Paper A

A Black-Oil and Compositional IMPSAT Simulator With Improved Compositional Convergence *

B017 A BLACK-OIL AND COMPOSITIONAL IMPSAT SIMULATOR WITH IMPROVED COMPOSITIONAL CONVERGENCE

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Abstract

A unified black-oil and compositional simulator has been developed, using an IMPSAT formulation within the framework of the Volume Balance Method. By new ways of determining explicit equations and variables, we obtain improved convergence over the traditional compositional formulations. In addition, simulator maintenance and development costs are reduced due to the unified formulation.

Application of the new formulation to simulation of a multiphase, multicomponent problem is presented in the paper.

Introduction

Reservoir Simulation in General

All reservoir simulators solve a set of differential equations. If the reservoir fluids consist of N_c chemical components (methane, ethane, water, etc.), N_c flow equations must be solved.

Two main types of simulators are currently commercially available: black-oil simulators and compositional simulators (e.g., [1]).

In a black-oil formulation, it is assumed that the hydrocarbon fluids may be sufficiently described by two components, a (pseudo) oil component and a (pseudo) gas component.

In a compositional formulation, an arbitrary number of hydrocarbon components can be included. This yields a more precise fluid description, but because of impractically large runtimes with the conventional formulations, black-oil simulators are often preferred to compositional simulators.

The development of multipurpose/general purpose simulators has for several years been subject to research (e.g., [2, 3, 4]). However, a successful unified black-oil and compositional simulator has not yet been presented in literature. This is mainly due to the lack of an inherent compositional formulation superior to the conventional. Improved compositional convergence is related to choice and treatment of variables and equations.

The starting point of any isothermal black-oil or compositional formulation is the set of N_c component conservation equations. These equations may be used in their conventional form, or in a modified form, as the N_c primary equations of the model.

With a fully implicit formulation, all the flow equations are solved implicitly (i.e., simultaneously) with respect to N_c primary variables. Fully implicit formulations are unconditionally stable, but require extensive computational effort. This motivates the use of approaches that are not fully implicit.

Let N_{impl} denote the number of implicit variables, and let N_{expl} denote the number of explicit variables, so that $N_{\text{impl}} + N_{\text{expl}} = N_c$. By fixing the explicit variables at the previous timestep, we are able to form N_{impl} equations determining the implicit variables at the new timestep. In the remaining equations we still fix the values of the explicit variables in the interblock flow terms, and make use of the determined values of the implicit variables. The explicit variables can then be determined one by one (explicitly).

Explicit treatment of variables may introduce stability problems that restrict timestep size. The stability criteria of a formulation depend on the choice of implicit and explicit variables and equations.

Conventional Formulations

In black-oil formulations where N_c equals N_p, the number of phases, one pressure and $N_p - 1$ saturations are chosen as primary variables. If one of the hydrocarbon phases (oil or gas) is not present, the corresponding saturation variable is replaced by the gas-oil ratio.

Because the number of flow equations is small, fully implicit black-oil simulations are often feasible. Alternatively, an IMPES approach is used: pressure is determined implicitly, while saturations are calculated explicitly. The motivation for treating pressure implicitly is that pressure changes spread instantly throughout the reservoir. Since the thermodynamic properties of a black-oil system depend only on pressure, the black-oil IMPES pressure equation is obtained by summing the black-oil conservation equations (thus eliminating the saturation terms from the accumulation term).

In many compositional problems, a fully implicit approach would require too much computational effort. Therefore, the conventional compositional

simulator uses an IMPES-like approach, where one pressure is calculated implicitly, and saturations and phase compositions are determined explicitly.

The sum of component conservation equations is not a suitable compositional IMPES pressure equation, since the thermodynamic properties of the accumulation terms are not solely dependent on pressure. In [5], Ács, Doleschall and Farkas presented a Volume Balance Method that correctly eliminates the saturation/concentration terms from the accumulation term of the pressure equation. The volume balance pressure equation is formed as a weighted sum of the component conservation equations, and is the unique IMPES pressure equation for compositional simulation (e.g., Coats, [6]).

The conventional compositional formulation uses pressure and component masses as primary variables, and does not reduce to black-oil IMPES when used with black-oil fluid properties.

New Compositional Approaches

IMPES is the fastest approach on a per-timestep basis, but it can have stability problems that restrict timestep size. This has given rise to the IMPSAT formulation, which is implicit in both pressure and saturations.

IMPSAT is motivated by Darcy's law, which is basically a relation between pressure and volumes (saturations). By solving for pressure and saturations implicitly, we obtain a good starting point for solving the total system consistently. The remaining variables to be determined should have little or no influence on the volume solution. Consequently, IMPSAT relaxes the timestep restrictions of the conventional IMPES approach.

IMPSAT (or IMPSAT-like) approaches reported in literature, [7, 8, 9, 10], differ in their choices of pressure and saturation equations, and in their choice of additional (explicit) primary variables and equations.

Watts, [7], generalized the Volume Balance Method of Ács, Doleschall and Farkas, and developed a set of volume balance saturation equations, formed as weighted sums of the component conservation equations. He showed that the volume balance saturation equations reduce to the conventional black-oil equations when used with black-oil fluid properties. In Watts' formulation, all phase compositions are treated explicitly when determining pressure and saturations. The following explicit update of $N_c - 1$ (independent) overall compositions is based on the N_c original component conservation equations. Consequently, $N_p + N_c - 1$ parameters are determined with only N_c flow equations. Watts commented that this inherent inconsistency may lead to inaccuracies.

In [8], Quandalle and Savary presented a consistent IMPSAT approach, addressing the shortcoming of Watts' approach. Here $N_c - N_p$ additional variables were introduced, referred to as Ci. These variables characterize the composition of the oil and gas phases at thermodynamic equilibrium. Instead of treating all phase compositions explicitly, only the Ci are fixed when determining pressure and saturations. The Ci are then determined explicitly by $N_c - N_p$ of the component conservation equations.

The Quandalle and Savary approach provides a certain adaptivity in the choice of Ci. In oil dominant regions, the Ci are chosen as $N_c - N_p$ of the oil mole fractions, while in gas dominant regions, the Ci are chosen among the gas mole fractions. In both cases the mole fractions corresponding to the lightest and the heaviest component are excluded. As additional primary equations for determining the Ci, Quandalle and Savary chose the corresponding $N_c - N_p$ component conservation equations.

Quandalle and Savary's choice of primary variables is based on the assumption that the gas saturation is closely related to the amount of the lightest component, while the oil saturation is related to the amount of the heaviest component. Consequently, the mole fractions of the lightest and the heaviest component should not be treated explicitly when determining pressure and saturations.

However, the lightest and the heaviest component may not always be representative of the gas and oil phase, respectively. For example, the total hydrocarbon composition may be evenly distributed between the components, and the lightest component may not always be the most volatile. The Quandalle and Savary approach is therefore not general.

The approaches of Watts and Quandalle and Savary are based on the Volume Balance Method. Branco and Rodríguez, [9], and Cao and Aziz, [10], used reduction of a linearized system of conservation equations to form pressure and saturation equations, keeping all phase compositions fixed. Cao and Aziz reported that the IMPSAT model is significantly more stable than the IMPES model, and in many cases substancially less expensive than the fully implicit model.

The Main Purpose of Our Work

We use the Volume Balance Method as a framework for forming a consistent IMPSAT approach. Improved convergence is related to choosing additional equations that are complementary to the volume balance equations, and additional variables that are complementary to pressure and saturations. Compared with the Quandalle and Savary approach, we introduce a more general and adaptive way of choosing additional equations and variables.

We also emphasize the fact that an IMPSAT approach within the framework of the Volume Balance Method provides a basis for a unified black-oil and compositional simulator.

Volume Balance Pressure and Saturation Equations (VBE)

We start by presenting the pressure and saturation equations of the Volume Balance Method. The N_c component conservation equations can be written on the form

$$\mathbf{g} = \left\{ \left(\frac{\partial n_i}{\partial t} - q_i + f_i \right) \Delta t \right\}_{i=1,2,\ldots,N_c} = \mathbf{0}. \quad (1)$$

Here n_i is the amount of component i, q_i is the source of component i, f_i is the outflux of component i and Δt is the timestep. Using a control volume discretization, (1) must hold for each control volume.

Following Watts, [7], we modify (1) into a set of N_p weighted sums of conservation equations:

$$\mathbf{W}_{\text{VBE}} \, \mathbf{g} = \mathbf{0}. \quad (2)$$

The $N_p \times N_c$ weight matrix $\mathbf{W}_{\text{VBE}}$ is of the form

$$\mathbf{W}_{\text{VBE}} = \left[\begin{array}{ccc} (\frac{\partial V_T}{\partial n_1})_{p,\mathbf{n}_{(1)}} & \cdots & (\frac{\partial V_T}{\partial n_{N_c}})_{p,\mathbf{n}_{(N_c)}} \\ (\frac{\partial V^o}{\partial n_1})_{p,\mathbf{n}_{(1)}} & \cdots & (\frac{\partial V^o}{\partial n_{N_c}})_{p,\mathbf{n}_{(N_c)}} \\ (\frac{\partial V^w}{\partial n_1})_{p,\mathbf{n}_{(1)}} & \cdots & (\frac{\partial V^w}{\partial n_{N_c}})_{p,\mathbf{n}_{(N_c)}} \end{array} \right]. \quad (3)$$

Here $(\partial V_T/\partial n_i)_{p,\mathbf{n}_{(i)}}$ is referred to as the total partial molar volume, and is a partial derivative of the total volume V_T with respect to the molar amount of component i, keeping pressure and the other component amounts fixed. Similarly, $(\partial V^j/\partial n_i)_{p,\mathbf{n}_{(i)}}$ is called the partial molar volume of phase j.

Note that (3) is formed assuming oil and water to be the primary phases, so $j = o, w$. Other choices are obviously possible.

After some rearrangements, Watts obtains a volume balance pressure equation,

$$\left(\frac{\partial(\phi V)}{\partial t} - \phi(\frac{\partial V_T}{\partial p})_{\mathbf{n}} \frac{\partial p}{\partial t} - \sum_{i=1}^{N_c} (\frac{\partial V_T}{\partial n_i})_{p,\mathbf{n}_{(i)}} q_i \right.$$
$$\left. + \sum_{i=1}^{N_c} (\frac{\partial V_T}{\partial n_i})_{p,\mathbf{n}_{(i)}} f_i \right) \Delta t = 0, \quad (4)$$

and volume balance saturation equations,

$$\left(\frac{\partial}{\partial t}(\phi V S^j) - \phi(\frac{\partial V^j}{\partial p})_{\mathbf{n}} \frac{\partial p}{\partial t} \right.$$
$$- \sum_{i=1}^{N_c} (\frac{\partial V^j}{\partial n_i})_{p,\mathbf{n}_{(i)}} q_i$$
$$\left. + \sum_{i=1}^{N_c} (\frac{\partial V^j}{\partial n_i})_{p,\mathbf{n}_{(i)}} f_i \right) \Delta t = 0. \quad (5)$$

Here ϕ is the porosity, and V is the size of the control volume. The saturation equations reduce to the conventional black-oil equations when used with black-oil fluid properties. Thus, the conventional black-oil formulation is inherent in the IMPSAT formulation when using the Volume Balance Method.

Additional Conservation Equations (ACE)

As stated earlier, we need N_c flow equations to solve the total compositional problem. To determine the form of the $N_c - N_p$ additional conservation equations, we generalize the weighting procedure of the Volume Balance Method. Consequently, instead of solving (1), we will solve the weighted system

$$\mathbf{W}\mathbf{g} = \left[\begin{array}{c} \mathbf{W}_{\text{VBE}} \\ \mathbf{W}_{\text{ACE}} \end{array} \right] \mathbf{g} = \mathbf{0}, \quad (6)$$

$$\begin{array}{l} \mathbf{W}_{\text{VBE}} : \; N_p \times N_c, \\ \mathbf{W}_{\text{ACE}} : \; (N_c - N_p) \times N_c. \end{array} \quad (7)$$

Obviously, to obtain the same solution as with (1), $\mathbf{W}$ has to be non-singular. In addition, we would like the additional conservation equations $\mathbf{W}_{\text{ACE}}\mathbf{g} = \mathbf{0}$ to be complementary to the volume balance equations. This is accomplished by the following procedure.

Let $\mathbf{W}_{\text{ACE}} = \left[\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{N_c - N_p} \right]^T$, where each $\mathbf{w}_i$ is a $N_c \times 1$ vector. Consider the following:

- The row space of $\mathbf{W}_{\text{VBE}}$ is the set of linear combinations of the rows of $\mathbf{W}_{\text{VBE}}$. The row space is a subspace of $\mathbb{R}^{N_c}$. Since the rows of $\mathbf{W}_{\text{VBE}}$ are linearly independent, the dimension of the row space is N_p.

- The nullspace of $\mathbf{W}_{\text{VBE}}$ is the set of solutions $\mathbf{x}$ to $\mathbf{W}_{\text{VBE}}\mathbf{x} = \mathbf{0}$. The nullspace is also a subspace of $\mathbb{R}^{N_c}$.

- The nullspace is the orthogonal complement of the row space. Its dimension is therefore $N_c - N_p$.

Obviously, if the rows of $\mathbf{W}_{\text{ACE}}$ are in the row space of $\mathbf{W}_{\text{VBE}}$, the rows of $\mathbf{W}$ will not be linearly independent, and $\mathbf{W}$ will be singular. On the other hand, if the rows of $\mathbf{W}_{\text{ACE}}$ form a basis for the nullspace of $\mathbf{W}_{\text{VBE}}$, the rows of $\mathbf{W}$ will span $\mathbb{R}^{N_c}$ and $\mathbf{W}$ will be non-singular.

By a singular value decomposition of $\mathbf{W}_{\text{VBE}}$ we may determine an orthonormal basis $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_{N_c - N_p}\}$ for the nullspace of $\mathbf{W}_{\text{VBE}}$. We choose $\mathbf{w}_i = \mathbf{v}_i$.

Consequently, with this choice, we can argue that the additional conservation equations $\mathbf{W}_{\text{ACE}}\mathbf{g} = \mathbf{0}$ are complementary to the volume balance equations $\mathbf{W}_{\text{VBE}}\mathbf{g} = \mathbf{0}$.

The thermodynamic interpretation of $\mathbf{W}_{\text{ACE}}$ is not yet clear, but its coefficients clearly depend on the state variables. At present, not knowing how to differentiate $\mathbf{W}_{\text{ACE}}$ with respect to the primary variables, our linearized system yields a quasi-Newton scheme.

The additional conservation equations are based on the approximation

$$\frac{\partial n_i}{\partial t} \simeq \frac{\partial n_i}{\partial p}\frac{\Delta p}{\Delta t} + \frac{\partial n_i}{\partial \mathbf{S}_p}\frac{\Delta \mathbf{S}_p}{\Delta t} + \frac{\partial n_i}{\partial \mathbf{x}_p}\frac{\Delta \mathbf{x}_p}{\Delta t} \quad (8)$$

in (1). Here $\mathbf{S}_p$ is the vector of primary saturations (e.g., $\mathbf{S}_p = \{S^o, S^w\}$), $\mathbf{x}_p$ are some $N_c - N_p$ additional primary variables, and Δu, $u \in \{p, \mathbf{S}_p, \mathbf{x}_p\}$, is the change $u^{n+1} - u^n$ in u over the timestep $\Delta t = t^{n+1} - t^n$. All derivatives in (8) are evaluated at time t^{n+1}.

Additional Primary Variables

From Darcy's law, we know that the determination of pressure and saturations resolves the main features of flow. However, if $N_c > N_p$, the phase compositions at equilibrium remain undetermined.

Phase compositions are represented by the mole fraction of component i in phase h, denoted

$$c_i^h = \frac{n_i^h}{n^h}. \quad (9)$$

Here n_i^h is the amount of component i in phase h, while n^h is the amount of phase h.

General framework

As our additional $N_c - N_p$ primary variables, we introduce a set of *primary mole fractions* by

$$(x_p)_m = \sum_{h=o,g}\sum_{i=1}^{N_{hc}} \omega_{mi}^h c_i^h, \quad (10)$$

where N_{hc} is the number of hydrocarbon components, m ranges from 1 to $N_c - N_p$, and $\omega_{mi}^h \in [-1, 1]$. The weights

$$\boldsymbol{\omega}_m = [\omega_{m1}^o, \ldots, \omega_{mN_{hc}}^o, \omega_{m1}^g, \ldots, \omega_{mN_{hc}}^g]^T \quad (11)$$

should be determined so that the primary mole fractions are complementary to pressure and saturations. This implies that the primary mole fractions can be assumed constant when determining pressure and saturations, and thereby be treated explicitly.

Stability considerations

The explicit treatment of primary mole fractions can be viewed as follows. Assume that a fully implicit formulation is formed, based on the variable set $\{p, \mathbf{S}_p, \mathbf{x}_p\}$, where $\mathbf{x}_p = \{(x_p)_1, \ldots, (x_p)_{N_c - N_p}\}$. Using a Newton-Raphson scheme to linearize the system of equations, we may update the phase compositions at the end of each Newton-Raphson iteration step k by

$$(c_i^h)^{(k)} = (c_i^h)^{(k-1)} + (\frac{\partial c_i^h}{\partial p})^{(k-1)}(\Delta p)^{(k)}$$
$$+ (\frac{\partial c_i^h}{\partial \mathbf{S}_p})^{(k-1)}(\Delta \mathbf{S}_p)^{(k)}$$
$$+ (\frac{\partial c_i^h}{\partial \mathbf{x}_p})^{(k-1)}(\Delta \mathbf{x}_p)^{(k)}. \quad (12)$$

Here $(\Delta u)^{(k)}$ denotes the change in the variable u during iteration step k. As the fully implicit formulation is unconditionally stable, (12) converges to a value $c_i^h \in [0, 1]$.

In an IMPSAT formulation, we first perform

$$(c_i^h)^{(k)} = (c_i^h)^{(k-1)} + (\frac{\partial c_i^h}{\partial p})^{(k-1)}(\Delta p)^{(k)}$$
$$+ (\frac{\partial c_i^h}{\partial \mathbf{S}_p})^{(k-1)}(\Delta \mathbf{S}_p)^{(k)} \quad (13)$$

during implicit steps, and then

$$(c_i^h)^{(k)} = (c_i^h)^{(k-1)} + (\frac{\partial c_i^h}{\partial \mathbf{x}_p})^{(k-1)}(\Delta \mathbf{x}_p)^{(k)} \quad (14)$$

during explicit steps. Consequently, the term that accounts for changes in the primary mole fractions is left out of (13), and we might get $(c_i^h)^{(k)} \notin [0, 1]$ when using that update. To avoid such instabilities, we must prevent the derivatives $\partial c_i^h / \partial u$, $u \in \{p, \mathbf{S}_p, \mathbf{x}_p\}$, from growing too large.

We find that

$$\frac{\partial c_i^h}{\partial u} = \sum_{k=1}^{N_{hc}} \left(\frac{\delta_{i,k} - c_i^h}{n^h}\right) \frac{\partial n_k^h}{\partial u}, \quad (15)$$

where $\delta_{i,k}$ is Kronecker's delta, so it will be sufficient to put restrictions on the derivatives $\partial n_k^h / \partial u$. For notational convenience, we represent these $2N_{hc}$ derivatives by the vector

$$\frac{\partial \mathbf{n}^{og}}{\partial u} = \left[\frac{\partial n_1^o}{\partial u}, \ldots, \frac{\partial n_{N_{hc}}^o}{\partial u}, \frac{\partial n_1^g}{\partial u}, \ldots, \frac{\partial n_{N_{hc}}^g}{\partial u}\right]^T. \quad (16)$$

If we have $2N_{hc}$ independent relations of the form

$$G = G(p, \mathbf{n}^o, \mathbf{n}^g) = 0, \quad (17)$$

we may differentiate with respect to u to obtain

$$\sum_{k=1}^{N_{hc}} \frac{\partial G}{\partial n_k^o}\frac{\partial n_k^o}{\partial u} + \sum_{k=1}^{N_{hc}} \frac{\partial G}{\partial n_k^g}\frac{\partial n_k^g}{\partial u} = -\frac{\partial G}{\partial p}\frac{\partial p}{\partial u}. \quad (18)$$

This yields a linear system of equations of the form

$$\mathbf{A}\frac{\partial \mathbf{n}^{og}}{\partial u} = \mathbf{b}_u, \quad (19)$$

where $\mathbf{A}$ is the same, regardless of u.

Consequently,

$$\left\|\frac{\partial \mathbf{n}^{og}}{\partial u}\right\| \leq \|\mathbf{A}^{-1}\| \|\mathbf{b}_u\| = \frac{\|\mathbf{b}_u\|}{\|\mathbf{A}\|} \operatorname{cond}(\mathbf{A}), \quad (20)$$

where $\|\cdot\|$ is some norm, and

$$\operatorname{cond}(\mathbf{A}) = \|\mathbf{A}\| \|\mathbf{A}^{-1}\| \quad (21)$$

is the condition number of $\mathbf{A}$. Assuming that $\|\mathbf{b}_u\|$ and $\|\mathbf{A}\|$ are always of the same size, $\|\partial \mathbf{n}^h / \partial u\|$ is minimal when $\operatorname{cond}(\mathbf{A})$ is minimal.

The properties of A

We use

$$G = \begin{cases} f_i^o - f_i^g \\ pV^h - n^h RTZ^h \\ \sum_{h=o,g} \sum_{k=1}^{N_{hc}} \omega_{mk}^h c_k^h - (x_p)_m \end{cases} \quad (22)$$

The relation $f_i^o - f_i^g = 0$, $i = 1, 2, \ldots, N_{hc}$, where f_i^h is the fugacity of component i in phase h, is the condition for chemical equilibrium. The relations $pV^h - n^h RTZ^h = 0$ represent the equation of state; R is the universal gas constant, T is absolute temperature and Z^h is the compressibility factor of phase h.

We observe that the coefficients $\partial G/\partial n_k^h$ derived from the fugacity equalities and the equation of state relations are independent of our choice of primary mole fraction weights, $\boldsymbol{\omega}_m$. Consequently, we may write

$$\mathbf{A} = \begin{bmatrix} \mathbf{B} \\ \mathbf{C} \end{bmatrix} \quad (23)$$

where the $(2N_{hc} - (N_c - N_p)) \times 2N_{hc}$ submatrix $\mathbf{B}$ is independent of $\boldsymbol{\omega}_m$.

The coefficients of the $(N_c - N_p) \times 2N_{hc}$ submatrix $\mathbf{C}$ are derived from the relations

$$\begin{aligned} \frac{\partial (x_p)_m}{\partial u} &= \sum_{h=o,g} \sum_{k=1}^{N_{hc}} \frac{\partial (x_p)_m}{\partial n_k^h} \frac{\partial n_k^h}{\partial u} \\ &= \begin{cases} 0 &, \quad u \in \{p, \mathbf{S}_p, \mathbf{x}_{p(m)}\} \\ 1 &, \quad u = (x_p)_m \end{cases} \end{aligned} \quad (24)$$

where $\mathbf{x}_{p(m)}$ contains all primary mole fraction except $(x_p)_m$. We find that

$$\begin{aligned} \frac{\partial (x_p)_m}{\partial n_k^h} &= \sum_{\alpha=o,g} \sum_{i=1}^{N_{hc}} \omega_{mi}^\alpha \frac{\partial c_i^\alpha}{\partial n_k^h} \\ &= \sum_{i=1}^{N_{hc}} \frac{1}{n^h} (\delta_{i,k} - c_i^h) \omega_{mi}^h \end{aligned} \quad (25)$$

so that

$$\mathbf{C} = \{c_{ij}\} \quad (26)$$

where

$$c_{ij} = \begin{cases} \sum_{k=1}^{N_{hc}} \omega_{ik}^o (\delta_{k,j} - c_k^o)/n^o, & j \in \mathcal{I}^o \\ \sum_{k=1}^{N_{hc}} \omega_{ik}^g (\delta_{k,j-N_{hc}} - c_k^g)/n^g, & j \in \mathcal{I}^g \end{cases} \quad (27)$$

Here

$$\mathcal{I}^o = \{1, 2, \ldots, N_{hc}\} \quad (28)$$

$$\mathcal{I}^g = \{N_{hc}+1, N_{hc}+2, \ldots, 2N_{hc}\} \quad (29)$$

Now we use the theory of orthogonal complements once again. To minimize the condition number of $\mathbf{A}$, we should choose the coefficients of $\mathbf{C}$ so that they span the nullspace of $\mathbf{B}$. This is obtained if

$$\frac{\partial (x_p)_m}{\partial n_k^h} = \sum_{i=1}^{N_{hc}} \frac{1}{n^h} \left(\delta_{i,k} - c_i^h \right) \omega_{mi}^h = \nu_{mk}^h \quad (30)$$

where $\boldsymbol{\nu}_m = \{\nu_{mk}^h\}$ are basis vectors for the null-space of $\mathbf{B}$.

Relation (30) yields a linear system of the form

$$\mathbf{H}\boldsymbol{\omega}_m = \mathbf{b}_m, \quad (31)$$

but, unfortunately, since $\sum_{i=1}^{N_{hc}} c_i^h = 1$, $\mathbf{H}$ is singular. This corresponds to a non-reducible total system of equations, and reflects the fact that an exact decoupling of pressure and saturations from the other state variables is physically unreasonable.

Now let the pseudoinverse of $\mathbf{H}$ be denoted $\mathbf{H}^+$. An approximate solution $\hat{\boldsymbol{\omega}}_m$ to $\mathbf{H}\boldsymbol{\omega}_m = \mathbf{b}_m$ is then given by $\hat{\boldsymbol{\omega}}_m = \mathbf{H}^+ \mathbf{b}_m$.

It is known that $\hat{\boldsymbol{\omega}}_m$ is a least-squares solution of $\mathbf{H}\boldsymbol{\omega}_m = \mathbf{b}_m$, not having any components in the nullspace of $\mathbf{H}$. When $\hat{\boldsymbol{\omega}}_m$ is inserted into $\mathbf{C}$, the rows of $\mathbf{C}$ approximately span the nullspace of $\mathbf{B}$, and $\text{cond}(\mathbf{A})$ becomes small. We choose to scale $\hat{\boldsymbol{\omega}}_m$ so that its largest element is 1 in absolute value. Consequently, $\omega_{mi}^h \in [-1, 1]$. The thermodynamic interpretation of $\hat{\boldsymbol{\omega}}_m$ is not yet clear.

As (22) shows, the above procedure is based on phase equilibrium thermodynamics. If only one hydrocarbon phase h is present, the fugacity equalities do not apply, and $N_c - N_p = N_{hc} - 1$, the number of independent mole fractions in the system. Then all sets of linearly independent weight combinations $\boldsymbol{\omega}_m$ are equivalent. Consequently, we may omit the above procedure, and choose $\mathbf{x}_p$ as $N_{hc} - 1$ of the mole fractions of phase h.

Sequential Approach

Assume that the primary variables at time t^n, $\{p^n, \mathbf{S}_p^n, \mathbf{x}_p^n\}$, have been determined. We seek a solution of the component conservation equations (1) at time t^{n+1}, that is,

$$\mathbf{g}(p^{n+1}, \mathbf{S}_p^{n+1}, \mathbf{x}_p^{n+1}) = \mathbf{0}. \quad (32)$$

With the IMPSAT formulation, we first solve the volume balance equations,

$$\mathbf{W}_{\text{VBE}} \mathbf{g}(p^{(k)}, \mathbf{S}_p^{(k)}, \mathbf{x}_p^{(k-1)}) = \mathbf{0}, \quad (33)$$

and then the additional conservation equations

$$\mathbf{W}_{\text{ACE}} \mathbf{g}(p^{(k)}, \mathbf{S}_p^{(k)}, \mathbf{x}_p^{(k,k-1)}) = \mathbf{0}. \quad (34)$$

Here $u^{(k)}$ is the k-th approximation of u^{n+1}, and we let $u^{(0)} = u^n$. The symbol $\mathbf{x}_p^{(k,k-1)}$ means that interblock flow terms are evaluated using $\mathbf{x}_p^{(k-1)}$ (interblock flow terms are not updated during the explicit iteration). Each step k is referred to as a *sequential step*.

At the end of sequential step k, we insert $\{p^{(k)}, \mathbf{S}_p^{(k)}, \mathbf{x}_p^{(k)}\}$ into (32). If the solution is not satisfactory, we proceed with step $k + 1$.

Expected Properties

In [10], Cao and Aziz reported that the IMPSAT formulation is significantly more stable than the IMPES formulation, and in many cases substantially less expensive than a fully implicit formulation. We expect the presented IMPSAT formulation to have similar properties, but we do not discuss stability criteria in this paper. Instead, we focus on how the choice of explicit variables and equations affects the computational costs per timestep.

The primary mole fraction weights $\boldsymbol{\omega}_m$ determine the properties of the variable set $\{p, \mathbf{S}_p, \mathbf{x}_p\}$. If the primary mole fractions are chosen complementary to pressure and saturations, $\mathbf{x}_p$ mainly determines equilibrium between phases, and not mass transfer between gridblocks. Likewise, if we choose additional conservation equations that are complementary to the volume balance equations, the explicit equations mainly take care of the conservation that is not resolved by the implicit equations. Recalling that the implicit equations describe the phase transport governed by Darcy's law, less effort should be required to establish the remaining conservation.

In sum, this means that the chances of solving (32) by a few sequential steps, are increased with the new approach. Consequently, if we compare the new approach to the approach of Quandalle and Savary, a reduction in computational costs can be expected, especially when the assumption that the lightest and the heaviest component are representative of the hydrocarbon phases, does not hold.

Numerical Results

Model Description

We consider a homogenous medium with a porosity of 0.2 and a permeability of 0.1 Darcy. We use a $10 \times 1 \times 10$ grid, in which each gridblock is $10 \times 10 \times 10$ m^3. The hydrocarbon phases consist of 5 different components; C1, C2, iC4, iC5, C7. The component properties are given in Table 1. All thermodynamic calculations are based on the Peng-Robinson equation of state.

	ω_i	T_{ci}	p_{ci}	V_{ci}	M_i
C1	0.008	190.6	46.00	99	16.043
C2	0.098	305.4	48.84	148	30.070
iC4	0.176	408.1	36.48	263	58.124
iC5	0.227	460.4	33.84	306	72.145
C7	0.337	536.5	29.45	476	96.000

Table 1: Acentric factor ω_i, critical temperature T_{ci} (K), critical pressure p_{ci} (bars), critical volume V_{ci} (cm^3/mole), molar mass M_i (g/mole).

Hydrocarbons are not allowed to dissolve in the water phase, and water is not present in the hydrocarbon phases. The water phase is assumed incompressible.

We set the connate water saturation to $S_{co}^w = 0.1$ and assume that the residual oil saturation is zero ($S_r^o = 0$). The relative permeabiities are given by

$$k_r^g = 0.1 \cdot \left(\frac{S^g}{1 - S_r^o - S_{co}^w} \right)^2, \qquad (35)$$

$$k_r^w = 0.1 \cdot \left(\frac{S^w - S_{co}^w}{1 - S_r^o - S_{co}^w} \right)^2 \qquad (36)$$

and

$$k_r^o = \frac{S^g \cdot k_r^{og}(S^o) + (S^w - S_{co}^w) \cdot k_r^{ow}(S^o)}{1 - S^o - S_{co}^w}, \quad (37)$$

where

$$k_r^{og} = 0.1 \cdot \left(\frac{S^o - S_r^o}{1 - S_r^o - S_{co}^w} \right)^2 \qquad (38)$$

and

$$k_r^{ow} = 0.1 \cdot \left(\frac{S^o - S_r^o}{1 - S_r^o - S_{co}^w} \right)^3. \qquad (39)$$

Phase viscosities are calculated by the approach of Lorentz et. al., [11]. Capillary pressure between any two phases is set to zero, and the reservoir temperature is 353.15 K (80 °C). We use no-flux boundary conditions.

The convergence criteria are as follows. The residual of the volume balance equations and the residual of the additional conservation equations are scaled by the volume of a gridblock, and the 2-norm is required to be less than 10^{-6} for convergence. For each of the component conservation equations we scale the residual by the amount of the corresponding component, and require the result to be less than 10^{-5} in 2-norm for convergence.

Test case

We initialize at equilibrium, with a gas-oil contact 40 m from the reservoir top and a water-oil contact 20 m from the reservoir bottom. The pressure at the gas-oil contact honours a total hydrocarbon composition of $\mathbf{z} = [0.2, 0.2, 0.25, 0.2, 0.15]^T$, i.e., evenly distributed between the components. Due to the zero capillary pressure assumption, the hydrostatic equilibrium is less accurate over the fluid contacts.

An injection well is located at the bottom left corner block, injecting water at a constant rate of 0.1 % of the total pore volume per day. A producer is located at the top right corner block. The pressure at the producer is fixed at the initial pressure, and everything that flows into the production block is produced.

We advance simulations to 200 days, with 40 timesteps of 5 days.

Solution at the end of the simulation

The state of the system at the end of the simulation, represented by pressure p, water saturation S^w and the mole fraction of the lightest component (C1) in oil, is presented in Figure 1. The solutions are plotted cellwise.
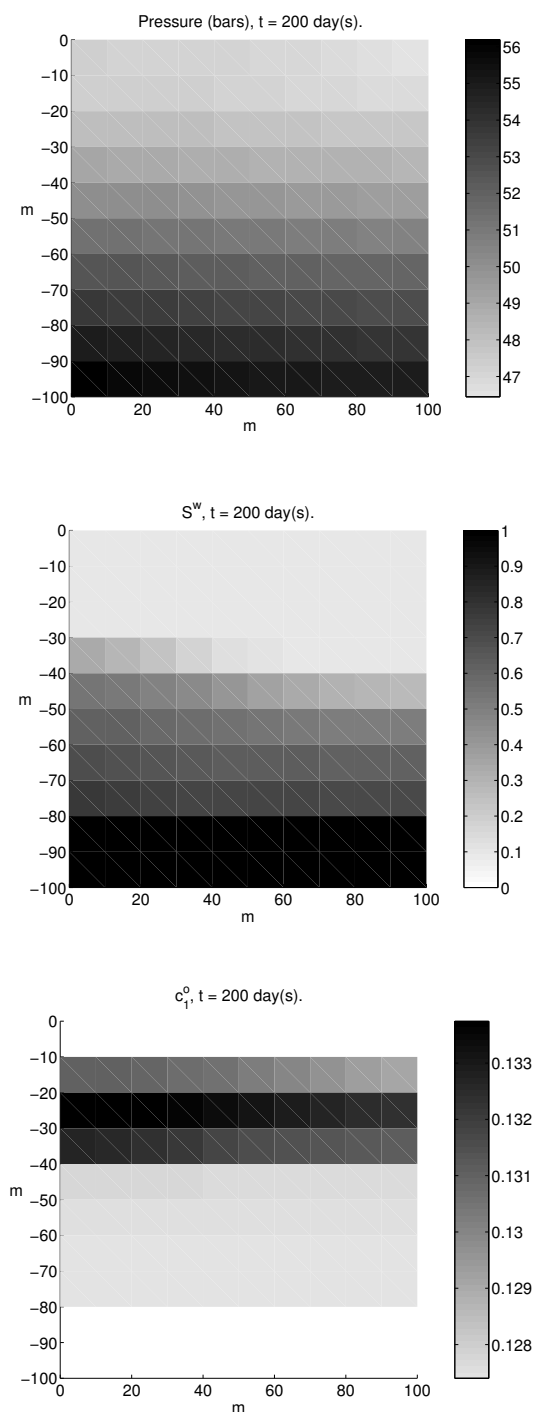
A comparison between the new approach and the approach of Quandalle and Savary

The test case was run both with the new approach (abbreaviated NA) and an implementation of the approach of Quandalle and Savary (abbreaviated QS).

Figure 2 gives a comparison between the two approaches. The first plot shows the number of sequential steps needed for convergence, and the other plots show the relative reduction of implicit and explicit steps when using NA.
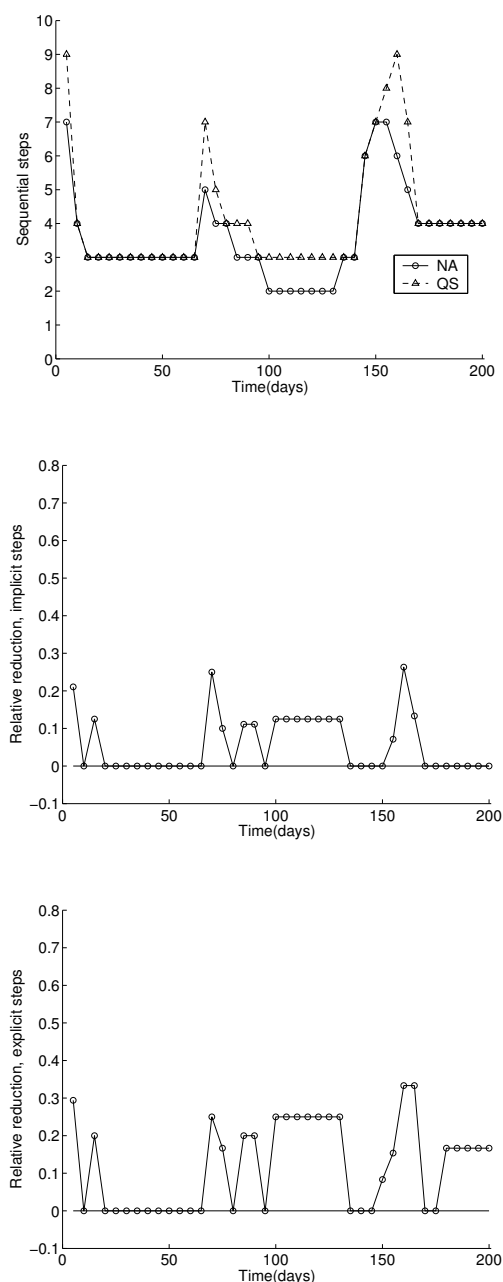

Figure 1: State at the end of the simulation.

Figure 2: A comparison between NA and QS.

Comments

The simulation results shown in Figure 1 look reasonable, and indicate the capabilities of the current implementation.

The fluid sample used for the test case has an even distribution of components. Hence, a reduction in computational costs is expected when using NA. As Figure 2 shows, the reduction can, at some stages, be up to about 30 %, which is a considerable improvement. At other stages, the two approaches perform equally well.

Simulations run on similar fluid samples show similar behaviour, suggesting that NA can be significantly better than QS.

Conclusions

A new, consistent IMPSAT formulation has been developed, implemented and tested. The formulation is based on the Volume Balance Method, and incorporates the conventional black-oil formulation. Consequently, it may serve as a basis for a unified black-oil and compositional reservoir simulator.

An IMPSAT formulation is generally more stable than an IMPES formulation, and requires less computational effort than a fully implicit formulation.

The presented explicit variables and equations have properties that are complementary to pressure and saturations and the volume balance equations, respectively. This may reduce computational costs, as fewer steps are required to obtain convergence.

The new approach takes local thermodynamics into account, and is robust, yet effective. It is not based on any assumptions on the component distribution, and is flexible and adaptive in the sense that the choice of additional primary variables may vary in the reservoir.

The calculation of equation and variable weights introduces an additional computational cost not present in previously presented IMPSAT formulations. However, the calculations are inexpensive, as they are non-iterative and operate on matrices of the same size as the number of components. Consequently, a reduced number of iteration steps with the new approach yields a total computational gain.

Further Work

The thermodynamic interpretation of the new explicit variables and equations is not yet clear. This is an important objective for further research, and includes finding a relation between the two sets of weights, and analyzing which set contributes the most to the improvement in different cases.

We should also investigate the inclusion of an extra implicit variable in the case of a missing hydrocarbon phase. Such a variable would correspond to the gas-oil ratio in black-oil models. Quandalle and Savary, [8], report the use of a variable Co for this purpose, chosen as the oil mole fraction of the lightest component in oil regions, and as the gas mole fraction of the heaviest component in gas regions. Using experience from the determination of primary mole fractions, one could possibly determine an implicit variable with better properties than Co.

For the presented test case, the new approach is superior to the approach of Quandalle and Savary. This will not hold in general. Extensive testing is needed to establish the differences between the methods, and to analyze for which cases the new approach can give a considerable improvement.

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