Numerical modeling of a compositional flow for chemical EOR and its stability analysis

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\section*{ABSTRACT}

A new two-dimensional surfactant flooding simulator for a three-component (water, petroleum, chemical), two-phase (aqueous, oleous) system in porous media is developed and analyzed. The compositional physical model is governed by a system of non-linear partial differential equations composed of Darcy’s and mass conservation equations. The system is then numerically solved by a finite difference method using the IMPE (IMPlicit Pressure and Explicit Concentration) scheme. Physical properties are described by a set of concentration-dependent algebraic equations. Additionally, a novel numerical stability analysis is presented in order to study the robustness of the new simulator. The oil recovery factor showed a strong dependency on the surfactant properties and phase behavior, which should be carefully evaluated. In order to achieve this, the new simulator utilizes and modifies a simplified ternary diagram to model accurately the component partitioning. Results showed that surfactant partitioning is the most relevant parameter in the recovery process. Numerically speaking, the simulator behaved according to the results obtained in the matrix stability analysis. Using the non-iterative IMPEC, a critical time value was found beyond which the system yielded large oscillatory values for the produced flowrates. The simulator can be employed to design and optimize chemicals used in enhanced oil recovery (EOR) processes before field application.

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1. Introduction

Oil has been and remains the main source of energy, and the economies of many countries depend greatly on it [1–4]. After traditional exploitation techniques, up to 50% of the original oil in place (OOIP) can be recovered [3,5–7]. Additional recovery methods, known as enhanced oil recovery (EOR), then target the remaining oil still trapped [8]. The most utilized EOR techniques are [6]: thermal (combustion in-situ - continuous/cyclic steam injection); chemical (polymers, surfactants and/or caustic); miscible (CO\textsubscript{2} injection, inert gas or miscible solvent); and others (such as microbial EOR).

Surfactant flooding for enhanced oil recovery is not new, but has been used for more than 40 years [7,9–15]. Surfactants (or amphiphiles) adsorb on the oil/water interface and reduce the interfacial tension (IFT) and capillary pressure, which is responsible for the trapped oil in pores (capillary trapping) [16]. The target in designing surfactants for recovering oil processes is to achieve low interfacial tension at low surfactant concentrations, and acceptable adsorption levels on the
formation rock [17,18]. Ultra-low interfacial tensions of less than $10^{-3}$ mN/m have been reported with less than 0.1 wt.% surfactant concentration. Nevertheless, experiments carried out by Yu et al. [19] demonstrated that it is not required to achieve ultra-low IFT values to improve the oil recovery. A multicomponent and multiphase system is then present in the reservoir. Several authors have studied how to deal mathematically with this kind of flow [20–27]. This research has led to the development of simulators like UTCHEM (University of Texas at Austin), CMG (Stars) and Eclipse (Schlumberger), as well as several others that can be found in the literature [28–36].

Nevertheless, commercial simulators are usually based on complex chemical models requiring a deep knowledge of both the components involved and their interactions with the porous medium. The outcome is a complex system of non-linear differential equations which might cause numerical stability problems if all these factors are not carefully evaluated. Moreover, simulators reported in the literature [28–30] do not perform a detailed study of component partitioning and phase behavior since they are based on what we consider an insufficient number of parameters to describe the latter. Thus, the synthesis of new chemicals for EOR may be based on incorrect results. Furthermore, these simulators [31,32] were developed in one-dimensional models, restricting their application to specific cases, since they do not take into account certain effects like the areal sweeping efficiency. On the other hand, three-dimensional fields may cause the system to lose numerical efficiency due to the fact that a larger non-linear system of equations must be solved. In addition to this, the vertical permeability is usually considered negligible with respect to the horizontal permeabilities. Hence, the computational cost is increased but the results may not show a significant difference in comparison to two-dimensional models. In consequence,

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it is deemed that the development of new models that can satisfy both requirements is necessary: a detailed modeling of the chemical phase behavior to be injected in the porous medium as well as a sufficiently robust numerical model to avoid the appearance of numerical instabilities. These are the objectives of the present work. In order to fulfill this, a novel numerical simulator was developed to study the tertiary recovery in a two-dimensional oil field, taking as a starting point and expanding the work developed by Porcelli and Bidner [31]. A simplified ternary phase diagram is employed in order to determine the value of the volumetric concentration ratios necessary to solve the compositional model.

The study of the two-phase system was chosen due to the fact that these present greater difficulties when determining the component partitioning parameters. Indeed, in three-phase systems (water–oil–microemulsion), the treatment is relatively simple and most simulators use the same approach: aqueous and oleous phases are considered pure, and the composition of the microemulsion is assumed to be constant and only expressed as a function of salinity and temperature. Due to the previous factors, the simulation of three-phase systems in fields with high salinity or thermal gradients may cause numerical instability issues, rendering the numerical method ineffective. By contrast, in two-phase systems components volume concentrations respond to a more complex model. In this case the phase behavior plays an important role in the amount of recoverable oil. That is why it is considered important to study and model a two-phase system. The influence of factors that can alter the behavior of the model (e.g. salinity expressed as the concentration of monovalent or divalent cations, temperature) is taken into account when choosing the partitioning factors. After presenting the algorithm and the results of the simulation, a numerical stability analysis of the model is presented. This study allows determination of the robustness of the model and the drawing of conclusions about its applicability in EOR processes. To the best of our knowledge, this stability analysis based on the perturbation method is also a novel approach in determining the numerical conditions which guarantee convergence in this kind of simulation.

The novelty of this work resides then in the development of a new simulator for a two-dimensional oil field capable of simulating the flow of a two-phase, three-component system. The component partitioning is modeled in an accurate, but yet relatively simple and robust way, solving the problems described in previous simulators. This was done by increasing the number of parameters used to describe the chemical behavior, but avoiding the creation of a complex system of non-linear equations which would complicate the numerical solving. This will lead to a new set of optimum design parameters to be used during the synthesis of future surfactants. In addition to this, the numerical stability of the simulator was assessed using a perturbation technique which has not been previously applied in EOR systems of these characteristics.

2. Theoretical development

2.1. Model description

The physical model represents a reservoir ($\Omega$) of known geometric characteristics (Fig. 1), which has an absolute permeability ($K$) and porosity ($\phi$), both considered as constants for the purpose of the simulation. Nevertheless, the absolute permeability may be modeled also as a variable field in both directions. The domain $\Omega$ is then decomposed in a system of $n_x \times n_y$ blocks to perform the numerical simulation. The flow is considered isothermal, Newtonian, incompressible and 2-dimensional (since it is assumed that the vertical permeability is negligible when compared to horizontal ones); it is also considered that the system is in local thermodynamic (phase) equilibrium. Darcy’s law is valid and gravitational forces are negligible compared to the viscous and capillary forces [32].
Surfactant EOR flooding involves the flow of fluids in two phases (aqueous and oleous), and various components (water, chemical and petroleum). These components are, in fact, mixtures of pure components: petroleum is a mixture of many hydrocarbons, water contains dissolved salts and the chemical may be composed of surfactants, polymers, alcohols, etc. Regarding the presence of polymers in the chemical component, even though it is well reported that polymer solutions exhibit non-Newtonian viscoelastic behavior, at low concentrations and/or low molecular weights they can be considered as non-elastic Newtonian fluids [3,8,14].

The recovery process involves injecting in a first stage an aqueous solution with the surfactant followed by a water bank to drive the surfactant plug, sweeping the mobilized oil into the producing wells. The model is represented by a system of nonlinear partial differential equations: the mass conservation equation for each component, and Darcy’s equation for two-phase flow. The physical properties considered are: phase behavior (represented in a ternary diagram), interfacial tension between the phases (IFT), residual phase saturations, relative permeabilities, rock wettability, phase viscosities, capillary pressure, adsorption on the formation, and dispersion. Analyzing these properties has made it clear that the IFT depends, mathematically speaking, on the partitioning of the surfactant and therefore on the phase behavior. Chemically speaking, the presence of the surfactant at the fluid-fluid interface is the reason for the IFT reduction. Also residual saturations and relative permeabilities are affected by the phase behavior. The viscosity of each phase depends on the volumetric concentrations of each of the three components, which is also a function of phase behavior. In conclusion, the first step in the successful development of a numerical simulator for chemical flooding is to have a model that allows us to predict accurately the phase behavior and component partitioning in the reservoir [26,27,37,38].

2.2. Flow equations

The balance equations are applied on a representative element volume (REV) of the porous medium. Darcy’s equation for each phase, and mass conservation equation for each component are applied [8,32,39]. Considering Darcy’s equation first:

$$\vec{u}^j = -K \frac{k_i^j}{\mu_j} \cdot \nabla p^j; \quad j=a,o.$$

(1)

The sum of Eq. (1) for each phase renders the total Darcy velocity,

$$\vec{u} = \vec{u}^a + \vec{u}^o = -\frac{\lambda^2}{\mu^o} \cdot \nabla p^o - \frac{\lambda^a}{\mu^a} \cdot \nabla p^a,$$

(2)

where $p_c$ is the capillary pressure for the water–oil system and the j-phase total mobilities are also introduced and defined as

$$\lambda^j = \frac{\lambda}{\mu_j} \quad \text{and} \quad \lambda^j = K \frac{k_i^j}{\mu_j}; \quad j=a,o.$$

(3)

The mass conservation equation for each component is now presented considering the flux by advection and diffusion mechanisms, plus source/sinks terms, adsorption, and finally the accumulation rate within the REV. It yields:

$$\phi \cdot \frac{\partial z_i}{\partial t} + \nabla \cdot \sum_j V_i^j \cdot \vec{u}^j - \nabla \cdot \sum_j D_i^j \cdot \nabla \cdot V_i^j = -\phi \cdot \frac{\partial Ad_i}{\partial t} + q_i; \quad i=p,c,w.$$

(4)

In addition to the advective movement described by Darcy phase velocities, components may also move due to dispersive forces. The hydrodynamic dispersion tensor which takes into account these effects is expressed as [39,40]

$$D_i^j = dm_i^j \cdot \phi \cdot S_i^j \cdot \delta_{ij} + |\vec{u}^j| \cdot \left[ \frac{dt^j}{|\vec{u}^j|^2} \begin{bmatrix} (u_i^j)^2 & u_i^j \cdot u_j^j \cdot u_i^j \cdot u_j^j \cdot (u_i^j)^2 \end{bmatrix} + dt^j \cdot \begin{bmatrix} 1 - \frac{(u_i^j)^2}{|u_i^j|^2} & -u_i^j \cdot u_j^j \cdot \frac{(u_i^j)^2}{|u_i^j|^2} \\ u_i^j \cdot u_j^j \cdot \frac{(u_i^j)^2}{|u_i^j|^2} & 1 - \frac{(u_i^j)^2}{|u_i^j|^2} \end{bmatrix} \right].$$

(5)

The previous equations are completed with a set of algebraic expressions from the macroscopic balance made in the domain [40].

$$z_i = \sum_j V_i^j \cdot S_i^j,$$

(6)

$$\sum_j S_i^j = 1,$$

(7)

$$\sum_i V_i^j = 1,$$

(8)

$$\sum_i z_i = 1,$$

(9)

$$\sum_j D_i^j \cdot \nabla \cdot V_i^j = 0.$$

(10)
The first step is to obtain an equation for the pressure of one phase (oleous or aqueous) by introducing the capillary pressure. This is achieved by adding Eq. (4) for the three components and taking into account the constraints established by Eqs. (2), (7)–(10). Thus,

$$\vec{\nabla} \cdot (\lambda \cdot \nabla p^i) = \phi \cdot \frac{\partial}{\partial t} \left( \sum_i \lambda_i \right) - \vec{\nabla} \cdot (\lambda^o \cdot \nabla p_o) + q_t$$

(11)

The numerical model as it was presented has 16 unknowns, which are: Darcy velocities \((u^a, a)\), pressures \((p_e, p^o, a)\) and saturation of each phase \((S^a, a)\), volumetric \((V_{p, w, c})\) and overall concentrations \((z_p, w, c)\) of each component. However, so far we have presented 13 equations: Eq. (1) for each phase, Eqs. (2) and (4) for two components, Eq. (6) for each component, Eqs. (7) and (8) for each phase, Eqs. (9), and (11). The remaining equations, necessary for the system to be numerically determined, are obtained from the equations describing the phase behavior and component partitioning.

2.3. Physical properties

2.3.1. Chemical component partition

The numerical simulation of our model involves a two-phase, three pseudo-component system (each of these is composed by several elementary components, but they are treated as a single “pseudo-component”), which can be represented in a ternary phase diagram, where the chemical compound is located in the apex, while the water and oil occupy the lower vertices. The composition of a mixture is determined by any point inside the triangle [27,31]. As the concentration of the chemical increases oil and water become miscible, so that the triangle can be divided into two zones (in two-phase systems): upper miscible and immiscible in the bottom. The curves delimiting these regions are determined by volumetric concentration ratios which are,

Solubilization coefficient = \( L_{pc}^a = \frac{V_p^a}{V_c^a} \).

swelling coefficient = \( L_{wc}^o = \frac{V_w^o}{V_c^o} \).

partition coefficient = \( K_c = \frac{V_c^o}{V_c^o} \).

(12, 13, 14)

Depending on the value of \( K_c \), two different behaviors are observed: Larson Type II (-) (for \( K_c < 1 \)), and Larson Type II (+) systems (for \( K_c > 1 \)). These values play a major role in the EOR process. They should be correctly measured to predict recovery factors with existing surfactants, or be the cardinal values when designing new chemical products. The partition coefficient value depends on the composition of the injected chemical and the water characteristics, such as temperature and salinity. Fig. 2 shows the original and simplified ternary diagrams used for this simulation.

2.3.2. Interfacial tension

The interfacial tension of the system depends on the presence and concentration of the chemical component as well as the Larson system present in the reservoir. In this simulation a simplified IFT correlation will be used [26,31,32,37,38].

For Larson II (-) systems (oil/water emulsion):

$$\log(\sigma) = \log(F) + (1 - L_{pc}^o) \cdot \log(\sigma^H) + \frac{G_1}{1 + L_{pc}^o} \cdot L_{pc}^o; \quad L_{pc}^o < 1,$$

$$\log(\sigma) = \log(F) + \frac{G_1}{1 + L_{pc}^o}, \quad L_{pc}^o \geq 1.$$

(15)

For Larson II (+) systems (oil emulsion/water):

$$\log(\sigma) = \log(F) + (1 - L_{wc}^o) \cdot \log(\sigma^H) + \frac{G_1}{1 + L_{wc}^o} \cdot L_{wc}^o; \quad L_{wc}^o < 1,$$

$$\log(\sigma) = \log(F) + \frac{G_1}{1 + L_{wc}^o}, \quad L_{wc}^o \geq 1.$$  

(16)

where \( G_1 \) and \( G_2 \) are input parameters, and the term \( F \) is calculated according to the following equation:

$$F = \frac{1 - e^{-\sqrt{\sum_i z_i \cdot (V_{p, w, c} V_i^o - V_i^o)^2}}}{1 - e^{-\sqrt{2}}}.$$

(17)

In chemical recovery process, the presence of the surfactant causes the decrease of IFT, allowing the mobilization of oil trapped in the reservoir, so it can be inferred that the residual saturations of the phases depend on the IFT. The IFT of the water–oil system (no surfactant present) is considered constant throughout the simulation.
Fig. 2. Ternary phase diagrams for type II(−) (left) and II(+) (right) systems (top) and their simplified representations (bottom) (Adapted from [32]).
2.3.3. Residual saturation

As explained in the previous section, the residual saturations \( S_{fr} \) depend on the IFT in the system. This relationship is ruled by a dimensionless group, the capillary number, defined by:

\[
N_{ve} = \frac{u \cdot K}{\kappa \cdot \sigma}
\]  

(18)

Then, the functionality between the capillary number and the residual saturation is described by the following model [31]:

\[
\frac{S_{fr}}{S_{frH}} = \begin{cases} 
1 & \text{if } N_{ve} < 10^{(1/T_1 - T_2)} \\
T_1 \cdot [\log(N_{ve}) + T_2] & \text{if } 10^{(1/T_1 - T_2)} \leq N_{ve} \leq 10^{T_2} \\
0 & \text{if } N_{ve} > 10^{T_2}, 
\end{cases}
\]  

(19)

where \( T_1 \) and \( T_2 \) are constants based on experimental observations. The piecewise function is defined by parameters which depend on the fluids (e.g., rheology, viscoelasticity) and the porous medium under study. The relationship between the residual saturation after chemical and water flooding processes is known as normalized saturation of phase \( j \). The form of Eq. (19) for both phases determines what is known as capillary desaturation curves (Fig. 3). The plot shows that the aqueous phase requires much higher values of \( N_{ve} \) to achieve their full desaturation [8].

2.3.4. Relative permeabilities

Relative permeabilities play a major role in oil recovery processes since they directly affect Darcy phase velocities. The model used to calculate the relative permeabilities is taken from [35,36]. These are expressed as a function of the phase and residual saturations defined by Eqs. (7) and (19), respectively, and calculated according to the following formula:

\[
k_j = k_j^0 \cdot \left( \frac{S_j - S_{fr}}{1 - S_{fr} - S_{fr}} \right)^{e_j}; \quad j = o, a; \quad j' = a, o; \quad j \neq j'.
\]  

(20)

where \( k_j^0 \) and \( e_j \) represent the end point and the curvature of the function \( k_j(S_j) \), respectively. These values are calculated by the following equations:

\[
k_j^0 = k_{jH}^0 + (1 - k_{jH}^0) \cdot \left( 1 - \frac{S_j}{S_{frH}} \right); \quad j = o, a; \quad j' = a, o; \quad j \neq j'.
\]  

(21)

\[
e_j = e_{jH} + (1 - e_{jH}) \cdot \left( 1 - \frac{S_j}{S_{frH}} \right); \quad j = o, a; \quad j' = a, o; \quad j \neq j'.
\]  

(22)

where \( k_{jH}^0 \) and \( e_{jH} \) are the endpoint values of curvature and relative permeability function system for water–oil without surfactant, respectively.
2.3.5. Phase viscosities

The viscosity of each phase depends on its composition as a function of the volumetric concentration of each component, according to the following function [32,35,36]:

\[ \mu^j = V^j_w \cdot \mu^{ow} + e^{α_1(V^j_w + V^j_o)} + V^j_p \cdot \mu^{oh} \cdot e^{α_1(V^j_w + V^j_o)} + V^j_c \cdot α_3 \cdot e^{α_2(V^j_w + V^j_o)}; \quad j = 0, a, \]

where \( α_k \) are constants and \( \mu^{oh} \) and \( \mu^{ow} \) are values of viscosity in the water–oil system without surfactant, respectively.

2.3.6. Capillary pressure

The capillary pressure is defined by the difference between the non-wetting phase (oleous) and the wetting phase (aqueous). The functionality describing this parameter is the following power law equation [8,38]:

\[ p_c = C \cdot \sqrt{\frac{φ \cdot \sigma}{σ^H}} \cdot \left( \frac{1 − S^o − S^w}{1 − S^w − S^o} \right)^n, \]

where \( C \) is a constant parameter and \( n \) defines the curvature of the function. The capillary pressure parameter \( C \) relates the capillary forces in the three component system (petroleum, water and chemical) to the capillary forces in the oil–water system.

2.3.7. Adsorption

The adsorption process occurs when surfactant monomers and/or micelles form onto the surface of the formation rock. In order for these monomers to aggregate and form the micelles, the surfactant concentration must exceed the critical micelle concentration (CMC). This phenomenon will cause a loss of surfactant in the porous medium, making the whole process economically unfeasible in case of high rates of adsorption. The adsorption isotherm is rather dependent on the type of surfactant, the characteristics of the rock and the type of electrolytes present in the solution [41]. The adsorption of the surfactant by the rock used in this simulator is described by the Langmuir monolayer model [24]:

\[ Ad_i = \frac{a_1 \cdot V^j_i}{1 + a_2 \cdot V^j_i} \quad \text{if} \quad \frac{∂V^j_i}{∂t} ≥ 0 \]

\[ \frac{∂Ad_i}{∂t} = 0 \quad \text{if} \quad \frac{∂V^j_i}{∂t} < 0 \]

\[ V^j_i = \max(V^j_o, V^j_a), \]

where \( a_1 \) and \( a_2 \) are constant parameters and \( Ad_i \) is a dimensionless parameter representing the adsorbed volume of chemical component per unit of volume of the porous media. Since it was assumed the fluids are incompressible, adsorption is formulated on a volume basis. The term \( a_1 \) is a function of the salinity present in the reservoir, and \( a_2 \) is used to describe the adsorption process: when \( a_2 = 0 \) is linear adsorption, and \( a_2 \neq 0 \) represents a Langmuir adsorption process. The main difference in the latter lies in the fact that linear adsorption does not limit the amount of surfactant loss in the rock whilst, as \( a_2 \) increases, the adsorption losses are diminished.

2.4. Initial and boundary conditions

At the start of the flooding, the residual saturation and initial pressure \( (p_i) \) in the reservoir are considered to be constant throughout the domain. It is also assumed that there is no chemical present. Thus:

\[ t = 0; \quad ∀(x,y) ∈ Ω : \quad z_e = 0; \quad z_p = S^{ow}; \quad p^p = p_i, \]

A ‘no flow’ boundary condition is imposed on the contour \((Γ)\), since it is assumed that the porous medium is surrounded by an impermeable rock layer. In the case of the advective flux this condition is satisfied if the transmissibilities (or mobilities) are zero on the boundary. For the diffusive flux, Fick’s law on the contour \((Γ)\) is applied, thus yielding:

\[ \text{Injecting Well} \Rightarrow \begin{cases} 0 ≤ t ≤ t_{in} : z_e = z_{in} \\ t > t_{in} : z_{in} = z_{w}, z_e = 0. \end{cases} \]

\[ \text{Boundaries} \Rightarrow \lambda_{m,n}^j = 0 \land \frac{∂z_i}{∂n} = 0; \quad i = p, c; \quad ∀t \land ∀(m,n) ∈ Γ. \]

2.5. Nondimensionalization of the transport equations

It is important in every physical model to establish the influence and degree of dominance of the different phenomena involved. Thus, the dimensionless forms of Darcy and mass conservation equations were derived (Eqs. (29) and (30)) and expressed using the Capillary (Eq. 18) and Peclet numbers (Eq. 31). The dimensionless variables and derivatives are represented using a breve symbol \( ˘ \).

\[ \nabla \cdot \left( \left( \frac{k^p}{N_{pc}^p} + \frac{k^c}{N_{pc}^c} \right) \cdot \nabla \bar{p}^o \right) = \phi \cdot \frac{∂}{∂t} \left( \sum_j Ad_j \right) - \nabla \cdot \left( \frac{k^c}{N_{pc}^c} \cdot \nabla \bar{p}_c \right) + t_{ref} \cdot q_t. \]
\[ \phi \frac{\partial z_i}{\partial t} + \nabla \cdot \left( \sum_j V_i^j \cdot \hat{u}^j - \nabla \cdot \sum_j \frac{1}{Pe_i} \cdot \nabla V_i^j \right) = -\phi \cdot \frac{\partial Ad_i}{\partial t} + \epsilon_{\text{ref}} \cdot q_i. \]  

(30)

\[ Pe_i = \frac{l_{\text{ref}} \cdot u_{\text{ref}}}{D_i}. \]  

(31)

The Capillary number describes the relationship between viscous and capillary forces and affects the pressure equation. The objective in a surfactant flooding is to make these forces of a similar order so the trapped oil can be displaced. The Peclet number defines the relative importance of the diffusion mechanism in the transport process. With negligible diffusion coefficients the Peclet number is high \((Pe_i \gg 1)\) and then advection dominates the process. Increasing this coefficient renders lower Peclet numbers \((Pe_i \approx 1)\) or \(Pe_i < 1\) and diffusion mechanisms can no longer be neglected.

2.6. Discretization of the partial differential equations

The physical description led to a system of parabolic partial differential equations, which are discretized using a finite difference method. The pressure equation is implicitly discretized using a centered scheme, with pressures evaluated in nodes and transmissibilities in the element boundaries. Therefore, the equations (11) (neglecting capillary pressure effects), (2) and (1) are discretized as follows:

\[ \lambda_{x,m+1/2,n}^{(n+1),[k]} \cdot \left( p_{m+1/2,n}^{a} - p_{m,n}^{a} \right)^{(n+1),[k+1]} - \lambda_{x,m-1/2,n}^{(n+1),[k]} \cdot \left( p_{m-1/2,n}^{a} - p_{m,n}^{a} \right)^{(n+1),[k+1]} + \ldots + \lambda_{x,m,n}^{(n+1),[k]} \cdot \left( p_{m,n}^{a} - p_{m-1/2,n}^{a} \right)^{(n+1),[k+1]} \]

(32)

\[ u_{m,n}^{(n+1),[k+1]} = \left[ -\frac{\lambda_{x,m,n}^{(n+1),[k]}}{2} \cdot \left( p_{m+1,n}^{a} - p_{m,n}^{a} \right)^{(k+1)} - \frac{\lambda_{y,m,n}^{(n+1),[k]}}{2} \cdot \left( p_{m,n+1}^{a} - p_{m,n}^{a} \right)^{(k+1)} \right] \cdot \hat{i} \]

(33)

\[ q_{m,n}^{a,(n+1),[k+1]} = \left[ -\frac{\lambda_{x,m,n}^{(n+1),[k]}}{2} \cdot \left( p_{m+1,n}^{a} - p_{m,n}^{a} \right)^{(k+1)} \right] \cdot \hat{i} + \ldots + \left[ -\frac{\lambda_{y,m,n}^{(n+1),[k]}}{2} \cdot \left( p_{m,n+1}^{a} - p_{m,n}^{a} \right)^{(k+1)} \right] \cdot \hat{j}. \]

(34)

To calculate source/sink terms well models are commonly used in reservoir simulation [42]. It was assumed that production wells operate at a constant total flow rate, whereas injectors operate at a constant bottomhole pressure. Hence, the flowrate in injectors is equal to

\[ Q = \left[ P_{I,m,n}^{a,\text{wf}} - P_{m,n}^{a,(k+1)} \right]^{(n+1)}. \]

(35)

The productivity ratio (PI) for two-dimensional systems is calculated as

\[ P_{I,m,n}^{a,\text{wf}} = \frac{2 \cdot \pi \cdot \sqrt{k_x \cdot k_y \cdot \Delta z}}{0.15802 \cdot \ln \left( \frac{l_x}{k_x} \right) + s \cdot \mu_{m,n}^a}. \]

(36)

The equivalent radius \(r_o\) is calculated using the Peaceman model [42]:

\[ r_o = 0.28 \cdot \frac{\left( \frac{k_x}{l_x} \right)^{1/4} \cdot \Delta x^2 + \left( \frac{k_y}{l_y} \right)^{1/4} \cdot \Delta y^2}{\left( \frac{k_x}{l_x} \right)^{1/4} + \left( \frac{k_y}{l_y} \right)^{1/4}}. \]

(37)

Due to the scheme chosen (quarter five-spot), the wells are located in boundary blocks. This affects the value of the equivalent radius. The Peaceman model was extended to take into account this and other factors (e.g. non-square grids and non-Darcy effects). This correction has been already addressed in the literature [40] and it has been considered in the simulator.

Finally, the discretized overall concentration equation for petroleum and chemical components is introduced. In this case, an explicit model is employed using the upwind method for advective terms and a centered method for the diffusive terms. The longitudinal and transversal dispersive terms will be neglected.
\[
\frac{\phi}{\Delta t} \left( x_i^{(n+1)} - x_i^{(n)} \right) + \frac{1}{\Delta x} \sum_j \left( u_j^{(k+1)} \cdot V_j^{(k)} - u_j^{(k+1)} \cdot V_j^{(k+1)} \right) = \cdots \\
+ \frac{1}{\Delta y} \sum_j \left( u_j^{(k+1)} \cdot V_j^{(k)} - u_j^{(k+1)} \cdot V_j^{(k+1)} \right) = \cdots \\
- \frac{\phi}{\Delta x^2} \sum_j \left[ (S^j \cdot d m^j)_{m+1/2,n} \cdot (V_j^{(k+1)} - V_j^{(k+1)}) - (S^j \cdot d m^j)_{m-1/2,n} \cdot (V_j^{(k+1)} - V_j^{(k+1)}) \right]^{(n+1),[k]} = \cdots \\
- \frac{\phi}{\Delta y^2} \sum_j \left[ (S^j \cdot d m^j)_{m,n+1/2} \cdot (V_j^{(k+1)} - V_j^{(k+1)}) - (S^j \cdot d m^j)_{m,n-1/2} \cdot (V_j^{(k+1)} - V_j^{(k+1)}) \right]^{(n+1),[k]} = \cdots \\
\frac{\phi}{\Delta t} \left( A_d^{(n)} - A_d^{(n+1)} \right)_{m,n} + q_{i,m,n}^{(n+1),[k]}. 
\]

Eq. 38 is the typical advection-diffusion discretized equation, used in hydraulic and fluid study in porous media. Adjective terms are of hyperbolic nature, and being discretized with the upwind method causes a numerical dispersion in the solution of overall concentrations, affecting the oil recovery factor. This may be solved using higher order numerical methods and/or flux-limiting techniques [43,44].

2.7. Solution algorithm

The discretization led to a non-linear system, solved by an implicit-explicit coupled method known as IMPEC (IMplicit Pressures and Explicit Concentrations). The complexity lies in that many auxiliary properties are functions of parameters being calculated for the corresponding time step. This is overcome by using an iterative method in each time step (iterative IMPEC). A maximum tolerance is set for the difference between two consecutive iterations in determine parameters within the same time step. When this tolerance is met, the values in the previous time step \( (n - 1) \) and \( k = k_{\text{max}} \), are used as starting values for the next step \( (n = 1, k = 1) \).

1. The aqueous phase pressure is calculated evaluating Eq. (32) in the domain.
2. The oil phase pressure is calculated using the capillary pressure.
3. Darcy velocities are calculated with Eqs. (2), (33) and (34).
4. Flowrates in the wells are calculated with Eqs. (35)–(37).
5. Overall compositions of the petroleum and chemical components are calculated with Eq. (38).
6. Overall concentration of water, volume fractions and phase saturations are calculated with Eqs. (6) \( (i = w), (7), (8) \) \( (j = o, a), (9), (12)–(14) \).
7. Finally the norm for the overall concentration of two components \( (i = p, c) \) is calculated with Eq. (39).

\[
e_i = \max_{\forall m,n,\omega} \left| z_i^{(n),[k+1]} - z_i^{(n),[k]} \right|. 
\]

2.8. Validation of the model

In order to validate our new simulator, we have considered a two-dimensional field which is operated under a waterflooding scheme. The data and geometrical characteristics were adopted from Najafabadi [45] and compared to the results obtained in UTCHEM and GPAS (a fully implicit, parallel EOS compositional reservoir simulator). The model dimensions are 201 m \( \times 201 m \times 30.5 m \) and it is discretized in a 10 \( \times \) 10 gridblock scheme. The permeability is 100 mD and constant throughout the reservoir. At the beginning of the process, the water saturation is 0.3. In Fig. 4 we plot the result of the oil recovery factor for the validation process and we compare it with the results obtained by Najafabadi [45]. Although the new simulator presents larger numerical dispersion than UTCHEM, the final oil recovery factor is comparable to the latter. The major differences are observed when the waterfront reached the production well \( (\sim 0.5 \text{ PV}) \) yielding an oil recovery factor slightly lower than the value in UTCHEM, mainly due to numerical errors. This numerical diffusion is not negligible but does not modify the final values in the new simulator and these are still accurate in terms of front location and cumulative oil production. This waterflooding test validates the behavior of the new simulator in two-dimensional fields.

3. Numerical simulator

3.1. Introduction

The simulator has been programmed in MathWorks MATLAB to solve the non-linear system of equations that results from evaluating Eq. (32) (aqueous phase pressure) in the domain. This system (Eq. (40)) is solved using the conjugate gradient method (CGM), chosen due to its fast convergence to the solution [46].
Thanks to the compositional formulation employed, this simulator can also be used for secondary recovery processes (waterflooding). The governing equations are then easily modified to take this into account. Using the general system described in 2.2, the new set of equations is obtained for the calculation of the saturations:

\[ V_{p,c}^o = 0 \Rightarrow V_{w,c}^o = 1; \quad V_{w,c}^o = 0 \Rightarrow V_p^o = 1. \]  

(41)

\[ z_i = \sum_j S_j^i \cdot V_j^i \Rightarrow \begin{cases} z_c = 0 \\ z_p = S_p^o \cdot V_p^o + S_o^o \cdot V_p^o = S_o^o \\ z_w = S_w^o \cdot V_w^o + S_o^o \cdot V_w^o = S_o^o, \end{cases} \]  

(42)

\[ S_{i,m,n}^{(n+1)} = S_{i,m,n}^{(n)} + \Delta t \cdot \sum_{k=1} \left\{ q_{i,m,n}^{(n+1)} \right\}_{k} - \left[ \frac{1}{\Delta x} \left( \frac{4}{3} \left( u_{i,m,n}^{(k+1)} - u_{i,m,n}^{(k+1)} \right) - \frac{1}{2} \left( u_{i,m,n}^{(k+1)} - u_{i,m,n}^{(k+1)} \right) \right) \right\}_{n}. \]  

(43)

Eq. (43) takes the form of the implicit pressure and explicit saturation (IMPES) method. The main difference is that traditional IMPES method is not iterative unlike the model developed here, which has an effect on the calculation time. Nevertheless, the feature of being an iterative method gives better numerical stability and robustness than the IMPES method. The new simulator has also the option to perform waterflooding simulations based on an iterative or a non-iterative method.

The formulation for a tertiary recovery process has been already developed and presented. This simulator aims to reproduce a process of chemical surfactant flooding in a reservoir with known physical and geometric characteristics.

3.2. Data

In order to perform the simulation a series of properties were established emulating a recovery in an oil reservoir. These are presented in Table 1. The operating conditions for the wells are showed in Table 2. Ancillary parameters introduced in Table 3 were adopted on the basis of a previous work [32]. They represent in an acceptable way the fluid properties and components’ behavior in the reservoir.

3.3. Simulation of a waterflooding process

3.3.1. Iterative process

The first part of the analysis covers the study of a waterflooding process in a reservoir that is supposed to have been exploited in its primary stage and now oil production has declined enough to make this exploitation no longer profitable. It is expected that, since the IFT shall not change due to the absence of a surfactant, the capillary number and residual saturations of the phases will not change, therefore the oil saturation will decrease eventually to the residual oil saturation, and then remain constant throughout the secondary recovery. The scenario is as follows: a reservoir that recently finished the primary recovery stage, with an average oil saturation well above the residual. The geometric scheme is completed with a system of two wells (quarter five-spot geometry - Fig. 1). To analyze its behavior, a waterflooding over a period of 8,000 days was performed. This period was set to guarantee the occurrence of each component breakthroughs as well as to achieve a pseudo steady state operating conditions in the producing well. These results were based on simulations for the following time steps: 25 days, 10 days, 5 days and 2.5 days. Table 4 shows the values of total oil production achieved for
Table 1
General parameters used for the simulations.

| Geometrical data of the reservoir |  |
|----------------------------------|--|--|--|--|--|
| Length in axis X                 | 900 m | 900 m | Layer thickness |
| n_x                              | 15 blocks | 15 blocks | 20 m            |
| Rock properties                  |  |
| Porosity                         | 0.25 | 500 mD | 500 mD |  |
|Initial conditions                |  |
| S_w (waterflood/EOR)             | 0.80/0.36 | S_w = S_w^H (EOR) | 0.35 | S_w = S_w^H | 0.15 |
|Simulation data                   |  |
| Total time                       | 8000 days | Chemical inj. time | 500 days | z_xi | 0.1 |
|Physical data of the phases       |  |
|μ_{ori}                           | 1 cP | μ_{ori} | 10 cP | IFT | 20 mN/m|
|Water density                     | 1020 kg/m³ |  |

<table>
<thead>
<tr>
<th>Table 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical data</td>
</tr>
<tr>
<td>Number of wells</td>
</tr>
<tr>
<td>Well radius</td>
</tr>
<tr>
<td>Skin factor</td>
</tr>
<tr>
<td>Operating conditions</td>
</tr>
<tr>
<td>Total flowrate</td>
</tr>
<tr>
<td>Bottomhole pressure</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ancillary parameters for the simulations.</td>
</tr>
<tr>
<td>IFT</td>
</tr>
<tr>
<td>G₁</td>
</tr>
<tr>
<td>G₂</td>
</tr>
<tr>
<td>Capillary pressure</td>
</tr>
<tr>
<td>Adsorption</td>
</tr>
<tr>
<td>Residual saturation</td>
</tr>
<tr>
<td>Relative permeabilities</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cumulative oil productions in the iterative simulation for different time steps.</td>
</tr>
<tr>
<td>Time step (Days)</td>
</tr>
<tr>
<td>-----------------------------------</td>
</tr>
<tr>
<td>25</td>
</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>2.5</td>
</tr>
</tbody>
</table>

each simulation and the average number of iterations per time step IMPEC demanded to converge. An important conclusion from Table 4 is that for the iterative IMPEC exists, for each grid configuration, an optimum time step. The latter minimizes the computational time without compromising the accuracy, as it usually happens with implicit techniques working with big time steps.  

Fig. 5 shows the pressure and oil saturation profiles at the end of the waterflooding process. The remanent oil reached maximum values in the corners where total Darcy velocities are nearly zero (where pressure gradients become negligible), and no displacement took place in this area. Fig. 6 illustrates the behavior of the process in terms of cumulative oil produced, oil/water flow rates, and the fractional flow. As was expected, it shows a steadily increasing behavior in the fractional flow, reaching eventually the economic limit for the process.  

In conclusion, the iterative method has a calculation sequence that makes it equivalent to a fully implicit method, ensuring stability, as it will be analyzed later. But like all implicit method, its accuracy decreases as the time step increases, as is shown in Table 4, where the maximum difference between the results obtained with the time steps tested is roughly 10.70%.
3.3.2. Non-iterative process

The same procedure is now presented, under the same operating conditions, but using a non-iterative approach, which renders the traditional IMPES method. When a time step was set in 30 days, the process became unstable. The stability limit of the process was found in a time step of approximately 22 days at the beginning of the process, which will be verified in the stability analysis. Hereunder the results for \( t = 25 \) days are presented (Figs. 7 and 8).

It was observed that, as the time step increased, oscillations began to appear at the beginning of the simulation, which later tended to fade out progressively until they completely disappeared (Fig. 8). Such oscillations undoubtedly have their origin in numerical instabilities due to the explicit calculation process of the phase saturations. The cumulative oil production was 714380 m\(^3\), which represents a difference of 0.4% when compared to the value obtained with the implicit scheme. Similar behavior was encountered in the pressure and oil saturation patterns, which was expected since the simulation parameters were not changed (Fig. 7). However, Fig. 8 shows the mentioned instabilities at the beginning of the simulation in the water/oil flowrates as well as in the fractional flow, but not reflected in the cumulative oil production.

Finally, a series of simulations have been performed with the non-iterative IMPES changing both parameters simultaneously, time and spatial steps. In order to do this, a criterion was established so as to modify these values without introducing...
Fig. 8. Cumulative oil production (left), oleous/aqueous produced flowrates (middle), and fractional flow (right) for a non-iterative waterflooding process.

<table>
<thead>
<tr>
<th>Spatial step (m)</th>
<th>Time step (days)</th>
<th>Cumulative oil production (m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>90</td>
<td>55</td>
<td>722,340</td>
</tr>
<tr>
<td>75</td>
<td>42</td>
<td>721,980</td>
</tr>
<tr>
<td>60</td>
<td>28</td>
<td>720,750</td>
</tr>
<tr>
<td>50</td>
<td>20</td>
<td>720,740</td>
</tr>
<tr>
<td>45</td>
<td>16</td>
<td>717,890</td>
</tr>
</tbody>
</table>

Table 5
Cumulative oil productions during a waterflooding applying CFL condition.

Numerical instabilities. As the process to be analyzed is a purely advective, without the presence of diffusion mechanisms, the CFL (Courant–Friedrichs–Lewy) condition was adopted, so the equation relating time and spatial steps yields:

\[
\frac{2 \cdot Cr}{\phi} \approx 1 \Rightarrow \Delta t \approx \frac{\phi}{2 \cdot U} \cdot \Delta x.
\]

(44)

Using the non-iterative method coupled with this concept, a new set of results for the different conditions was obtained, indicating a correspondence between the relationships chosen for the study (Table 5). The CFL condition allowed obtaining production values without the appearance of numerical oscillations, and guaranteed at the same time accuracy in the results.

3.4. Simulation of a chemical flooding process

From the results obtained during waterflooding processes, it is inferred that long after the whole operative cycle of the production well, oil is still flowing out. However, oil flowrates therefrom may go below limit values that make the exploitation itself to become uneconomical, since injection plus production associated costs become larger than the income from oil production. This limit is known as minimum operating flow. This flow does not have a certain fixed value, depending on the country, the region and the present oil price. To mobilize the remaining oil, tertiary recovery processes must be applied, in this case, a chemical surfactant flooding. For this type of process the non-iterative method cannot be used, as the resulting system of equations involves more physical parameters in the simulation that depend on each other. Therefore, an iterative IMPEC calculation must be carried out.

The situation is now different from that in the previous cases: a reservoir with an initial saturation equal to the remaining oil saturation after the waterflooding process. After an initial period with an aqueous surfactant solution being injected, a water bank is employed to drive the surfactant slug and oil bank towards the producing well. The chemical concentration profile is shape similar to a wave propagation in a two-dimensional field, which travels with a speed equal to Darcy velocities in each block (Fig. 9). For this first stage of simulation, the mechanisms of adsorption, diffusion/dispersion and capillary pressure are neglected. It is also envisaged that numerical diffusion mechanisms, along with the physical diffusion mechanisms, if enabled, will cause a deformation and widening of the surfactant slug. The simulation was done with a time step of 10 days in a Larson II(–) system (Fig. 2) (\(L_{yc}^0 = 1, L_{yc}^0 = 1\) and \(K_c = 0.5\)) (Figs. 9 and 10). During an initial period, oil production was nearly zero due to the low residual saturation after waterflooding in the area surrounding the well. Then after approximately 2,000 days, the oil bank mobilized by the surfactant reached the vicinity of the production well (oil breakthrough) (Fig. 9). Fig. 10 shows that after the EOR process a partial desaturation below the waterflooding residual saturation took place, increasing the recovery factor of the oil field. Approximately 500 days after the oil breakthrough the same phenomenon occurred with the surfactant (chemical breakthrough), reaching after displacing the remaining oil the producing well (Fig. 11). Analyzing the process from a numerical point of view, the model behaved as mentioned above: the iterative method granted implicit properties to the numerical scheme, hereby ensuring the stability of the method. Also, the period of greater instability for the process was when the chemical breakthrough occurred, as seen in Fig. 11, when the simulator employed a larger number of iterations. During the injection period the IMPEC method reached convergence.
with an average of 2.14 iterations per time step, mainly due to the small time step chosen for the simulation. This average dropped, as expected, to 1.69 during the water injection period. This value might have been lower but the chemical breakthrough period demanded a larger number of iterations per time step to reach convergence.

4. Numerical stability analysis

A numerical stability analysis is performed to check the stability and robustness of the new simulator for EOR flooding. As explained above, the simulator can operate under two possible conditions: iterative and non-iterative. Conceptually, these conditions use the concepts of numerical simulation under explicit and implicit schemes. The non-iterative method calculates the concentration data of the time step in the study using data from the previous step, which gives an explicit character; however, the iterative method calculates concentrations using information, despite previous iterations, always cor-
responding to the time step in study, which gives a fully implicit character. What is explained below is the stability analysis for these methods in order to validate the theoretical results obtained during the simulations.

4.1. Explicit method

The stability perturbation analysis is performed on Eq. (43), based on the following assumptions: diffusive/dispersive or adsorption effects and source/sink terms are not taken into account. Thus the equation, when applied to the case of secondary recovery is as follows:

$$
S_{i,m,n}^{(n+1)} = S_{i,m,n}^{(n)} - \frac{\Delta t}{\phi} \left[ \frac{1}{\Delta x} \left( u_{x,m,n}^{[k+1]} - u_{x,m-1,n}^{[k+1]} + \frac{1}{\Delta y} \left( u_{y,m,n}^{[k+1]} - u_{y,m-1,n}^{[k+1]} \right) \right) \right]^{(n)},
$$

$$
S_{i,m,n}^{(n+1)} = S_{i,m,n}^{(n)} - \frac{\Delta t}{\phi} \left[ \frac{1}{\Delta x} \cdot f(S_{i,m,n}^{(j)}) + \frac{1}{\Delta y} \cdot g(S_{i,m,n}^{(j)}) - \frac{1}{\Delta x} \cdot f(S_{m-1,n}^{(j)}) - \frac{1}{\Delta y} \cdot g(S_{m,n-1}^{(j)}) \right]^{(n)}. \tag{45}
$$

Eq. (45) is the basic equation for analysis. To study the stability, we introduce a perturbation $\epsilon$ in the saturation at time step $n$, and study the behavior of the disturbance in the following time steps. If the former increases in amplitude, for this particular process, the method is considered unstable; on the contrary, if the disturbance tends to decrease and fade out, the method is stable. So the perturbed equation is:

$$
S_{i,m,n}^{(n+1)} + \epsilon_{i,m,n}^{(n+1)} = S_{i,m,n}^{(n)} + \epsilon_{i,m,n}^{(n)} - \frac{\Delta t}{\phi} \cdot \left[ \frac{1}{\Delta x} \cdot f(S_{i,m,n}^{(j)} + \epsilon_{i,m,n}) + \frac{1}{\Delta y} \cdot g(S_{i,m,n}^{(j)} + \epsilon_{i,m,n}) - \frac{1}{\Delta x} \cdot f(S_{m-1,n}^{(j)} + \epsilon_{i,m-1,n}) - \frac{1}{\Delta y} \cdot g(S_{m,n-1}^{(j)} + \epsilon_{i,m,n-1}) \right]^{(n)}, \tag{46}
$$

Now a Taylor series expansion for functions $f$ and $g$ up to first order is introduced. Thus:

$$
S_{i,m,n}^{(n+1)} + \epsilon_{i,m,n}^{(n+1)} = S_{i,m,n}^{(n)} + \epsilon_{i,m,n}^{(n)} - \frac{\Delta t}{\phi} \cdot \left[ \frac{1}{\Delta x} \cdot f(S_{i,m,n}^{(j)}) \cdot \epsilon_{i,m,n} + \frac{\partial}{\partial S} f(S_{i,m,n}^{(j)}) \cdot \epsilon_{i,m,n} - \frac{1}{\Delta x} \cdot f(S_{m-1,n}^{(j)}) \cdot \epsilon_{i,m-1,n} - \frac{1}{\Delta y} \cdot g(S_{m,n-1}^{(j)}) \cdot \epsilon_{i,m,n-1} \right], \tag{47}
$$

Combining Eqs. (45) and (47), and also assuming that the spatial discretizations in both axes are equal, the general equation of the perturbation method is obtained.

$$
\epsilon_{i,m,n}^{(n+1)} = \epsilon_{i,m,n}^{(n)} - \frac{\Delta t}{\phi \cdot \Delta x} \cdot \left[ \frac{\partial}{\partial S} f(S_{i,m,n}^{(j)}) \cdot \epsilon_{i,m,n} + \frac{\partial}{\partial S} g(S_{i,m,n}^{(j)}) \cdot \epsilon_{i,m,n} - \frac{1}{\Delta x} \cdot f(S_{m-1,n}^{(j)}) \cdot \epsilon_{i,m-1,n} - \frac{1}{\Delta y} \cdot g(S_{m,n-1}^{(j)}) \cdot \epsilon_{i,m,n-1} \right]^{(n)}; \quad \text{and} \quad r = \frac{\Delta t}{\phi \cdot \Delta x}. \tag{48}
$$

$$
\epsilon_{i,m,n}^{(n+1)} = r \cdot \frac{\partial}{\partial S} f(S_{i,m,n}^{(j)})^{(n)} \cdot \epsilon_{i,m,n}^{(n)} + \epsilon_{i,m,n}^{(n)} \cdot \left[ 1 - r \cdot \left[ \frac{\partial}{\partial S} f(S_{i,m,n}^{(j)}) + \frac{\partial}{\partial S} g(S_{i,m,n}^{(j)}) \right] \right]^{(n)} + \ldots
$$

$$
+ r \cdot \frac{\partial}{\partial S} g(S_{i,m,n}^{(j)})^{(n)} \cdot \epsilon_{i,m,n-1}^{(n)} + \epsilon_{i,m,n}^{(n)} \cdot \epsilon_{i,m,n-1}^{(n)} + \ldots \tag{49}
$$

With Eq. (49) the perturbation matrix is assembled evaluating it throughout the reservoir. The matrix of amplification is lower triangular, and can be written in blocks as follows:

$$
\tilde{\epsilon}^{(n+1)}_{j} = \begin{bmatrix}
A_{1}^{j} & 0 & \cdots & 0 \\
B_{1}^{j} & A_{2}^{j} & \cdots & 0 \\
0 & \cdots & 0 & \ddots \\
0 & \cdots & 0 & B_{m-1}^{j}
\end{bmatrix} \cdot \epsilon^{(n)}_{j}, \tag{50}
$$

wherein sub-matrices $A$ and $B$ are a lower triangular and a diagonal matrices, respectively, of dimensions $n_{x} \times n_{y}$, and the constituent elements are those from Eq. (49). The stability condition required in these systems is that the absolute value of the eigenvalues of the amplification matrix should be less than 1. This condition can be met as follows:
\[
\varepsilon^{j,(n+1)} = \mathbf{G} \cdot \varepsilon^{j,(n)} \Rightarrow \| \varepsilon^{j,(n+1)} \| = \| \mathbf{G} \cdot \varepsilon^{j,(n)} \| \leq \| \mathbf{G} \| \cdot \| \varepsilon^{j,(n)} \| = \ldots
\]
\[
\| \mathbf{G} \| \cdot \| \varepsilon^{j,n-1} \| \leq \| \mathbf{G} \|^{2} \cdot \| \varepsilon^{j,n-2} \| \leq \ldots \leq \| \mathbf{G} \|^{n+1} \cdot \| \varepsilon^{j,0} \|.
\]

(51)

In order for the model to be stable, the perturbation in the initial time step should tend to zero as \( n \) tends to infinity; this is achieved only if the norm of the amplification matrix is less than 1, which can also be met if all the eigenvalues of this matrix are lower in module 1. In the case of this matrix:

**Eigenvalues of** \( \mathbf{G} \Rightarrow \lambda_{i} = 1 - r \cdot (f'_{i} + g'_{j}) \); \( i \in [1; nx \cdot ny] \), \( m \in [1; nx] \), \( n \in [1; ny] \).

(52)

**Characteristic equation of** \( \mathbf{G} \Rightarrow \prod_{i,j=1}^{nx \cdot ny} \left[ 1 - r \cdot (f'_{i} + g'_{j}) \right] = 0. \)

(53)

**To achieve stability** \( \Rightarrow |\lambda_{i}| < 1 \Rightarrow \left\{ \begin{array}{l}
1 - r \cdot (f'_{i} + g'_{j}) < 1 \\
1 - r \cdot (f'_{i} + g'_{j}) m,n < 1
\end{array} \right. \)

(54)

The first condition for stability does not allow obtaining any relationship between the values of spatial and temporal steps, thus it only remains to check the sign of the derivatives of the functions. With respect to the second stability condition, it is obtained as:

\[
r < \frac{2}{(f' + g'_{m,n})} \Rightarrow \text{To achieve stability} \Rightarrow \Delta t < \frac{2 \cdot \Delta x \cdot \phi}{\max_{m,n} (f' + g'_{m,n})}.
\]

(55)

We have hereby obtained an equation that allows establishment of the relationship between space and time steps to ensure the stability of our simulator, using the non-iterative scheme. The system is conditionally stable, as it is usually found when using explicit numerical schemes. The problem here lies in finding the values of the derivatives of functions \( f \) and \( g \) with respect to the saturation. The most relevant part of this analysis is to find the cell(s) where these functions will reach their maximum values. Since they are related to Darcy velocities, the region where these values reach a maximum are near the source/sink cells.

Take as example the case of a waterflooding process in a reservoir. As was shown in Fig. 8, some oscillations were attributed to a numeric behavior appearing at the beginning of the simulation. To demonstrate this, the above formulation was analyzed on the blocks that were considered critical regarding functions \( f \) and \( g \), and calculated the maximum time step which ensures stability. Results yielded a critical time step of \( \Delta t = 22 \) days at the beginning of simulation, with values taken in the production well block. At the beginning of the simulation the critical time step was lower than the time step chosen causing instabilities, as seen in Fig. 8, which then disappeared as the critical time step became higher than the time step. This is due to the fact that the problem is non-linear, and the stability condition depends on the value of the functions in the time step under study.

4.2. Implicit method

The stability of the iterative method is now presented. The basic concepts are the same as in the explicit method, and therefore will not be analyzed here. The major change is in the previous section, the amplification matrix elements were based on values from the previous time step; now, these elements belong to the time step being calculated. Thus, the

\[
S^{(n+1)}_{i,m,n} = S^{(n)}_{i,m,n} - \frac{\Delta t}{\phi} \cdot \left[ \frac{1}{\Delta x} \cdot f(S^{i}_{m,n}) + \frac{1}{\Delta y} \cdot g(S^{i}_{m,n}) - \frac{1}{\Delta x} \cdot f(S^{i}_{m-1,n}) - \frac{1}{\Delta y} \cdot g(S^{i}_{m,n-1}) \right]^{(n+1)},
\]

(56)

\[
S^{(n+1)}_{i,m,n} + \varepsilon^{(n+1)}_{i,m,n} = S^{(n)}_{i,m,n} + \varepsilon^{(n)}_{i,m,n} - \frac{\Delta t}{\phi} \cdot \left[ \frac{1}{\Delta x} \cdot f(S^{i}_{m,n}) + \frac{\partial}{\partial s} f(S^{i}_{m,n}) \cdot \varepsilon_{i,m,n} \right] + \ldots
\]

\[
+ \frac{1}{\Delta y} \cdot \left[ g(S^{i}_{m,n}) + \frac{\partial}{\partial s} g(S^{i}_{m,n}) \cdot \varepsilon_{i,m,n} \right] - \frac{1}{\Delta x} \cdot \left[ f(S^{i}_{m-1,n}) + \frac{\partial}{\partial s} f(S^{i}_{m-1,n}) \cdot \varepsilon_{i,m-1,n} \right] - \ldots
\]

\[
- \frac{1}{\Delta y} \cdot \left[ g(S^{i}_{m,n-1}) + \frac{\partial}{\partial s} g(S^{i}_{m,n-1}) \cdot \varepsilon_{i,m,n-1} \right]^{(n+1)}.
\]

(57)

\[
\varepsilon^{(n+1)}_{i,m,n} = \frac{\Delta t}{\phi \cdot \Delta x} \cdot \left[ \frac{\partial}{\partial s} f(S^{i}_{m,n}) \cdot \varepsilon_{i,m,n} + \frac{\partial}{\partial s} g(S^{i}_{m,n}) \cdot \varepsilon_{i,m,n} \right] - \ldots
\]

\[
- \frac{\partial}{\partial s} f(S^{i}_{m-1,n}) \cdot \varepsilon_{i,m-1,n} - \frac{\partial}{\partial s} g(S^{i}_{m,n-1}) \cdot \varepsilon_{i,m,n-1} \right]^{(n+1)} = \varepsilon^{(n)}_{i,m,n} \quad \text{and} \quad r = \frac{\Delta t}{\phi \cdot \Delta x}.
\]

(58)
\[
\epsilon^{(n)}_{i,m,n} = -r \frac{\partial}{\partial S} f(S_{m-1,n}^{(n+1)}) \cdot \epsilon^{(n+1)}_{i,m-1,n} + \epsilon^{(n+1)}_{i,m,n} \cdot \left\{ 1 + r \cdot \left[ \frac{\partial}{\partial S} f(S_{m,n}^{(n)}) + \frac{\partial}{\partial S} g(S_{m,n}^{(n)}) \right] \right\}^{(n+1)} - \cdots
\]

The amplification matrix remains lower triangular, and the block form is as follows:
\[
\epsilon^{j,(n+1)} = \begin{bmatrix}
A^1_{j} & 0 & \cdots & 0 \\
B^1_{j} & A^2_{j} & 0 & \cdots \\
0 & \cdots & \cdots & \cdots \\
0 & \cdots & \cdots & B^{n,1}_{j} & A^{n,1}_{j}
\end{bmatrix}^{(n)} = \epsilon^{j,(n)}.
\]

Now we calculate the eigenvalues for the amplification matrix.

**Eigenvalues of** \( \mathbb{C} \Rightarrow \lambda_i = 1 + r \cdot (f'_S + g'_S)_{m,n} \); \( i \in [1; n_x \cdot n_y] \), \( m \in [1; n_x] \), \( n \in [1; n_y] \).

**Characteristic equation of** \( \mathbb{C} \Rightarrow \prod_{i,j=1}^{i \cdot j \cdot n, m \cdot n} \left[ 1 + r \cdot (f'_S + g'_S)_{i,j} \right] = 0. \)

The eigenvalues of the amplification matrix were obtained, but they still refer to the time step being calculated; to establish conditions for stability, the matrix must be inverted, and then the new eigenvalues must be computed. However, we use a property stating that if a lower triangular matrix has non-zero determinant the eigenvalues of the inverse are the inverses of the eigenvalues. Thus:

**Eigenvalues of** \( \mathbb{C}^{-1} \Rightarrow \lambda_i = \frac{1}{1 + r \cdot (f'_S + g'_S)_{m,n}} \); \( i \in [1; n_x \cdot n_y] \), \( m \in [1; n_x] \), \( n \in [1; n_y] \).

**Characteristic equation of** \( \mathbb{C}^{-1} \Rightarrow \prod_{i,j=1}^{i \cdot j \cdot n, m \cdot n} \left[ \frac{1}{1 + r \cdot (f'_S + g'_S)_{i,j}} \right] = 0. \)

To achieve stability \( \Rightarrow |\lambda_i| < 1 \Rightarrow \begin{cases} \frac{1}{1 + r \cdot (f'_S + g'_S)_{m,n}} < 1 \\ -1 < \frac{1}{1 + r \cdot (f'_S + g'_S)_{m,n}} \end{cases} \).

As in the explicit case, the first condition for stability does not allow obtaining values or a relationship between spatial and temporal steps. Regarding the second condition, it yields:

\[
-r < \frac{2}{(f'_S + g'_S)_{m,n}} \Rightarrow \text{To achieve stability} \Rightarrow \Delta t > -\frac{2 \cdot \Delta x \cdot \phi}{\max_{v,m,n} (f'_S + g'_S)_{m,n}}.
\]

Since the right side of the inequality (66) is negative, any time step will satisfy the condition of stability, hence the method is unconditionally stable, which is consistent with the results obtained during this work.

5. Conclusions

In this study, we have proposed a novel two-dimensional simulator for a three pseudo-components, two phase flow, applied to chemical enhanced oil recovery using surfactants. Moreover, we have discussed a numerical stability analysis of the system of equations which, to the best of our knowledge, has never been presented for this system in surfactant EOR. The simplification of the ternary diagram was shown to be a valid and simple approach to model the surfactant properties and phase behavior, which are known to play a major role in surfactant EOR process. When considering only these parameters, we have found that the partition coefficient is the most influential in the oil recovery factor, followed in a lesser degree by the swelling and solubilization ratios. The importance of the different phenomena analyzed (e.g. dispersion, adsorption, capillary pressure) was relevant only when they affected significantly the surfactant concentration profile.

Besides the sensitivity analysis of the physical parameters during the recovery process we have also presented the numerical stability and robustness analysis of the new simulator. The iterative IMPEC scheme yielded stable results, independent of the time step chosen. However, this came at the expense of a higher computational time. On the other hand, the non-iterative IMPEC was sensitive to the time step selected, showing some oscillations in the flowrates in the production well during the start-up period, which progressively faded out.

Surfactant EOR simulations showed the potential of chemical EOR methods to sweep the residual oil by means of reducing the IFT. The model employed with the ternary diagram may provide a simple way to design chemicals with specific properties before experimental or field tests be performed. Avenues for future research include the use of higher-order discretization schemes so as to reduce numerical round-off errors as well as including salt as a fourth component and studying its influence on both the surfactant properties and the recovery process.
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