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Preface

This supplementary volume contains the proceedings of the 9th conference on Discrete Optimization and Operations Research and scientific school on Modern Optimization and Equilibrium, held in Vladivostok, Russia, during September 19 - 23, 2016. It was organized by the Far Eastern Federal University, Sobolev Institute of Mathematics, Krasovsky Institute of Mathematics and Mechanics, Novosibirsk State University, and the Higher School of Economics in Nizhny Novgorod.

Previous conferences took place at the Sobolev Institute of Mathematics, Novosibirsk, in 1996, 1998, 2000, 2002, and 2004. The 6th conference was held in the Russian Far East in a picturesque on the shore of the Japanese Sea near Vladivostok in 2007. The 7th one, in 2010, was held in the Mountain Altay. The 8th event took place in Novosibirsk again.

This event is a part of series of regular international conferences on optimization and operations research that covers a wide range of topics in mathematical programming and its applications, integer programming and polyhedral combinatorics, bi-level programming and multi-criteria optimization, optimization problems in machine learning and data mining, discrete optimization in scheduling, routing, bin packing, locations, and optimization problems on graphs, computational complexity, and polynomial time approximation. The main purpose of the conference and scientific school is to provide a forum where scientists and young researchers can exchange ideas, identify promising directions for research and application domains, and foster new collaborations.

In response to the call for papers, we received 181 submissions. Papers included in this volume were carefully selected by the Program Committee on the basis of reports from two or more reviewers from 17 countries such as Belarus, Belgium, France, Germany, India, Israel, Italy, Kazakhstan, Netherlands, Russian Federation, Spain, Sweden, Taiwan, Turkey, Ukraine, United Kingdom, United States. Only 82 submissions were selected for inclusion in this volume. The conference also featured ten invited talks by the following eminent speakers:

- Vladimir Mazalov from the Institute of Applied Mathematical Research of the Karelian Research Centre RAS, Russia; Title of the talk: *Behavioral equilibrium in transportation networks*;
- Evripidis Bampis from the Université Pierre et Marie Curie, France; Title of the talk: *Algorithmic issues in energy-efficient computation.*
- Vitaly Strusevich from the University of Greenwich, Old Royal Naval College, United Kingdom; Title of the talk: *Handling scheduling problems with controllable parameters by methods of submodular optimization.*
- Fedor Fomin from the University of Bergen, Norway; Title of the talk: *Modern trends in parameterized algorithms*
- Panos Pardalos from the University of Florida, USA; Title of the talk: *A new information theory perspective on network robustness*
- Jun Pei from School of Management, Hefei University of Technology, China; Title of the talk: *Coordinated scheduling of deteriorating jobs in a two-stage supply chain.*
- Yair Censor from the University of Haifa, Israel; Title of the talk: *Linear and non-linear superiorization: A methodology between feasibility-seeking and optimization.*

– Athanasios Migdalas from the Lulea University of Technology, Sweden; Title of the talk: *Location modeling in the presence of firm and customer competition.*
– Vadim Shmyrev from the Sobolev Institute of Mathematics, Russia; Title of the talk: *Iterative approach for piecewise linear exchange model*;
– Alexandr Kononov from the Sobolev Institute of Mathematics, Russia; Title of the talk: *Short survey on minimization graph correlation clustering;*

and eight tutorials:

– Adil Erzin from the Sobolev Institute of Mathematics, Russia; Title of the talk: *Computational geometry and combinatorial optimization problems in the context of wireless sensor networks optimization*;
– Alexandr Kononov from the Sobolev Institute of Mathematics, Russia; Title of the talk: *How to design approximation schemes for intractable optimization problems*;
– Yury Kochetov from the Sobolev Institute of Mathematics, Russia; Title of the talk: *Discrete Location Problems;*
– *Nenad Mladenovic from the University of Valenciennes, France; Title of the talk: Developing variable neighborhood and formulation space search procedures;*
– *Michael Khachay from the Krasovsky Institute of Mathematics and Mechanics, Russia; Title of the talk: Effective algorithms for some actual generalizations of geometrical traveling salesman problems;*
– *Oleg Khamisov from the Melentiev Institute of Energy Systems, Russia; Title of the talk: Modeling of the energy markets with network restrictions;*
– *Michael Batsyn from the National Research University Higher School of Economics, Russia; Title of the talk: Optimization problems in the transportation logistics;*
– *Alexandr Strekalovsky from the Matrosov Institute for System Dynamics and Control Theory, Russia; Title of the talk: Theory and methods of nonlinear optimization.*

We thank all Program Committee members and external reviewers for their cooperation. We also thank the Organizing Committee members and our sponsors: the Russian Foundation for Basic Research, the Far Eastern Federal University, Novosibirsk State University, the Laboratory of Algorithms and Technologies for Networks Analysis, the Higher School of Economics in Nizhny Novgorod for supporting our project.

September 2016

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Abstract. In this paper we develop a new mathematical formulation for chemical compositional reservoir simulation, and provide a comparison of its results on alkaline-surfactant-polymer flooding with those of UTCHEM simulator. Our research has found that the existing chemical compositional model estimates the adsorption effect on the transport of a component reasonably well but it does not satisfy the principle of mass conservation. Since the total mass conservation equation follows from summing the species-conservation equations over all components, the obtained equation violates the principle of total mass conservation as well. With these partial differential equations as governing equations, several simulators have been developed. In this work, we propose an approach to model the change in pore volume due to adsorption that satisfies the mass conservation law, and allows applying a sequential solution approach.

Keywords: chemical compositional model,surfactant, porosity, adsorption

1 Introduction

Chemical flooding is one of the most promising and broadly applied enhanced oil recovery (EOR) processes. Chemical flooding can be further subdivided into alkaline flooding, surfactant flooding, polymer flooding, and alkaline-surfactant-polymer (ASP) flooding. Alkali reduces adsorption of the surfactant on the rock surfaces and reacts with acids in the oil to create natural surfactant. Surfactants are chemicals that used to reduce the interfacial tension between the involved fluids, increasing oil mobility. ASP flooding is a form of chemical EOR method that can allow operators to extend reservoir pool life and extract incremental reserves currently inaccessible by conventional methods. While ASP flooding has a high efficiency it is technical, costly, and risky. Model studies can assist in this evaluation.

Most multiphase compositional models reported in the literature [1], [2], [3], [4] and [5] are limited in their applicability in one way or another (single species, equilibrium mass transfer, and lack of miscibility modeling etc). The mathematical formulation

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developed in this work is extended from the UTCHEM model formulation for use in chemical flooding studies that does not have these common limitations.

Sequential schemes are very suitable for chemical compositional flow problems which include a large number of chemical components. Only the implicit pressure and explicit composition (IMPEC) formulation was used for chemical compositional reservoir simulation so far, but there is no obvious reason why the sequential formulation can't be used as well. Because of explicit solution of compositions, the size of time steps is limited to stabilize the general procedure.

Chen et al. [6] presented a numerical approach that solves both pressure and compositions implicitly. Though the approach was claimed to be sequential and extended from the IMPEC approach used in UTCHEM model [7], the mathematical formulations for the governing equations did not undergo any change in their model.

The basic equations used in UTCHEM model that describe multiphase, multicomponent flow in permeable media are the species-conservation, pressure (an overall mass-continuity), and energy conservation equations. Accumulation terms in the species-conservation equations used in UTCHEM model account for the reduction in pore volume caused by adsorption.

During the process of this research, it was revealed that this commonly used approach estimates the adsorption effect on the transport of a component reasonably well but it does not satisfy the species-conservation equation. Since the total mass conservation equation follows from summing the species-conservation equations over all components, the obtained equation violates the principle of total mass conservation as well. In recent years with use of these governing equations several simulators were developed for simulation of the chemical flooding processes [6], [7], [8] and [9].

In this work we introduce a new approach to model the reduction in pore volume due to adsorption that satisfies the conservation equations. In certain situations, such as significant change in the effective pore size due to adsorption, these enhancements are essential to properly model the physical phenomena occurring in petroleum reservoirs. In addition, this new approach for modeling the adsorption effect on the transport of a component makes it possible to develop a new mathematical formulation for the sequential chemical compositional reservoir simulation.

2 Mathematical model

Consider a bulk volume V_b at some point within a porous medium domain. Let us assume that this representative elementary volume (REV) is made up of $n_p + 1$ phases (n_p fluid phases and a solid phase consisting of rock grains or soil) with n_c chemical species. Conceivably, at least, each species can exist in any phase and can transfer between phases via evaporation, condensation, dissolution, adsorption and so forth.

In our model formalism, each pair (i, α), with i chosen from the species indices and α chosen from the phases, is a constituent. Each constituent (i, α) has its own intrinsic mass density $\rho_{i\alpha}$, measured as mass of i per unit volume of α, and its own average velocity $\overrightarrow{u}_{i\alpha}$. Each phase α has its own volume fraction ϕ_α. The volume fraction of phase α, ϕ_α, is the volume of phase α divided by the bulk volume V_b.

If the index n_c represents the species and the index n_p+1 represents the phases making up the solid phase, then in terms of the above defined mechanical variables the mass balance for each constituent (i, α) is

$$\frac{\partial}{\partial t}(\phi_\alpha \rho_{i\alpha}) + \nabla \cdot (\phi_\alpha \rho_{i\alpha} \overrightarrow{u}_{i\alpha}) = R_{i\alpha} + r_{mi\alpha} + q_{i\alpha}, \quad \left\{ \begin{array}{c} i = 1, ..., n_c, \\ \alpha = 1, ..., n_p + 1. \end{array} \right\} \tag{1}$$

From left to right in Eq. (1), the terms are now the accumulation, transport, and source terms, the last consisting of three types. The mass fraction of component i in phase α in V_b is defined to be $\omega_{i\alpha}$. The parameter $\omega_{i\alpha}$ is the mass of component i in phase α divided by mass of the phase. Hence, $\sum_{i=1}^{n_c} \omega_{i\alpha} = 1$. With that definition,

$$\rho_{i\alpha} = \rho_\alpha \omega_{i\alpha}, \qquad \{ i = 1, ..., n_c, \quad \alpha = 1, ..., n_p + 1, \} \tag{2}$$

where ρ_α is intrinsic mass density of phase α.

The source term $R_{i\alpha}$ accounts for the rate of mass generation ($R_{i\alpha} > 0$) and consumption ($R_{i\alpha} < 0$) of component i in phase α, either through chemical or biological reactions. There is no general function for $R_{i\alpha}$. An example of a first-order reaction rate for radioactive decay or biodegradation is

$$R_{i\alpha} = -k_i \phi_\alpha \rho_\alpha \omega_{i\alpha}, \qquad \{ i = 1, ..., n_c, \quad \alpha = 1, ..., n_p + 1, \} \tag{3}$$

where k_i is the decay constant or reaction rate coefficient in units of inverse time.

The second source term $r_{mi\alpha}$ expresses the rate of mass transfer of component i from or into the phase α owing to vaporization or condensation. Adsorption is described through isotherms.

The last source term in Eq. (1) $q_{i\alpha}$ represents physical sources (wells).

Substitution of Eqs.(2) and (3) into Eq. (1) gives:

$$\begin{gathered} \frac{\partial}{\partial t}(\phi_\alpha \rho_\alpha \omega_{i\alpha}) + \nabla \cdot (\phi_\alpha \rho_\alpha \omega_{i\alpha} \overrightarrow{u}_{i\alpha}) = -k_i \phi_\alpha \rho_\alpha \omega_{i\alpha} + r_{mi\alpha} + q_{i\alpha}, \\ \{ i = 1, ..., n_c, \quad \alpha = 1, ..., n_p + 1. \} \end{gathered} \tag{4}$$

From definition, volume fractions must obey the constraint $\sum_{\alpha=1}^{n_p+1} \phi_\alpha = 1$. It is well known that the porosity ϕ is defined as the fraction of the bulk permeable medium that is pore space, that is, the pore volume V_p divided by the bulk volume V_b. The fact that the all fluid phases jointly fill the voids (pores) implies the relation $\sum_{\alpha=1}^{n_p} \phi_\alpha = \phi$.

The phase saturation S_α is defined as the fraction of the pore volume occupied by phase α, that is, volume of phase α V_α divided by the pore volume V_p. The saturation of fluid phase α can also be defined as $S_\alpha = \phi_\alpha / \phi$. For fluid phases such as liquids and vapors, $\phi_\alpha = \phi S_\alpha$, $\alpha = 1, ..., n_p$, where ϕS_α also called the fluid content. For the solid (s) phase $\phi_s = 1 - \phi$, which is the grain volume divided by the bulk volume V_b. We can rewrite equation (4) in the following form by noting that the porosity is $\phi = 1 - \phi_s$ and defining the fluid saturations $S_\alpha = \phi_\alpha / \phi, \alpha = 1, ..., n_p$:

$$\begin{gathered} \frac{\partial}{\partial t}(\phi S_\alpha \rho_\alpha \omega_{i\alpha}) + \nabla \cdot (\phi S_\alpha \rho_\alpha \omega_{i\alpha} \overrightarrow{u}_{i\alpha}) = -k_i \phi S_\alpha \rho_\alpha \omega_{i\alpha} + r_{mi\alpha} + q_{i\alpha}, \\ \{ i = 1, ..., n_c, \quad \alpha = 1, ..., n_p, \} \end{gathered} \tag{5}$$

for the fluids, and if we fix a coordinate system in which $\vec{u}_{is} = 0$, and note that $q_{is} = 0$, then the momentum balance for the solid phase reduces to

$$\frac{\partial}{\partial t}((1-\phi)\rho_s\omega_{is}) = -k_i(1-\phi)\rho_s\omega_{is} + r_{mis}, \qquad \{i = 1, ..., n_c.\} \tag{6}$$

The statistical average apparent velocity of constituent (i, α) owing to both convection and dispersion is the sum of the barycentric velocity of phase α and the diffusion velocity of species i in phase α:

$$\vec{u}_{i\alpha} = \vec{u}_{\alpha} + \vec{u}_{i\alpha}, \qquad \{i = 1, ..., n_c, \quad \alpha = 1, ..., n_p.\} \tag{7}$$

Since phase velocities are typically more accessible to measurement than species velocities, it is convenient to rewrite the constituent mass balance equation (5) as

$$\begin{aligned} \frac{\partial}{\partial t}(\phi S_\alpha \rho_{i\alpha}) + \nabla \cdot (\phi S_\alpha \rho_{i\alpha} \vec{u}_{i\alpha}) + \nabla \cdot \vec{J}_{Di\alpha} = -k_i \phi S_\alpha \rho_{i\alpha} + r_{mi\alpha} + q_{i\alpha}, \\ \{i = 1, ..., n_c, \quad \alpha = 1, ..., n_p,\} \end{aligned} \tag{8}$$

where $\vec{J}_{Di\alpha} = \phi S_\alpha \rho_{i\alpha} \vec{u}_{i\alpha}$ stands for the diffusive flux of constituent (i, α).

So far, the mathematical formulation of the mass conservation equations developed above is essentially the same as the standard formulation described in [7]; where it differs is in the treatment of average velocity in the governing equations. Here we start to deviate from the standard formulation.

The fluxes of component i in phase α with respect to volume-averaged velocity $\vec{J}_{Di\alpha} = -\phi S_\alpha \bar{\bar{K}}_{i\alpha} \cdot \nabla(\rho_\alpha \omega_{i\alpha})$ and mass-averaged velocity $\vec{J}_{Di\alpha} = -\phi S_\alpha \bar{\bar{K}}_{i\alpha} \cdot \nabla(\omega_{i\alpha})$ owing to hydrodynamic dispersion alone were presented in [10]. The flux with respect to bulk volume-averaged velocity is proposed in this work:

$$\vec{J}_{Di\alpha} = -\bar{\bar{K}}_{i\alpha} \cdot \nabla(\phi S_\alpha \rho_\alpha \omega_{i\alpha}), \qquad \{i = 1, ..., n_c, \quad \alpha = 1, ..., n_p,\} \tag{9}$$

Two components of $\bar{\bar{K}}_{i\alpha}$ for a homogeneous, isotropic permeable medium [11] are

$$\begin{aligned} (K_{xx})_{i\alpha} &= \frac{D_{i\alpha}}{\tau} + \frac{\alpha_{l\alpha} u_{x\alpha}^2 + \alpha_{t\alpha}(u_{y\alpha}^2 + u_{z\alpha}^2)}{|\vec{u}_\alpha|}, \\ (K_{xy})_{i\alpha} &= \frac{(\alpha_{l\alpha} - \alpha_{t\alpha}) u_{x\alpha} u_{y\alpha}}{|\vec{u}_\alpha|}, \end{aligned} \qquad \left\{ \begin{aligned} i &= 1, ..., n_c, \\ \alpha &= 1, ..., n_p, \end{aligned} \right\} \tag{10}$$

where the subscript l refers to the spatial coordinate in the direction parallel, or longitudinal, to bulk flow, and t is any direction perpendicular, or transverse, to l. $D_{i\alpha}$ is the effective binary diffusion coefficient of component i in phase α [12], $\alpha_{l\alpha}$ and $\alpha_{t\alpha}$ are the longitudinal and transverse dispersivities, and τ is the permeable medium tortuosity.

A general set of partial differential equations (11) for the conservation of component i in fluid phase α is obtained upon substitution of the definition for flux (Eq. (9)) into Eq. (8):

$$\begin{aligned} &\frac{\partial}{\partial t}(\phi S_\alpha \rho_\alpha \omega_{i\alpha}) + \nabla \cdot (\phi S_\alpha \rho_\alpha \omega_{i\alpha} \vec{u}_{i\alpha}) - \bar{\bar{K}}_{i\alpha} \cdot \nabla(\phi S_\alpha \rho_\alpha \omega_{i\alpha}) = \\ &= -k_i \phi S_\alpha \rho_\alpha \omega_{i\alpha} + r_{mi\alpha} + q_{i\alpha}, \qquad \{i = 1, ..., n_c, \quad \alpha = 1, ..., n_p,\} \end{aligned} \tag{11}$$

The term $r_{mi\alpha}$ is difficult to calculate without detailed analysis of the transport occurring within the phases. One typically simplifies the equations by using overall compositional balance equations. Overall compositional balance equations can be obtained by summing Eqs. (6) and (11) over the solid and n_p fluid phases:

$$\begin{aligned}&\frac{\partial}{\partial t}\left[\sum_{\alpha=1}^{n_p}\phi S_\alpha\rho_{i\alpha}+(1-\phi)\rho_{is}\right]+\nabla\cdot\sum_{\alpha=1}^{n_p}(\phi S_\alpha\rho_{i\alpha}\overrightarrow{u}_\alpha)-\\&-\nabla\cdot\sum_{\alpha=1}^{n_p}[\bar{\bar{K}}_{i\alpha}\cdot\nabla(\phi S_\alpha\rho_{i\alpha})]=-k_i\left[\sum_{\alpha=1}^{n_p}\phi S_\alpha\rho_{i\alpha}+(1-\phi)\rho_{is}\right]+Q_i,\\&\qquad\{i=1,...,n_c,\}\end{aligned}\tag{12}$$

where $Q_i=\sum_{\alpha=1}^{n_p}q_{i\alpha}$ is the injection/production rate for component i per bulk volume. We have $\sum_{\alpha=1}^{n_p+1}r_{mi\alpha}=0$, a relation following from the inability to accumulate mass at a volumeless phase interface.

In equation (12), expressing the content of component i in phase α in terms of volume fraction

$$\left.\begin{aligned}&\rho_\alpha\omega_{i\alpha}=\rho_i c_{i\alpha},\quad \alpha=1,...,n_p\\&(1-\phi)\rho_s\omega_{is}=\phi\rho_i\hat{c}_i,\end{aligned}\right\}\qquad\{i=1,...,n_c,\}\tag{13}$$

we get

$$\begin{aligned}&\frac{\partial}{\partial t}\left[\phi\rho_i\left(\sum_{\alpha=1}^{n_p}S_\alpha c_{i\alpha}+\hat{c}_i\right)\right]+\nabla\cdot\phi\rho_i\sum_{\alpha=1}^{n_p}(S_\alpha c_{i\alpha}\overrightarrow{u}_\alpha)-\\&-\nabla\cdot\sum_{\alpha=1}^{n_p}\left[\bar{\bar{K}}_{i\alpha}.\nabla(\phi\rho_i S_\alpha c_{i\alpha})\right]=-k_i\phi\rho_i\left(\sum_{\alpha=1}^{n_p}S_\alpha c_{i\alpha}+\hat{c}_i\right)+Q_i,\\&\qquad\{i=1,...,n_c,\}\end{aligned}\tag{14}$$

where ρ_i is the component mass density in units of mass of i per unit volume of i, $c_{i\alpha}$ is the component concentration in units of volume of i in phase α per unit volume of α, and $\hat{c}_i$ is the adsorbed component concentration, measured as volume of i in phase α per unit pore volume. The linear, Freundlich and Langmuir adsorption isotherm models are applied to calculate the adsorbed concentrations $\hat{c}_i$. In our definition

$$\sum_{i=1}^{n_c}\left(\sum_{\alpha=1}^{n_p}S_\alpha c_{i\alpha}+\hat{c}_i\right)=1,\tag{15}$$

but

$$\sum_{i=1}^{n_c}\sum_{\alpha=1}^{n_p}S_\alpha c_{i\alpha}\neq 1,\tag{16}$$

unlike existing model. To account for the reduction in pore volume caused by adsorption, the coefficient $(1-\sum_{i=1}^{n_{cv}}\hat{c}_i)$ is introduced into the overall compositional balance equation (14) in UTCHEM model. The coefficient represents reduction in pore volume due to adsorption, $\hat{c}_i$ is the adsorbed concentration of species i, and n_{cv} is the total number of volume-occupying components. During the process of this research, it was revealed that even though this approach estimates the adsorption effect on the transport of a component reasonably well, it does not satisfy the species-conservation equation since the coefficient is multiplied only to the first summand of the accumulation term in Eq. (14). It is well known that an equation remains balanced when both sides of an equation are multiplied by the same nonzero quantity.

In the present work we introduce a new approach to model the reduction in pore volume due to adsorption that satisfies the continuity equation. Let us denote the modified volume fraction of phase α due to adsorption by $\hat{\phi}_\alpha$. Porosity $\hat{\phi}$ is defined as the fraction of the bulk permeable medium that is pore space remaining after adsorption. This porosity is related to the original porosity ϕ as follows:

$$\hat{\phi} = \phi\left(1 - \sum_{i=1}^{n_{cv}} \hat{c}_i\right). \tag{17}$$

The saturation of fluid phase α is defined as $S_\alpha = \hat{\phi}_\alpha / \hat{\phi}$. Now using the same derivation procedure as carried out above, we obtain

$$\begin{aligned} &\frac{\partial}{\partial t}\left[\hat{\phi}\rho_i\left(\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} + \hat{c}_i\right)\right] + \nabla\cdot\hat{\phi}\rho_i\sum_{\alpha=1}^{n_p}(S_\alpha c_{i\alpha}\overrightarrow{u}_\alpha) - \\ &-\nabla\cdot\sum_{\alpha=1}^{n_p}\left[\bar{\bar{K}}_{i\alpha}\cdot\nabla(\hat{\phi}\rho_i S_\alpha c_{i\alpha})\right] = -k_i\hat{\phi}\rho_i\left(\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} + \hat{c}_i\right) + Q_i, \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \{i = 1, ..., n_c,\} \end{aligned} \tag{18}$$

The phase flux from Darcy's law is

$$\overrightarrow{u}_\alpha = -\frac{\bar{\bar{k}} k_{r\alpha}}{\hat{\phi} S_\alpha \mu_\alpha}(\nabla p_\alpha - \gamma_\alpha \nabla z), \qquad \{\alpha = 1, ..., n_p,\} \tag{19}$$

where $\bar{\bar{k}}$ is the permeability tensor, $k_{r\alpha}$ is the relative permeability of fluid phase α, μ_α is the dynamic viscosity of fluid phase α, p_α is the pressure in fluid phase α, γ_α is the specific weight for fluid phase α, and z represents depth.

Variation of pore volume with pore pressure p can be taken into account by the pressure dependence of porosity. The porosity depends on pressure due to rock compressibility, which is often assumed to be constant and can be defined as

$$\phi = \phi_R[1 + c_f(p_1 - p_s)], \tag{20}$$

where ϕ_R is the porosity at a specific pressure p_s, p_1 is the water phase pressure, and c_f is the pore compressibility at p_s.

A slightly compressible fluid has a small but constant compressibility. For a slightly compressible fluid, the component density ρ_i can be written as:

$$\rho_i = \rho_{iR}[1 + c_i^0(p_1 - p_R)], \qquad \{i = 1, ..., n_c,\} \tag{21}$$

where ρ_{iR} is the density of component i at the standard pressure p_R, a constant value, c_i^0 is the compressibility of component i.

Now since reference density ρ_{iR} is constant for each component we can divide through both sides of Eq. (18) by ρ_{iR}. In terms of the dimensionless density $\bar{\rho}_i = \rho_i/\rho_{iR}$ Eq. (18) can be written as:

$$\frac{\partial}{\partial t}\left[\hat{\phi}\bar{\rho}_i\left(\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} + \hat{c}_i\right)\right] + \nabla\cdot\hat{\phi}\bar{\rho}_i\sum_{\alpha=1}^{n_p}(S_\alpha c_{i\alpha}\vec{u}_\alpha) - \\ -\nabla\cdot\sum_{\alpha=1}^{n_p}\left[\bar{\bar{K}}_{i\alpha}\cdot\nabla(\hat{\phi}\bar{\rho}_i S_\alpha c_{i\alpha})\right] = -k_i\hat{\phi}\bar{\rho}_i\left(\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} + \hat{c}_i\right) + \frac{Q_i}{\rho_{iR}}, \\ \{i = 1, ..., n_c,\} \tag{22}$$

We sum the mass balance equations above over the n_c components to obtain the equation of continuity, or conservation of total mass. The equation of continuity is

$$\phi F_t(\tilde{c}_i, \hat{c}_i) + \hat{\phi}_R c_t \frac{\partial p_1}{\partial t} + \nabla\cdot\left\{\hat{\phi}\sum_{\alpha=1}^{n_p}(S_\alpha\vec{u}_\alpha\sum_{i=1}^{n_c}\bar{\rho}_i c_{i\alpha})\right\} = \sum_{i=1}^{n_c}\frac{Q_i}{\rho_{iR}}, \tag{23}$$

where we used that

$$\sum_{i=1}^{n_c}\nabla\cdot\vec{J}_{D i\alpha} = 0, \qquad \{\alpha = 1, ..., n_p,\} \tag{24}$$

(net dispersive flux in a phase is zero), and according to the total reaction definition

$$\sum_{i=1}^{n_c}\left(\sum_{\alpha=1}^{n_p} R_{i\alpha} + R_{is}\right) = 0. \tag{25}$$

The total compressibility, c_t, is

$$c_t = \left(1 - \sum_{i=1}^{n_{cv}}\hat{c}_i\right)\left\{c_f + \left[1 + c_f(2p_1 - p_s - p_R)\right]\sum_{i=1}^{n_c}(c_i^0\tilde{c}_i)\right\}, \tag{26}$$

and

$$F_t(\tilde{c}_i, \hat{c}_i) = (p_1 - p_R)\frac{\partial}{\partial t}\left[\left(1 - \sum_{i=1}^{n_{cv}}\hat{c}_i\right)\sum_{i=1}^{n_c} c_i^0\tilde{c}_i\right] - \frac{\partial}{\partial t}\left(\sum_{i=1}^{n_{cv}}\hat{c}_i\right). \tag{27}$$

We define the overall concentration $\tilde{c}_i$ as

$$\tilde{c}_i = \sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} + \hat{c}_i, \qquad \{i = 1, ..., n_c,\} \tag{28}$$

and by definition

$$\sum_{i=1}^{n_c}\tilde{c}_i = 1. \tag{29}$$

The pressure equation is developed by substituting Darcy's law (Eq. (19)) for the phase flux term of Eq. (23), using the definition of capillary pressure $p_{c\alpha 1} = p_\alpha - p_1, \alpha = 2, ..., n_p$. The pressure equation in terms of the reference phase (phase 1) pressure is

$$\begin{aligned}\hat{\phi}_R c_t \frac{\partial p_1}{\partial t} - \nabla \cdot \left(\bar{\bar{k}} \lambda_{rTc} \nabla p_1\right) = \nabla \cdot \left(\bar{\bar{k}} \sum_{\alpha=2}^{n_p} \lambda_{r\alpha c} \nabla p_{c\alpha 1}\right) - \\ -\nabla \cdot \left(\bar{\bar{k}} \sum_{\alpha=1}^{n_p} \lambda_{r\alpha c} \gamma_\alpha \nabla z\right) - \phi F_t(\tilde{c}_i, \hat{c}_i) + \sum_{i=1}^{n_c} \frac{Q_i}{\rho_{iR}},\end{aligned} \tag{30}$$

where

$$\lambda_{r\alpha c} = \lambda_{r\alpha} \sum_{i=1}^{n_c} \bar{\rho}_i c_{i\alpha}, \qquad \{\alpha = 1, ..., n_p,\} \tag{31}$$

and total relative mobility is

$$\lambda_{rTc} = \sum_{\alpha=1}^{n_p} \lambda_{r\alpha c}. \tag{32}$$

The extension of the LET correlations is used to represent the relative permeability and capillary pressure curves [13], [14].

Applying the mean value estimate for character sums in Eq. (22), we can write

$$\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} \vec{u}_\alpha = \vec{u}_i \sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha}, \qquad \{i = 1, ..., n_c,\} \tag{33}$$

and

$$\sum_{\alpha=1}^{n_p} \bar{\bar{K}}_{i\alpha} \cdot \nabla(\hat{\phi} \bar{\rho}_i S_\alpha c_{i\alpha}) = \bar{\bar{\bar{K}}}_i \cdot \sum_{\alpha=1}^{n_p} \nabla\left(\hat{\phi} \bar{\rho}_i S_\alpha c_{i\alpha}\right), \qquad \{i = 1, ..., n_c,\} \tag{34}$$

where $\vec{u}_i$ and $\bar{\bar{\bar{K}}}_i$ can be defined as some averages. Since differentiation and summation are interchangeable operations in this system, the sum of the gradients can be calculated as the gradient of the sum

$$\bar{\bar{\bar{K}}}_i \cdot \sum_{\alpha=1}^{n_p} \nabla\left(\hat{\phi} \bar{\rho}_i S_\alpha c_{i\alpha}\right) = \bar{\bar{\bar{K}}}_i \cdot \nabla\left(\hat{\phi} \bar{\rho}_i \sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha}\right), \qquad \{i = 1, ..., n_c.\} \tag{35}$$

Equation (22) can be written using Eqs. (33), (34), and (35) as below:

$$\begin{aligned}\frac{\partial}{\partial t}\left[\hat{\phi} \bar{\rho}_i \left(\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} + \hat{c}_i\right)\right] + \nabla \cdot \left(\hat{\phi} \bar{\rho}_i \vec{u}_i \sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha}\right) - \\ -\nabla \cdot \left[\bar{\bar{\bar{K}}}_i \cdot \nabla\left(\hat{\phi} \bar{\rho}_i \sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha}\right)\right] = -k_i \hat{\phi} \bar{\rho}_i \left(\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} + \hat{c}_i\right) + \frac{Q_i}{\rho_{iR}}, \\ \{i = 1, ..., n_c,\}\end{aligned} \tag{36}$$

This new mathematical formulation of species conservation equations makes it possible to apply a sequential solution approach to solve these equations implicitly for the total concentration $\sum_{\alpha=1}^{n_p} S_\alpha c_{i\alpha}$ of each component. A flash calculation is then performed to obtain the phase saturations and the concentrations of components in each phase. Numerical values of $\overrightarrow{u}_i$ and $\bar{\bar{\tilde{K}}}_i$ can be most simply calculated as the weighted averages

$$\overrightarrow{u}_i = \frac{\sum\limits_{\alpha=1}^{n_p} S_\alpha c_{i\alpha} \overrightarrow{u}_\alpha}{\sum\limits_{\alpha=1}^{n_p} S_\alpha c_{i\alpha}}, \quad \bar{\bar{\tilde{K}}}_i = \frac{\sum\limits_{\alpha=1}^{n_p} \bar{\bar{K}}_{i\alpha} \cdot \nabla(\hat{\phi}\rho_i S_\alpha c_{i\alpha})}{\nabla\left(\hat{\phi}\rho_i \sum\limits_{\alpha=1}^{n_p} S_\alpha c_{i\alpha}\right)}, \quad \{i = 1, ..., n_c,\} \qquad (37)$$

obtained from previous time-step values.

The sequential solution procedure is carried out in the following order: (a) solution of the pressure equation (30) implicitly, (b) solution of the transport system of equations (36) implicitly for the total concentration of each component.

Details about the derivation of the mathematical model formulation are provided in our previous publication [15].

3 Numerical Results

ASP flooding is the most promising EOR solution for one of the greatest challenges facing the oil industry worldwide: after conventional water flooding the residual oil (drops trapped by capillary forces) in reservoirs around the world is likely to be around 70% of the original oil in place. The mathematical formulation is evaluated in the modeling of a field scale ASP EOR process.

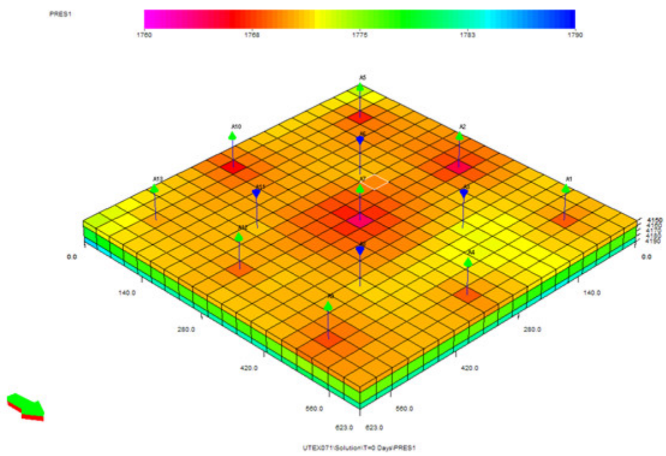

Fig. 1. Computational domain and well pattern illustration

As illustrated in Fig. 1, the ASP flooding pilot has 4 injection wells and 9 production wells in an inverted five-spot well pattern. The ASP process was conducted in a 4-slug sequence: pre-flush polymer flood, alkaline/surfactant slug, alkaline/surfactant/polymer slug, and a polymer drive. Total simulation time is 551 days. Reservoir properties include heterogeneous permeability and initial water saturation fields. The reservoir is at a depth of 4150 ft., has an average initial pressure of 1770 psi, and the porosity is assumed to be constant throughout the reservoir and equal to 0.3. Grid dimensions are $19 \times 19 \times 3$. The OOIP is 395,427 bbls, the crude oil viscosity is 40 cp, the initial brine salinity is 0.0583 meq/ml and the initial brine divalent cation concentration is 0.0025 meq/ml.

We use S3GRAF software, developed and licensed by Sciencesoft Ltd., for post-processing the output data.

Three flowing phases and eleven components are considered in the numerical simulations. The phases are water, oil and microemulsion, while the components are water, oil, surfactant, polymer, chloride anions, divalent cations (Ca++, Mg++), carbonate, sodium, hydrogen ion, and oil acid. The ASP interactions are modeled using the reactions: in situ generated surfactant, precipitation and dissolution of minerals, cation exchange with clay and micelle, and chemical adsorption. Note the detailed chemical reaction modeling, and the heterogeneous and multiphase petroleum reservoir under consideration.

A comparison with UTCHEM has also been performed. The matches between old and new formulations' numerical results for the matched variables are shown in Figs. 2-5 for the injected pore volume in the range 0 - 1.0 PV. Comparative studies show that

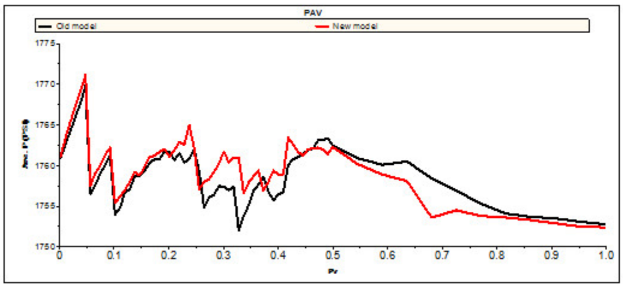

Fig. 2. Average pressure vs. total injected pore volume

the results obtained from IMPEC implementation of the newly proposed formulation are in a good agreement with that of UTCHEM simulator. In the scope of this research work, through its application to the above-mentioned numerical experiment and comparisons with UTCHEM model results, the newly developed formulation has proven to be reliable, practical, and accurate. The mathematical model and numerical simulation developed in this work can also be used to study the transport of contaminants and

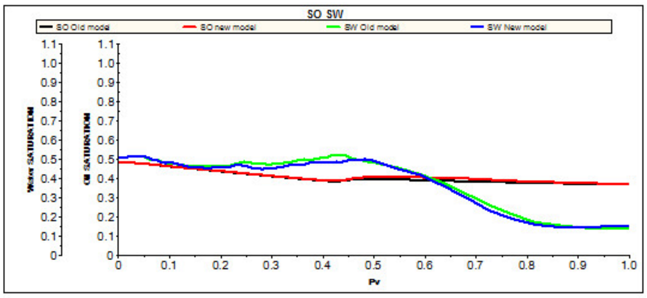

Fig. 3. Oil and water saturations vs. total injected pore volume

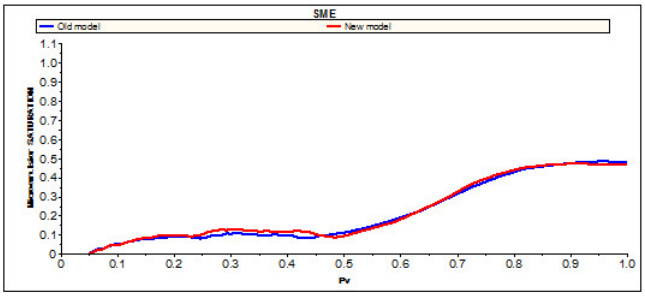

Fig. 4. Microemulsion saturation vs. injected pore volume

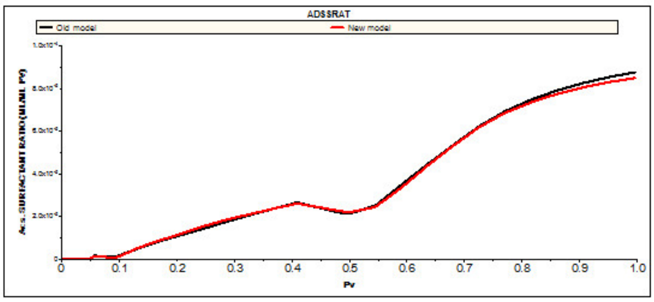

Fig. 5. Adsorbed surfactant ratio (ML per ML of pore volume) vs. injected pore volume

remediation of contaminated aquifers surfactants.

4 Conclusion

In the scope of this research work, a new mathematical model formulation for multicomponent, multiphase flow in porous media has been developed. During the process of this research, it was revealed that commonly used approach estimates the adsorption effect on the transport of a component reasonably well but it does not satisfy the mass conservation or continuity equation. In the present work we introduce a new approach to model the reduction in pore volume due to adsorption that satisfies the continuity equation. The mathematical formulation developed in the scope of this work is extended from the UTCHEM model formulation for use in chemical flooding studies. A comparison with UTCHEM has also been performed. Comparative studies show that the results obtained from IMPEC implementation of the newly proposed formulation are in a good agreement with that of UTCHEM simulator. The implementation of a sequential solution approach for chemical compositional reservoir simulation based on the formulation described in this paper is scheduled for the future.

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