Paper D

A Comparison of Two Different IMPSAT Models in Compositional Simulation *

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A Comparison of Two Different IMPSAT Models in Compositional Simulation

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Summary

The large computational costs of conventional compositional simulation have motivated the development of the IMPSAT (implicit pressure and saturations) model, which has been proposed as a model less expensive per timestep than the FIM (fully implicit) model, and more stable than the compositional IMPES (implicit pressure, explicit compositions) model.

The IMPSAT models proposed in the literature mainly differ in their choices of variables and equations supplementing the pressure and saturation part, and the explicit treatment of variables in the interblock flow terms. In this paper, we compare two different approaches, one approach in which phase mole fractions and a selection of component mass balance equations are the additional variables and equations, and one approach with isochoric (volume complementary) variables and equations. In the former, the phase mole fractions are treated explicitly in the interblock flow terms, while in the latter, the isochoric variables are treated explicitly. We investigate the performance of the two approaches, in terms of nonlinear iteration, stability and precision.

Our analysis shows that the use of complementary primary variables in the isochoric approach leads to an improved iterative scheme, in which a rigorous explicit treatment of primary variables is feasible. Consequently, a full Newton-Raphson scheme rather than a quasi-Newton scheme can be used, and fewer nonlinear iteration steps are required.

In addition, the introduction of isochoric variables leads to a better stability criterion than the one currently used in the mole fraction approach. Numerical results indicate that the new criterion can be used for the mole fraction approach as well, and that it may allow for significantly larger timesteps. Furthermore, the new criterion seems to give a reasonably precise estimate of the CFL stability limit of IMPSAT.

In cases where the isochoric variation involves large changes to the phase compositions and thus is important for the fluid flow, as is the case for retrograde gas condensate reservoirs, the mole fraction approach appears to be more stable than the isochoric approach. However, the improved stability is only seen when both stability criteria are violated. Consequently, for this improvement to be of practical use, a new stability criterion must be developed for the mole fraction approach.

The precision of the two compared IMPSAT approaches, measured by the amount of numerical diffusion, seems to be very similar.

Our conclusions are supported by numerical test examples.

Introduction

An isothermal compositional model involves the solution of N_c flow equations with respect to N_c primary variables in each gridblock, where N_c is the number of chemical components (including pseudo components) in the system.

Fluid flow is governed by Darcy's law, which is basically a relation in pressure and saturations. In addition, the requirement that the fluids must fill the pore volume (volume balance) is naturally given in terms of saturations. Consequently, pressure and N_p-1 saturations constitute a convenient set of N_p primary variables, where N_p is the number of fluid phases. Omitting one saturation ensures that the saturations sum to unity, which is the volume balance requirement.

We also note that, when pressure and saturations are used as primary variables, the compositional model reduces to the conventional black-oil model when used with saturated black-oil fluid properties. Having a unified black-oil and compositional simulator leads to reduced simulator development and maintenance costs.

For a consistent IMPSAT model, N_c-N_p additional primary variables must also be specified. Several consistent IMPSAT models have been presented in the literature, e.g., by Quandalle and Savary,[1] Branco and Rodríguez,[2] Cao and Aziz,[3,4] and Haukås *et al.*[5-7]

In the approaches of Quandalle and Savary,[1] Branco and Rodríguez[2] and Cao and Aziz,[3,4] a selection of phase mole fractions are the additional primary variables, and all of the phase mole fractions are treated explicitly in the interblock flow terms. Explicit treatment of variables implies that the interblock flow terms are evaluated with values of the variables from the previous time level. Consequently, interblock couplings vanish, and an explicit solution (one gridblock at a time) with respect to the explicit variables becomes feasible.

A stability criterion for explicit treatment of phase mole fractions was derived by Cao and Aziz.[3,4] They also provided a comparison of their IMPSAT model to the compositional IMPES model and the FIM model. Their conclusion was that the IMPSAT model with explicit phase mole fractions is much more stable than the IMPES model and in many cases substantially less expensive than the FIM model.

In the IMPSAT approach of Haukås *et al.*,[6,7] the N_c-N_p additional primary variables, referred to as the isochoric variables, are chosen to be complementary to volumes, and only the isochoric variables are treated explicitly in the interblock flow terms. Haukås *et al.*,[6,7] emphasise that the use

of complementary variables and equations yields a system that is better conditioned, and that the introduction of isochoric variables leads to an improved stability criterion.[6]

In this paper, we let the mole fraction approach be represented by the IMPSAT model of Cao and Aziz,[3,4] as implemented in General Purpose Research Simulator (GPRS),[4] and compare results obtained with GPRS to results obtained with our in-house simulator XPSIM, which is based on the isochoric IMPSAT approach of Haukås *et al.*[6,7]

We first give an overview of the equations and variables used in the two approaches, and the properties to be compared, i.e., the iterative schemes, the explicit treatment of variables and the stability criteria. Then the performance of the two models is compared by numerical test examples.

Equations and variables

In the following, we present the conservation requirements and constraints that are fulfilled by the two compared IMPSAT models at convergence of the nonlinear iteration. We also present the sets of primary and secondary variables used.

Conservation requirements and constraints

The control-volume discretized form of the N_c component conservation equations can be written

$$\Delta\vec{n} + \left(\vec{f} - \vec{q}\right)\Delta t = \vec{0}, \quad \text{.....(1)}$$

where $\vec{n}$, $\vec{f}$ and $\vec{q}$ are N_c-vectors of component mole numbers, discretized interblock flow terms and source terms, respectively, while t is time. Furthermore,

$$\Delta t = t^n - t^{n-1}, \quad \Delta\vec{n} = \vec{n}^{\,n} - \vec{n}^{\,n-1}, \quad \text{.....(2)}$$

which corresponds to a backward-difference approximation of the time derivative in the differential form of the mass balance equations.

For chemical equilibrium between the hydrocarbon phases, we require

$$\vec{f}^{\,o} - \vec{f}^{\,g} = \vec{0}, \quad \text{.....(3)}$$

where $\vec{f}^{\,o}$ is the N_{hc}-vector of oil fugacities, while $\vec{f}^{\,g}$ is the N_{hc}-vector of gas fugacities. N_{hc} is the number of hydrocarbon components. We note that if there is only a single hydrocarbon phase, (3) is redundant.

The fluids are supposed to fill the pore volume completely. We let the N_p-vector $\vec{V}$ represent the fluid volumes, and let the N_p-vector $\vec{V}_p$ represent the corresponding parts of the pore volume. Examples of representations of $\vec{V}$ and $\vec{V}_p$ for a three-phase system are

$$\vec{V} = \begin{bmatrix} V^o \\ V^g \\ V^w \end{bmatrix}, \quad \vec{V}_p = \phi V_b \begin{bmatrix} S^o \\ S^g \\ S^w \end{bmatrix}, \quad S^o + S^g + S^w = 1, \quad \text{.....(4)}$$

and

$$\vec{V} = \begin{bmatrix} V_T \\ V^g \\ V^w \end{bmatrix}, \quad \vec{V}_p = \phi V_b \begin{bmatrix} 1 \\ S^g \\ S^w \end{bmatrix}, \quad S^o + S^g + S^w = 1. \quad \text{.....(5)}$$

Here, superscripts *o*, *g* and *w* denote the oil, gas and water phases. In the latter representation, S^g and S^w have been chosen to be primary saturations. Other choices are of course possible.

Based on this notation, we introduce the general volume balance requirement

$$\vec{V}_p - \vec{V} = \vec{0}, \quad S^o + S^g + S^w = 1. \quad \text{.....(6)}$$

In addition, motivated by the notion of isochoric variables introduced by Haukås *et al.*,[6] we may include the isochoric balance requirement

$$\vec{x}_p - W_x\vec{n} = \vec{0}, \quad \text{.....(7)}$$

where the vector $\vec{x}_p$ is referred to as the isochoric variables, while the rows of the $(N_c - N_p) \times N_c$ matrix W_x are chosen to span the nullspace of the $N_p \times N_c$ matrix

$$W_v = \left(\frac{\partial\vec{V}}{\partial\vec{n}}\right)_p, \quad \text{.....(8)}$$

containing the partial molar volumes. During a timestep, W_x is kept fixed, usually at the previous time level.

As volumes are homogeneous functions of first degree in the mole numbers, we have

$$\vec{V} = W_V\vec{n}. \quad \text{.....(9)}$$

Then, since W_x spans the nullspace of W_V, which is the orthogonal complement of the row space of W_V, the isochoric variables $\vec{x}_p$ are complementary to volumes. Further details on the notion of complementary variables are provided by Haukås *et al.*[6]

We note that (7) only needs to be introduced when isochoric variables are used. It is therefore not included by Cao and Aziz.[3,4]

Primary and secondary equations

For both approaches, the mass balance equations (1) are referred to as the primary equations, meaning that they are fulfilled at the end of the nonlinear iteration. For the model of Haukås *et al.*,[6,7] the fugacity equalities (3) plus the volume balance requirement (6) and the isochoric balance requirement (7) are used as secondary equations. For the model of Cao and Aziz,[3,4] the fugacity equalities (3) are referred to as secondary equations. The volume balance is inherent. We return to a discussion of the fulfilment of secondary equations when considering the iterative schemes of the two approaches.

Primary and secondary variables

For the IMPSAT model of Haukås *et al.*,[6,7] the primary variables are

$$\vec{u}_p^{\,H} = (p, \vec{S}_p, \vec{x}_p), \quad \text{.....(10)}$$

where $\vec{S}_p$ contains N_p-*1* primary saturations, while the N_c–N_p isochoric variables $\vec{x}_p$ are defined by (7). The secondary variables are chosen as

$$\vec{u}_s^H = (\vec{n}^o, \vec{n}^g, n^w), \quad (11)$$

i.e., the mole numbers of the components in the oil, water and gas phases. The number of secondary variables is thus

$$N_s^H = N_c + N_{hc}(N_{hp} - 1), \quad (12)$$

which corresponds to the fugacity equalities (3), the volume balance requirement (6) and isochoric balance requirement (7).

For the IMPSAT model of Cao and Aziz,[3,4] the N_c primary variables can be written

$$\vec{u}_p^{CA} = (p, \vec{S}_p, \vec{c}_p), \quad (13)$$

where $\vec{c}_p$ contains N_c–N_p of the hydrocarbon phase mole fractions. The secondary variables are

$$\vec{u}_s^{CA} = \vec{c}_s, \quad (14)$$

containing the remaining hydrocarbon phase mole fractions, excluding one for each hydrocarbon phase since the phase mole fractions sum to unity. The number of secondary variables is thus

$$N_s^{CA} = N_{hc}(N_{hp} - 1), \quad (15)$$

which corresponds to the number of fugacity equalities (3).

Compared properties

In the following, we present the compared properties of the two IMPSAT approaches. These include the iterative schemes, the explicit treatment of variables and the stability criteria.

Iterative schemes

The iterative scheme used by Haukås *et al.*,[6,7] is based on a linearization of the volume balance requirement (6) and the isochoric balance requirement (7) with respect to the primary variables, combined with a linearization of the mass balance equations (1). Taking advantage of the fact that $\vec{V}_p$ is a function of pressure and saturations only, and assuming that $\vec{V} = \vec{V}(p, \vec{n})$, the linearization of (6) can be shown to yield[7]

$$\left[\left(\frac{\partial \vec{V}_p}{\partial p}\right)^{(k)} - \left(\frac{\partial \vec{V}}{\partial p}\right)_{\vec{n}}^{(k)}\right]\Delta p^{(k+1)} + \left(\frac{\partial \vec{V}_p}{\partial \vec{S}_p}\right)^{(k)} \Delta \vec{S}_p^{(k+1)}$$

$$+\left(\frac{\partial \vec{V}}{\partial \vec{n}}\right)^{(k)}\left[\left(\frac{\partial(\vec{f}-\vec{q})}{\partial(p,\vec{S}_p)}\right)^{(k)} \Delta\left(p, \vec{S}_p\right)^{(k+1)} - \left(\frac{\partial \vec{q}}{\partial \vec{x}_p}\right)^{(k)} \Delta \vec{x}_p^{(k+1)}\right]\Delta t$$

$$= -\left(\frac{\partial \vec{V}}{\partial \vec{n}}\right)^{(k)}\left[\Delta\vec{n} + \left(\vec{f} - \vec{q}\right)\Delta t\right]^{(k)}. \quad (16)$$

Similarly, a linearization of (7) yields[7]

$$\Delta x_p^{(k+1)} - W_x\left(\frac{\partial \vec{q}}{\partial \vec{x}_p}\right)^{(k)} \Delta t \; \Delta \vec{x}_p^{(k+1)}$$

$$= -W_x\left[\Delta\vec{n} + \left(\vec{f} - \vec{q}\right)\Delta t\right]^{(k)} \Delta t$$

$$-W_x\left[\left(\frac{\partial(\vec{f}-\vec{q})}{\partial(p,\vec{S}_p)}\right)^{(k)} \Delta\left(p, \vec{S}_p\right)^{(k+1)}\right]\Delta t. \quad (17)$$

We note that, due to the IMPSAT formulation, derivatives of the interblock flow terms $\vec{f}$ with respect to the isochoric variables vanish. For gridblocks which contain fully implicit and variable source terms $\vec{q}$, the equations (16) and (17) must be solved simultaneously. For all other gridblocks, the pressure and saturation equations are decoupled from the rest of the system.

The equations (16) and (17) can be interpreted as a preconditioning of the linearized mass balance equations by the partial volumes $\left(\partial \vec{V}/\partial \vec{n}\right)_p$ and the matrix W_x. The form (16) is very similar to the equations used in the volume balance method of Àcs, Doleschall and Farkas[8] and Watts.[9]

The iterative scheme used by Cao and Aziz[3,4] is based on a linearization of the mass balance equations (1) and the fugacity equalities (3) with respect to both the primary and the secondary variables. The linearized equations are combined into N_c equations with the N_c primary variables of the present iteration level as the only unknowns. Due to the IMPSAT formulation, the only derivatives of the interblock flow terms that are considered are those with respect to pressure and saturations. Subsequently, Cao and Aziz[3,4] use Gaussian elimination of the Jacobian to reformulate the first N_p equations into equations for which pressure and saturations are the only unknowns. The remaining N_c–N_p mass balance equations are kept in their original form.

The scheme of Cao and Aziz[3,4] deals with residuals of both (1) and (3) during the iteration, while the scheme used by Haukås *et al.*[6,7] involves the solution of the secondary equations, including the fugacity equalities (3), at every iteration step.

One reason why Haukås *et al.*[6,7] determine the phase equilibrium at every iteration step is that the calculation of the derivatives $\left(\partial \vec{V}/\partial p\right)_{\vec{n}}$ and $\left(\partial \vec{V}/\partial \vec{n}\right)_p$ requires that (3) is fulfilled.[7] Evidently, extra phase equilibrium calculations could increase the costs on a per-iteration basis, but they also exclude thermodynamic difficulties from the Jacobian. The latter increases the robustness, and may be advantageous in challenging thermodynamic cases.

Furthermore, due to the solution of the secondary equations with respect to the secondary variables at every iteration step, Haukås *et al.*[6,7] may treat the secondary variables as functions of the primary variables, rather than independent iteration variables. Consequently, Haukås *et al.*[6,7] may write any variable or relation *h* as

$$h = h\left(\vec{u}_p^H, \vec{u}_s^H\left(\vec{u}_p^H\right)\right), \quad (18)$$

which refers to a determination of the secondary variables with the primary variables $\vec{u}_p^H$ known in advance from the solution of (16) and (17). This allows for a rigorous explicit treatment of variables in the interblock flow terms, as discussed below.

Explicit treatment of variables in the interblock flow terms

The flow of component *i* in phase *j* through interface γ may be expressed by

$$f_{i,\gamma}^j = \left(\frac{c_i^j \xi^j k_r^j}{\mu^j} \right)_\gamma \sum_{\eta \in I_\gamma} t_{\eta,\gamma} \left(p_\eta^j - \rho_\gamma^j g D_\eta \right), \quad \text{.....(19)}$$

where the leftmost bracketed term is referred to as the generalized mobility and is evaluated upstream, according to the sign of (19). The components of the interblock flow terms $\vec{f}$ that appear in the mass balance equations are calculated as the sum of (19) over every interface of a gridblock and over all phases in which the component is present.

During a nonlinear IMPSAT iteration, (19) is to be evaluated with the current pressure and saturations, but with the remaining parts at the previous time level. For the IMPSAT model of Haukås *et al.*,[6,7] this is done rigorously, i.e., by using

$$\vec{u}_p^H = \left(p^{(k)}, \vec{S}_p^{(k)}, \vec{x}_p^{n-1} \right) \text{.....(20)}$$

in (18) when updating the interblock flow terms and the derivatives of those terms, and

$$\vec{u}_p^H = \left(p^{(k)}, \vec{S}_p^{(k)}, \vec{x}_p^{(k)} \right) \text{.....(21)}$$

in (18) when updating all other terms and derivatives.

For the IMPSAT model of Cao and Aziz,[3,4] both primary and secondary variables take part in the nonlinear iteration, and a form equivalent to (18) is not available. The interblock flow terms could possibly be updated by

$$\vec{f} = \vec{f} \left(p^{(k)}, \vec{S}_p^{(k)}, \vec{c}_p^{n-1}, \vec{c}_s^{n-1} \right), \quad \text{.....(22)}$$

but then densities and viscosities would only be updated with respect to pressure, thus introducing unnecessary stability limitations. Consequently, only the mole fractions c_i^j that appear explicitly in the generalized mobility of (19) are evaluated at the previous time level in the IMPSAT model of Cao and Aziz.[3,4] All other terms are evaluated fully implicitly, i.e., with all variables at the current iteration level.

However, in order to decouple the implicit and explicit part of the IMPSAT system of Cao and Aziz,[3,4] derivatives of (19) with respect to all mole fractions are neglected, including those of densities and viscosities. This leads to a quasi-Newton scheme rather than a full Newton-Raphson scheme.

Stability criteria

Explicit treatment of variables in an equation of hyperbolic nature may lead to an unstable solution, if the CFL stability criterion is violated. An unstable solution is characterized by increasing oscillations with time. Unfortunately, due to the complexity of the flow equations, only estimates of the true IMPSAT CFL limit can be derived.

The criterion used by Cao and Aziz[3,4] may be written

$$\frac{f_i}{n_i} \Delta t \le 1, \quad \text{.....(23)}$$

where f_i represents the gross flow rate of component *i* out of a gridblock, while n_i represents the amount of that component present in the gridblock. The interpretation of (23) is that the outflux is not allowed to exceed the component amount present in the gridblock. The corresponding predicted maximum stable timestep is thus

$$\max \Delta t^{CA} = \min_i \frac{n_i}{f_i}. \quad \text{.....(24)}$$

However, (23) and (24) do not reflect the fact that saturations are treated implicitly. To take the implicit saturation solution into account, Haukås *et al.*[6] introduce an isochoric projection operator

$$proj_{\pi_x} = \overline{W}_x^T \overline{W}_x, \quad \text{.....(25)}$$

and write their stability criterion as

$$\frac{\left(proj_{\pi_x} \vec{f} \right)_i}{\left(proj_{\pi_x} \vec{n} \right)_i} \Delta t \le 1. \quad \text{.....(26)}$$

The corresponding predicted maximum stable timestep is

$$\max \Delta t^H = \min_i \frac{\left(proj_{\pi_x} \vec{n} \right)_i}{\left(proj_{\pi_z} \vec{f} \right)_i}. \quad \text{.....(27)}$$

The rows of the $(N_c - N_p + 1) \times N_c$ matrix $\overline{W}_x$ are chosen to span the nullspace of the $(N_p - 1) \times N_c$ matrix $\overline{W}_V$, which is similar to the matrix W_V of partial volumes defined by (8), only that it excludes the derivatives of the phase volume that best accounts for the properties of the total volume. The reason for the exclusion of the total volume derivatives is that the total volume corresponds to pressure, which has an elliptic rather than a hyperbolic nature.

The interpretation of (26) is that the hyperbolic isochoric part of the outflux is not allowed to exceed the hyperbolic isochoric part of the mass present in the gridblock. Further details are provided by Haukås *et al.*[6]

We note that in the single phase (undersaturated) case, pressure is the only implicit variable. Consequently, IMPSAT reduces to IMPES, and (26) reduces to (23). Otherwise, (26) should predict maximum stable timesteps that are at least as large as those predicted by (23).

Test examples

In the following, we describe the test examples used for comparison of the IMPSAT model of Haukås *et al.*,[6,7] represented by the in-house simulator XPSIM, to the IMPSAT model of Cao and Aziz,[3,4] represented by GPRS.[4]

Fluid samples

We use two different fluid samples for the comparisons. The first sample contains 6 hydrocarbon components, and the fluid characterization is that of the Fifth SPE Comparative Solution Project.[10] The second sample contains 9 hydrocarbon

components, and the characterization is that provided by Arco Oil and Gas Company for the Third SPE Comparative Solution Project.[11] The runs with the first fluid sample are referred to as Case 1 runs, while the runs with the second fluid sample are referred to as Case 2 runs.

Initial conditions

The original initial temperatures and overall compositions[10,11] are used for all cases, but the initial datum pressure is adjusted so that two hydrocarbon phases are present in every gridblock initially. Consequently, we may compare the two IMPSAT models without having to take their reduction to IMPES in the undersaturated case into account. For Case 1, we use an initial pressure of 40 bars, while for Case 2, the initial pressure is set to 150 bars.

We note that the initial conditions of Case 2 correspond to a retrograde gas condensate reservoir. For such reservoirs, the isochoric part is important for the fluid flow. Case 2 is therefore expected to be especially challenging for the isochoric IMPSAT approach.

Grids

Each test case is simulated on a selection of grids. Most of the illustrative results are obtained on a 24×24×1 grid, with gridblock dimensions 100/3×100/3×10 m^3. To check the solution precision (numerical diffusion), we also use a 8×8×1 grid on the same domain, i.e., with gridblock dimensions 100×100×10 m^3. These 2D examples are referred to as Cases 1a and 2a. Furthermore, Case 1b is a 3D example with the original 7×7 ×3 grid,[10] while Case 2b is a 3D example with the original 9×9×4 grid.[11]

Other properties

For simplicity, we neglect water and rock compressibility, and use the analytical relative permeability relations

$$k_r^o = 0.4 \cdot \left(S^o\right)^{2.75}, \quad \text{.....(28)}$$

$$k_r^g = 0.4 \cdot \left(S^g\right)^{1.9}, \quad \text{.....(29)}$$

where k_r^j is the relative permeability of phase j. The thermodynamics is based on the Peng-Robinson equation of state,[12] while viscosities are calculated by the LBC method.[13]

For Cases 1a and 2a, a porosity of 0.2 is used, and the absolute permeability is 150 mD in both the x- and y-directions. For Cases 1b and 2b we use the original porosity and permeability fields.[10,11]

Injection and production scenario

An injector of the lightest component (methane) is located in gridblock (1,1,1), and we use a fixed bottom hole pressure producer in the opposite corner of the grid, i.e., in gridblock (24,24,1) for the 24 × 24 × 1 grid, etc. The injection rate is set to 0.2 std m^3/s for Cases 1a and 1b, and to 0.05 std m^3/s for Cases 2a and 2b. The bottom hole pressure is fixed at 20 bars for Cases 1a and 1b, and at 130 bars for Cases 2a and 2b.

Convergence criteria

The convergence criteria are

$$\left| \frac{\Delta\vec{n} + \left(\vec{f} - \vec{q}\right)\Delta t}{\vec{n}} \right| < 10^{-3}, \quad \text{.....(30)}$$

for the local mass balance (in every gridblock) and

$$\left| \frac{\vec{f}^{\,o} - \vec{f}^{\,g}}{\vec{f}^{\,g}} \right| < 10^{-3}, \quad \text{.....(31)}$$

for the phase equilibrium. Here, fractions of vectors are to be interpreted componentwise.

Timestep selection

Timesteps are governed by a formula due to Aziz and Settari,[14]

$$\Delta t^{n+1} = \Delta t^n \min_u \left[\frac{(1+\lambda)\Delta u^n}{\Delta u^* + \lambda \Delta u^n} \right], \quad \text{.....(32)}$$

where Δt^{n+1} is the next timestep, Δt^n is the previous timestep, Δu^n is the change in the variable u during the timestep, Δu^* is the target variable change during the next timestep and λ is a tuning factor. We use λ = 0.5, a target pressure change of 15.0 bars and a target saturation change of 0.1. The initial timestep is 0.5 days.

For stability, the timesteps are further restricted by (23) for the IMPSAT model of Cao and Aziz[3,4] and (26) for the IMPSAT model of Haukås *et al.*[6,7]. Instabilities are expected when the stability criteria are violated. As a measure of such a violation, we introduce the notion of CFL factors, meaning the numbers replacing unity in (23) and (26).

The simulation run is set to 1000 days for Case 1a, 500 days for Case 2a, and 800 days for Cases 1b and 2b.

Results

Nonlinear iteration

Table 1 shows the number of timesteps and nonlinear iteration steps for the simulation runs with XPSIM and GPRS.

We observe that the required number of iteration steps per timestep is greater for GPRS in all cases. This is mainly due to the quasi-Newton scheme used in GPRS. In addition, GPRS may require a significantly larger number of timesteps for simulation runs where (27) predicts significantly larger maximum stable timesteps than (24). This is the case for Case 1a, as discussed below.

Furthermore, experience shows that XPSIM handles strict convergence criteria (for instance residuals less than 10^{-6}) without severe convergence problems, while GPRS generally does not. This is actually the reason why the quite relaxed convergence limit of 10^{-3} had to be used.

	Timesteps		Iterations		Iterations/timestep	
	XPSIM	GPRS	XPSIM	GPRS	XPSIM	GPRS
Case 1a	162	309	330	1178	2.037	3.812
Case 1b	147	149	268	309	1.823	2.074
Case 2a	55	56	114	166	2.073	2.964
Case 2b	28	27	69	83	2.464	3.074

Table 1: Number of timesteps and nonlinear iteration steps, Cases 1a, 1b, 2a and 2b.

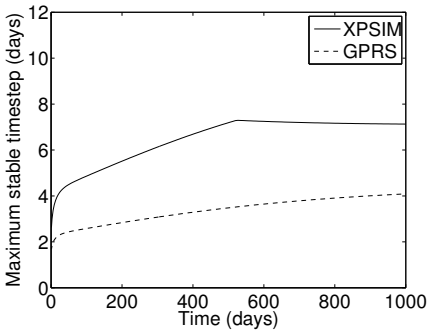

Figure 1: Predicted maximum stable timesteps during the simulation run of Case 1a, as calculated by (24) and (27).

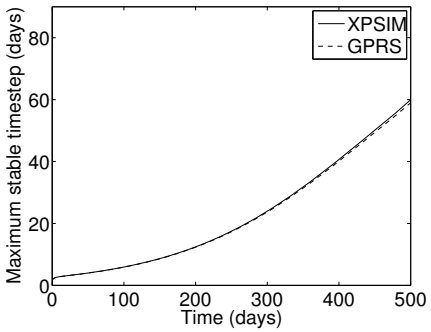

Figure 2: Predicted maximum stable timesteps during the simulation run of Case 2a, as calculated by (24) and (27).

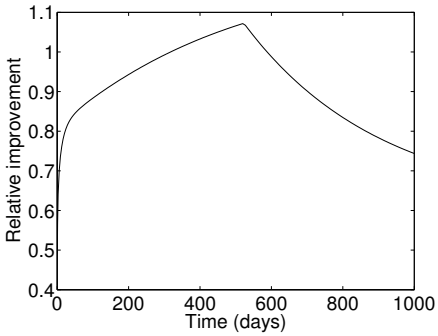

Figure 3: Relative timestep improvement during the simulation run of Case 1a, as calculated by (33).

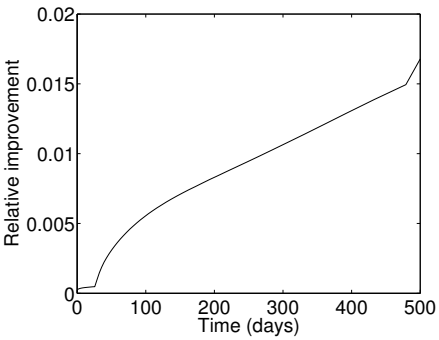

Figure 4: Relative timestep improvement during the simulation run of Case 2a, as calculated by (33).

Timestep improvement due to the new stability criterion

In Figure 1 and Figure 2, the predicted maximum stable timesteps for XPSIM and GPRS during the simulation runs of Cases 1a and 2a, respectively, are plotted. As mentioned, (27) predicts larger maximum stable timesteps than (24) does. The corresponding relative improvement is calculated as

$$relative\ \ improvement = \frac{\max \Delta t^{H} - \max \Delta t^{CA}}{\max \Delta t^{CA}}, \quad .....(33)$$

and is plotted in Figure 3 and Figure 4 for Cases 1a and 2a, respectively.

For Case 1a, the relative improvement is quite significant, ranging from 0.6 to more than 1.0. We note that a relative improvement of 1.0 corresponds to taking twice as large timesteps. For Case 2a, the improvement is insignificant (around 1 %).

Experience shows that a significant timestep improvement when using (27) instead of (24) often can be seen, but that the improvement is negligible for retrograde condensate reservoirs, e.g., Case 2. The latter should be expected, because the isochoric part is important to the fluid flow in retrograde condensate cases.

In addition, we note that the two stability criteria are approximately the same in gridblocks that are close to undersaturated. If these gridblocks experience high throughput rates, there is almost no gain in using (27) instead of (24). This is the case when 3D cases initialized at steady state are run for a shorter period of time, e.g., Cases 1b and 2b.

Stability criteria

The solution obtained with XPSIM for Case 1a shows no signs of instability unless (26) is violated. Furthermore, running GPRS with the same timesteps as used by XPSIM does not lead to stability problems either. This suggests that (26) could be adopted by GPRS as well, although its theoretical foundation is based on the IMPSAT model of Haukås *et al.*[6,7]

For a CFL factor of 3.0 when using (26) in Case 1a, an unstable solution is obtained, as illustrated in Figure 5 for the amount of the second component divided by the size of the pore volume. Generally, the increasing oscillations with time are first observed for the intermediate components. This is due to the fact that the lightest and heaviest components approximately correspond to the implicitly treated gas and oil saturations, respectively. Consequently, they are more stable than the intermediate components.

We observe that the oscillations in Case 1a are greatest for XPSIM. However, the origins of the oscillations are similar. Further investigations reveal that the instabilities occur for a CFL factor of approximately 2.5. Consequently, for Case 1a, criterion (26) is a reasonably good estimate of the true CFL limit for both the compared IMPSAT approaches.

For Case 2a with XPSIM, oscillations appear in the second component for a CFL factor of 2.0, as shown in Figure 6. Further testing indicates that the stability limit corresponds to a CFL factor of around 1.5. For Case 2a, criterion (26) is thus a good estimate of the true CFL criterion.

However, as Figure 6 shows, the solution obtained using the same timesteps for GPRS does not experience any oscillations, and is therefore more stable than the XPSIM solution. The reason for this is the use of

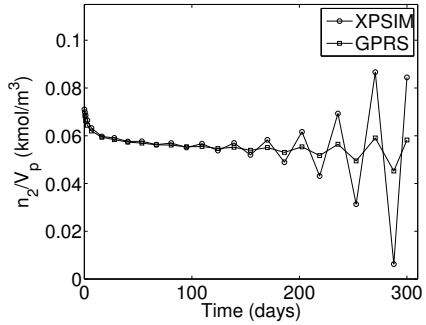

Figure 5: Detected instability, Case 1a, using a CFL factor of 3.0 in (26).

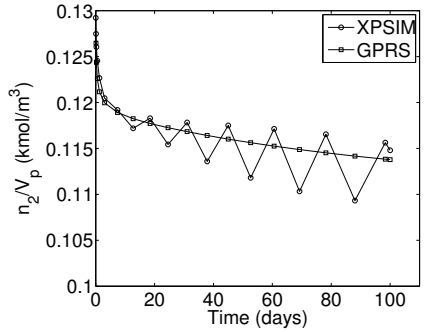

Figure 6: Detected instability, Case 2a, using a CFL factor of 2.0 in (26).

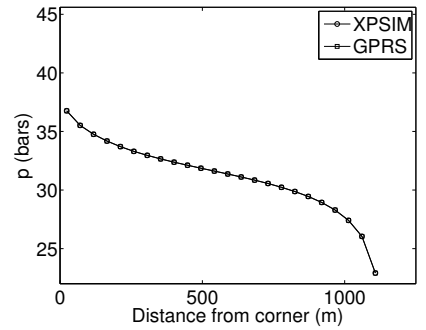

Figure 7: Pressure solution along diagonal from gridblock (1,1,1) to gridblock (24,24,1), Case 1a.

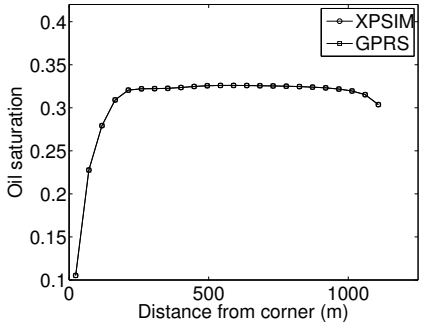

Figure 8: Oil saturation solution along diagonal from gridblock (1,1,1) to gridblock (24,24,1), Case 2a.

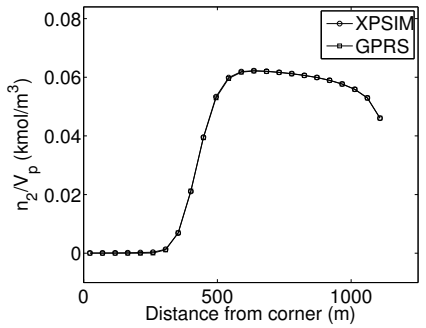

Figure 9: Normalized component amount along diagonal from gridblock (1,1,1) to gridblock (24,24,1), Case 1a.

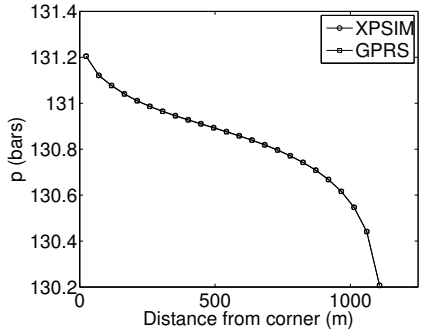

Figure 10: Pressure solution along diagonal from gridblock (1,1,1) to gridblock (24,24,1), Case 2a.

$$c_i^j = c_i^j\left(p^{(k)}, \vec{S}_p^{(k)}, \vec{x}_p^{n-1}\right), \quad \text{.....(34)}$$

in the update of interblock flow terms in XPSIM, rather than

$$c_i^j = \left(c_i^j\right)^{n-1}, \quad \text{.....(35)}$$

which is used by GPRS.

In retrograde gas condensate cases, the relation between pressure changes and changes in the isochoric variables is stronger than the relation between pressure changes and volume (saturation) changes. Consequently, a phase equilibrium corresponding to the form (34), where pressure and isochoric variables are evaluated at different time levels, must be used with care, i.e., the proper stability criterion (26).

With (35), the phase equilibrium is always evaluated with all variables at the same time level, and stability problems in retrograde gas condensate cases are not particularly severe. However, this feature is of no practical use unless a stability criterion that predicts larger maximum stable timesteps than (27) for retrograde gas condensate cases is developed.

Precision

On the 24×24×1 grid, the solutions obtained with GPRS and XPSIM with a CFL factor of 1.0 are indistinguishable, as shown for pressure, oil saturations and the pore volume normalized amount of the second component in Figure 7, Figure 8 and Figure 9 for Case 1a, and in Figure 10, Figure 11 and Figure 12 for Case 2a. The plots show gridblock solutions along the grid diagonal from block (1,1,1) to block (24,24,1).

Overall, no significant difference in the numerical diffusion of the two compared IMPSAT approaches was found. Figure 13 shows a comparison between the solution of the normalized amount of the second component on an 8×8×1 grid for XPSIM and GPRS together with a fully implicit (FIM)

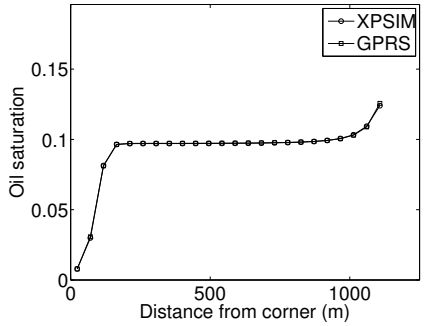

Figure 11: Oil saturation solution along diagonal from gridblock (1,1,1) to gridblock (24,24,1), Case 2a.

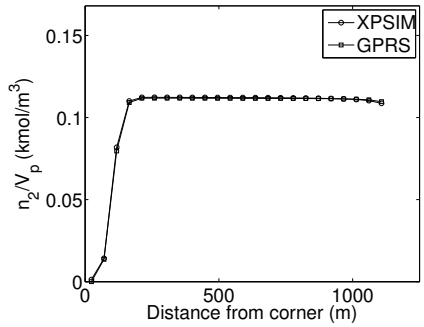

Figure 12: Normalized component amount along diagonal from gridblock (1,1,1) to gridblock (24,24,1), Case 2a.

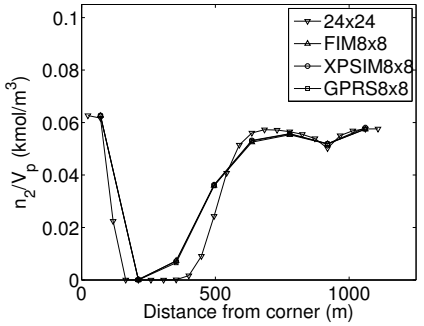

Figure 13: Normalized component amount along grid diagonal, Case 1a: Reference solution from block (1,1,1) to block (24,24,1) on a 24×24×1 grid, fully implicit solution (FIM) and IMPSAT solutions with XPSIM and GPRS from block (1,1,1) to block (8,8,1) on a 8×8×1 grid.

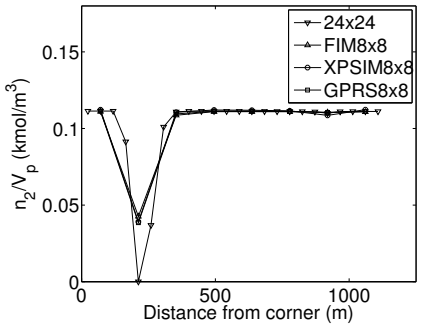

Figure 14: Normalized component amount along grid diagonal, Case 2a: Reference solution from block (1,1,1) to block (24,24,1) on a 24×24×1 grid, fully implicit solution (FIM) and IMPSAT solutions with XPSIM and GPRS from block (1,1,1) to block (8,8,1) on a 8×8×1 grid.

solution, compared to the reference solution on the 24×24×1 grid for Case 1a. Figure 14 shows the same comparison for Case 2a. In both cases, the FIM and IMPSAT results on the 8×8×1 grid are almost indistinguishable. We note that the locations of the injector and producer were changed so that they coincided in the two grids.

In addition, for the presented cases, the IMPSAT solutions appear to be very similar to the fully implicit solution. For the saturation fronts, this will always be the case, since saturations are determined implicitly.

Conclusions

We have investigated the performance of two different IMPSAT approaches, one mole fraction approach,[3,4] and one isochoric approach.[6,7] The compared properties are the performance of the iterative schemes, stability constraints and solution precision (numerical diffusion).

The isochoric approach leads to a full Newton-Raphson scheme rather than a quasi-Newton scheme, and therefore requires fewer nonlinear iteration steps than the mole fraction approach. However, some extra phase equilibrium calculations may be necessary, the costs of which have not been evaluated.

The stability criterion used with the isochoric approach predicts larger maximum stable timesteps than the criterion for the mole fraction approach, and experience shows that no instabilities occur unless both criteria are violated. Consequently, the stability criterion for the isochoric approach is better, and can apparently be applied to the mole fraction approach as well. The improvement may be significant, so that 50% to 100% larger timesteps can be taken. In addition, the IMPSAT stability criterion of the isochoric approach appears to be a reasonably precise estimate of the true CFL stability criterion.

For retrograde condensate reservoirs, the mole fraction approach is found to be more stable. However, to make the improvement of practical use, a new stability criterion must be developed. This is an interesting subject for further research.

No significant difference in the numerical diffusion of the two compared IMPSAT approaches has been found. A comparison of the numerical diffusion of fully implicit solutions and IMPSAT solutions could be further investigated.

Nomenclature

N_c = number of components,

N_{hc} = number of hydrocarbon components,

N_p = number of phases,

$\vec{c}$ = vector of mole fractions,

$\vec{f}$ = N_c-vector of component flow rates [mol/s],

$\vec{f}^{\,j}$ = N_{hc}-vector of component fugacities in phase j [Pa],
$\vec{n}$ = N_c-vector of component amounts [mol],
$\vec{n}^{\,j}$ = vector of component amounts in phase j,
$\vec{q}$ = N_c-vector of component source rates [mol/s],
$\vec{S}_p$ = N_p–1-vector of primary saturations,
$\vec{u}$ = vector of unknowns,
$\vec{V}$ = N_p-vector of fluid volumes [m^3],
$\vec{V}_p$ = N_p-vector of pore volume parts [m^3],
$\vec{x}_p$ = N_c-N_p-vector of isochoric variables [mol],
$proj_{\pi_x}$ = $N_c \times N_c$-matrix, hyperbolic isochoric projection,
W_V = $N_p \times N_c$-matrix of partial volumes [m^3/mol],
W_x = $(N_c - N_p) \times N_c$-matrix, complementary to W_V,
$\overline{W}_V$ = $(N_p - 1) \times N_c$-matrix of partial volumes [m^3/mol],
$\overline{W}_x$ = $(N_c - N_p + 1) \times N_c$-matrix, complementary to $\overline{W}_V$,
c_i^j = mole fraction of component i in phase j,
D_η = depth of gridblock η [m],
f_i = gross component flow rate out of a gridblock [mol/s],
$f_{i,\gamma}^j$ = rate of comp. i in phase j through interface γ [mol/s],
g = acceleration of gravity [m/s^2],
I_γ = the set of cells in the flux molecule of interface γ,
k_r^j = relative permeability of phase j,
n_i = amount of component i [mol],
p = pressure,
p_η^j = pressure of phase j in gridblock η [Pa],
S^j = saturation of phase j,
t = time [s],
$t_{\eta,\gamma}$ = transmissibility of gridblock η in I_γ [m^3],
V_b = bulk volume [m^3],
V^j = volume of phase j,
V_T = total fluid volume,
μ^j = viscosity of phase j [Pa s],
ξ^j = molar density of phase j [mol/m^3],
ρ_γ^j = mass density of phase j through interface γ [kg/m^3],
ϕ = porosity,

superscript n = evaluation at time level t^n.
superscript $n-1$ = evaluation at time level t^{n-1}.
superscript (k) = evaluation at iteration level k.
superscript $(k+1)$ = evaluation at iteration level $k+1$.
superscript j = phase,
superscripts o, g, w = oil phase, gas phase, water phase,
superscript CA = IMPSAT approach of Cao and Aziz,[3,4]
superscript H = IMPSAT approach of Haukås *et al.*,[6,7]
subscript p = primary,
subscript s = secondary.

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