g,\pi\}} \sum_{j \in I_+^\kappa} \beta_j^\kappa G^\kappa(\mathbf{u}, \mathbf{u}_j) - \sum_{\kappa=\{d,g,\pi\}} \sum_{j \in I_-^\kappa} \beta_j^\kappa G^\kappa(\mathbf{u}_j, \mathbf{u}), \quad (60b)$$

where F^d and G^d are given by (58). From the analysis presented in the previous sections, there are good reasons to believe that the single cell problem given by the system of equations (60) is well posed. This question deserves further investigations as the well posedness of the single cell problem is a strong indication of good robustness properties of the corresponding discretization in term of choices of numerical fluxes.

7 Concluding Remarks

A series of numerical experiments that demonstrate the efficiency and scalability of the operator-splitting, Gauss–Seidel approach for polymer flooding are reported in [10]. All experiments reported in [10] were run with the numerical flux (41), and although this flux does not theoretically guarantee a well-posed scheme, we did not encounter any convergence problems, even for quite large time steps. A topic for future research would therefore be to conduct a thorough numerical study to compare the stability and accuracy of the two fluxes, (41) and (47b).

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