An Efficient Approach to Adaptive-Implicit Compositional Simulation With an Equation of State

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Summary. This paper describes a robust and efficient method for solving the equations corresponding to an equation-of-state (EOS) compositional model. The method is developed for an adaptive-implicit simulator in which only a small number of blocks need to be solved implicitly while the remaining blocks are solved explicitly. The salient features of the method are decoupling of the solution of flow equations from the flash calculations and switching from explicit to implicit formulations on the basis of a stability criterion. The performance of the adaptive-implicit approach is compared with that of a fully implicit approach and an explicit-transmissibility approach. Results show that the adaptive-implicit approach is two to three times faster than the other two methods.

Introduction

Most EOS compositional models described in the literature use explicit transmissibilities. Because of the complexity of the equations and the use of large numbers of components (around 10), the explicit formulation has been the only feasible approach to field-scale simulation. This was demonstrated in the Third SPE Comparative Solution Project,[1] where all the simulators used were explicit. The drawback of the explicit formulation is the timestep size limitation, which excludes its application in coning studies. Some attempts have been made to develop a fully implicit EOS compositional model.[2,3] The application of such a model was restricted to very small problems, however, and no field-scale runs were reported.

Bertiger and Kelsey[4] described the use of the adaptive-implicit method in an EOS compositional model. The adaptive-implicit method, introduced by Thomas and Thurnau,[5] is based on the idea that, at a given time during a simulation, only some gridblocks need to be solved implicitly, while the remaining gridblocks are solved explicitly. Thus, during a simulation, blocks are switched automatically between explicit and implicit to allow the use of large timesteps. The alignment of equations and variables used by Bertiger and Kelsey[4] is similar to that of Coats.[2] Their test examples also were restricted to relatively small systems.

This paper describes a robust and efficient formulation of an adaptive-implicit EOS compositional model. The salient features of the formulation are the selection of primary equations and variables and decoupling of the solution of the flow equations and the volume-consistency equation from the flash calculations. The flow equations and the volume-consistency equations are converged with Newton's method, while the phase-equilibrium equations can be solved by any technique (e.g., Newton's method and quasi-Newton successive substitution[6]). This is a departure from previous Newton's method approaches to compositional simulation where the flow and phase-equilibrium equations are converged simultaneously. These approaches are described by Fussell and Fussell[7] and Young and Stephenson[8] for explicit-transmissibility models and by Coats[2] and Chien *et al.*[3] for fully implicit models. The desirable features of the present approach are discussed later. Furthermore, the switching from explicit to implicit formulations is based on a stability criterion rather than on a threshold criterion as in the approach of Thomas and Thurnau[5] and Forsyth and Sammon[9] for black-oil systems.

The performance of the adaptive-implicit approach developed in this paper is compared with the performances of both an explicit-transmissibility approach and a fully implicit approach. The Third SPE Comparative Solution Project[1] with 10 components and 324 gridblocks was used in the comparison. It is felt that this problem provides a rigorous test for an adaptive-implicit formulation because it was originally designed for explicit-transmissibility models. Thus, neither the gridblocks nor the problem were selected so that an explicit-transmissibility model would perform poorly (e.g., coning or gas percolation problems).

Equations

Flow Equations. The material-balance, finite-difference equations for the components in the oil and gas phases and for the water component are

$$\Psi_i \equiv \Delta T_o^m y_{io}^m(\Delta p^{n+1} - \gamma_o^m \Delta D) + \Delta T_g^m y_{ig}^m(\Delta p^{n+1} + \Delta P_{cog}^m - \gamma_g^m \Delta D) + q_i^{n+1} - (V/\Delta t)[N_i^{n+1} - N_i^n] = 0, \quad i = 1 \ldots n_c \quad \ldots\ldots(1)$$

and

$$\Psi_{n_c+1} \equiv \Delta T_w^m(\Delta p^{n+1} - \Delta P_{cwo}^m - \gamma_w^m \Delta D) + q_{n_c+1}^{n+1} - (V/\Delta t)[N_{n_c+1}^{n+1} - N_{n_c+1}^n] = 0, \quad \ldots\ldots(2)$$

where $N_i (i = 1 \ldots n_c)$ denotes the moles of Component i per unit of reservoir volume and N_{n_c+1} denotes the moles of water per unit of reservoir volume. No mass transfer is assumed to occur between the hydrocarbon and water phases. Note that the N_i represent the bulk molar density of Component i in the total gridblock volume. Superscripts n and $n+1$ denote the old and current time levels, respectively. Superscript m refers to n for explicit gridblocks and $n+1$ for implicit gridblocks.

The N_i are related to the phase molar densities, saturations, and compositions as follows:

$$N_i = \phi(\rho_o S_o y_{io} + \rho_g S_g y_{ig}) \quad \ldots\ldots(3)$$

and

$$N_{n_c+1} = \phi \rho_w S_w. \quad \ldots\ldots(4)$$

Volume-Consistency Equation. A volume-consistency equation, which equates the sum of the phase volumes per unit reservoir volume to the porosity, relates the pressure and molar densities in each gridblock:

$$\Psi_p \equiv N_o^{n+1}/\rho_o^{n+1} + N_g^{n+1}/\rho_g^{n+1} + N_w^{n+1}/\rho_w^{n+1} - \phi^{n+1} = 0. \quad \ldots\ldots(5)$$

This equation involves only variable values in the gridblock in question and at the $n+1$ time level.

Thermodynamic Equilibrium Equations. Given $N_i (i = 1 \ldots n_c)$, the pressure, p, and temperature, T, the phase compositions and splits can be obtained by solving the thermodynamic equilibrium equations:

$$g_i \equiv \ln f_{ig} - \ln f_{io} = 0, \quad i = 1 \ldots n_c \quad \ldots\ldots(6)$$

for either N_{ig}, the moles of Component i in the gas phase, or N_{io}, the moles of Component i in the oil phase. In Eq. 6, f_{im} denotes the fugacity of Component i in Phase $m (m = o,g)$.

Saturation Equation. Because the saturations correspond to phase volume fractions by definition, they can be obtained from

$$S_m = (N_m/\rho_m) \Big/ \left[\sum_q (N_q/\rho_q) \right], \quad m = o,g,w, \quad q = o,g,w. \quad \ldots\ldots(7)$$

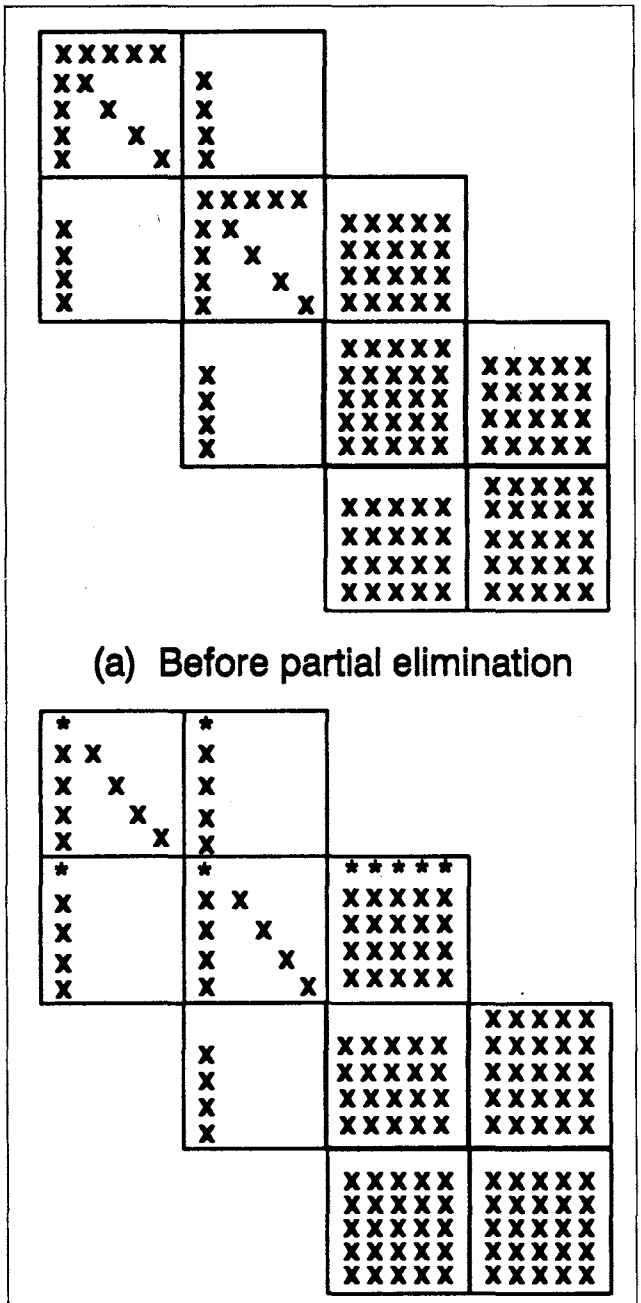

Fig. 1—Incidence matrix for a 1D three-hydrocarbon-component system [(*) denotes elements that have been modified in the partial elimination].

Solution Method

Primary Equations and Variables. Eqs. 1, 2, 5, and 6 form a system of $n_b(2n_c+2)$ nonlinear equations that can be solved simultaneously for the variables $(p, N_1 \ldots N_{n_c}, N_{n_c+1}, N_{1g} \ldots N_{n_cg})_k^{n+1}$ with $k=1 \ldots n_b$, where n_b is the number of gridblocks. In this approach, the flow and phase-equilibrium equations are solved simultaneously and the oil and gas phases are not in equilibrium until convergence is achieved. This was basically the approach taken by Fussell and Fussell[7] and Young and Stephenson[8] for explicit-transmissibility compositional models and by Coats[2] and Chien *et al.*[3] for fully implicit compositional models.

Our experience in phase-behavior computation shows that the solution of the thermodynamic equilibrium equations is by itself a difficult task. It often involves some complex logic during the iteration,[5,10] and solving the flow and equilibrium equations together adds a high level of complexity to the solution method. Therefore, it was decided to iterate on Eqs. 1, 2, and 5 for the $n_b(n_c+2)$ primary variables $(p, N_1 \ldots N_{n_c+1})_k^{n+1}$, $k=1 \ldots n_b$, and to converge the equilibrium equations after each iteration of the primary variables. This approach is reminiscent of the non-Newtonian method for explicit-transmissibility models described in Refs. 11 and 12. However, in this paper, Newtonian iteration is used. The computation of the partial derivatives required in the Jacobian is described later.

The approach taken here separates the task of solving the flow equations from that of solving the equilibrium equations. This is a desirable feature because the development of flash calculation methods can be carried out independently from the solution method for the flow equations and the simulator can easily be expanded to include three-phase flash calculations. It also allows the use of various methods for flash calculations (e.g., Newton's method, quasi-Newton methods, quasi-Newton successive substitution,[6] or a switch from one method to another as described in Refs. 13 through 16. Complex logic for a phase stability test[6,16] can also easily be implemented.

Jacobian Evaluation. Let F and x be the flow equations and primary unknowns. The elements of F and x corresponding to gridblock k are

$$F_k \equiv (\Psi_p, \Psi_1 \ldots \Psi_{n_c}, \Psi_{n_c+1})_k^T, \quad k=1 \ldots n_b. \quad \ldots\ldots\ldots\ldots (8)$$

and $$x_k \equiv (p^{n+1}, N_1^{n+1} \ldots N_{n_c}^{n+1}, N_{n_c+1}^{n+1})_k^T, \; k=1 \ldots n_b. \quad \ldots\ldots (9)$$

The Ψ are defined in Eqs. 1, 2, and 5. The well constraint equations and flowing bottomhole pressures are also included in F and x, respectively, after the reservoir equations and variables, as discussed in Refs. 17 and 18. Solution of the equations with Newton's method corresponds to the iterative scheme

$$x^{k+1} = x^k - [(\partial F/\partial x)^k]^{-1} F^k, \quad \ldots\ldots\ldots\ldots\ldots\ldots (10)$$

where $(\partial F/\partial x)$ represents the Jacobian of F with respect to x and superscript k denotes the iteration level.

The partial derivatives of $(\Psi_1 \ldots \Psi_{n_c+1})$ with respect to $(p, N_1 \ldots N_{n_c+1})^{n+1}$ for explicit blocks are straightforward and are evaluated by analytical differentiation. The partial derivatives of $y_{io}^{n+1}, y_{ig}^{n+1} (i=1 \ldots n_c), \rho_o^{n+1}, \rho_g^{n+1}, S_o^{n+1}, S_g^{n+1}$ (and of all properties that depend on these variables) with respect to p^{n+1} and $N_j^{n+1} (j=1 \ldots n_c)$ involve the derivatives of the equilibrium equations with respect to the last primary variables. (The dependence of S_w^{n+1} on p^{n+1} and N_i^{n+1} can be seen from Eq. 7.) Those derivatives are obtained as described below.

The simplest approach would involve the shifting of each primary variable by a small amount and performing a flash calculation after each shift. This would require an unnecessarily large computational effort. Consequently, the following analytical approach is used. Because Eq. 6 is satisfied at equilibrium, we can write for each gridblock containing an oil and a gas phase

$$(\partial g/\partial p)\mathrm{d}p + (\partial g/\partial N)\mathrm{d}N + (\partial g/\partial N_g)\mathrm{d}N_g = 0 \quad \ldots\ldots\ldots\ldots (11)$$

where $$N \equiv (N_1 \ldots N_{n_c})^T \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (12)$$

and $$N_g \equiv (N_{1g} \ldots N_{n_c,g})^T. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (13)$$

In the differentiation in Eq. 11, the moles of Component i in the oil phase, N_{io}, are treated as the dependent variables. Expressions for the partial derivatives are given in the Appendix. Replacing the variations in Eq. 11 by finite quantities (i.e., Δp, ΔN, ΔN_g), and rearranging gives

$$\Delta N_g = -(\partial g/\partial N_g)^{-1}[(\partial g/\partial p)\Delta p + (\partial g/\partial N)\Delta N]. \quad \ldots\ldots\ldots (14)$$

Eq. 14 provides the desired variation of the flash-calculation results to small variations of the primary variables. It allows an efficient evaluation of the phase splits corresponding to small variations in the primary variables in a numerical differentiation scheme. Once ΔN_g is known, the gas and oil compositions can readily be computed and the phase properties can be evaluated. This approach allows the inclusion of analytical derivatives in a numerical differentiation scheme. Through this scheme, analytical derivatives

are inserted in the Jacobian in the same manner as when analytical differentiation is used.[19]

Jacobian Structure and Partial Elimination. For simplicity, consider a three-hydrocarbon-component system ($n_c=3$) in a 1D grid system. Let Gridblocks 1 and 2 be explicit and Gridblocks 3 and 4 be implicit. Criteria for selecting implicit and explicit blocks are discussed in a subsequent section.

Fig. 1a shows the incidence matrix of the Jacobian. Note that because of the selection of equations and primary variables, the explicit diagonal blocks are sparse and simple to factorize. For all explicit diagonal blocks, the diagonal elements are used to eliminate the elements in the first row. This gives rise to the incidence matrix depicted in **Fig. 1b**, where the asterisk denotes the elements that have been modified in the partial elimination. Fig. 1b also shows that $(p)_1$, $(p)_2$, $(p, N_1, N_2, N_3, N_4)_3$ and $(p, n_1 \ldots N_4)_4$ can further be decoupled from the remaining variables and solved by a preconditioned iterative method described in Ref. 20.

Selection of Implicit Blocks and Switching Criteria. A recently described[21] method based on the Courant-Friedrichs-Lewy criterion was used to designate gridblocks as implicit or explicit. This is a stability-based criterion in which the component front velocity of largest magnitude in a given gridblock is compared with a "discretization velocity" computed from the block geometry and the timestep size. The front velocities are obtained by solving a generalized eigenvalue problem in each block. This criterion is generally too computationally costly to be applied to every gridblock in each timestep; instead, it is applied to all implicit blocks, to all explicit blocks that neighbor implicit blocks, and to all blocks in which a mobile phase first appears. Wellblocks are always treated implicitly.

TABLE 1—GAS-CONDENSATE COMPOSITION (mol%)

C_1	67.93
C_2	9.90
C_3	5.91
C_4	5.17
C_5	2.69
C_6	1.81
C_7 through C_9	3.99
C_{10} through C_{11}	1.22
C_{12} through C_{14}	0.80
C_{15+}	0.58

Comparison of Different Methods

Outline. A comparison of the adaptive-implicit, the fully implicit, and the explicit-transmissibility approaches was carried out with the problem in the Third SPE Comparative Solution Project[1] as the test example. The fully implicit technique used the same solution method as in the adaptive-implicit approach except that all gridblocks were implicit for the whole run. For the explicit-transmissibility method, all gridblocks except the wellblocks were explicit. Newtonian iterations were used in all cases.

Problem Description. The test problem was Case No. 1 of the Third SPE Comparative Solution Project, which corresponds to a gas-cycling process in a gas-condensate reservoir. The problem specification is given in Ref. 1. The gas is produced at a separator rate of 6,200 Mscf/D for 15 years. During the first 10 years, part of the produced separator gas is reinjected at a rate of 4,700 Mscf/D.

TABLE 2—PERFORMANCE OF VARIOUS METHODS WITH TEST EXAMPLE FROM THE THIRD SPE COMPARATIVE SOLUTION PROJECT

Method	Normalized Execution Time	Number of Timesteps	Average Timestep Size (days)	Total Number of Iterations	Average Fraction of Implicit Blocks
Adaptive-implicit	1.00	40	136.9	135	0.078
Explicit-transmissibility	2.43	186	29.4	388	0.010
Fully implicit	3.10	37	148.0	80	1.00

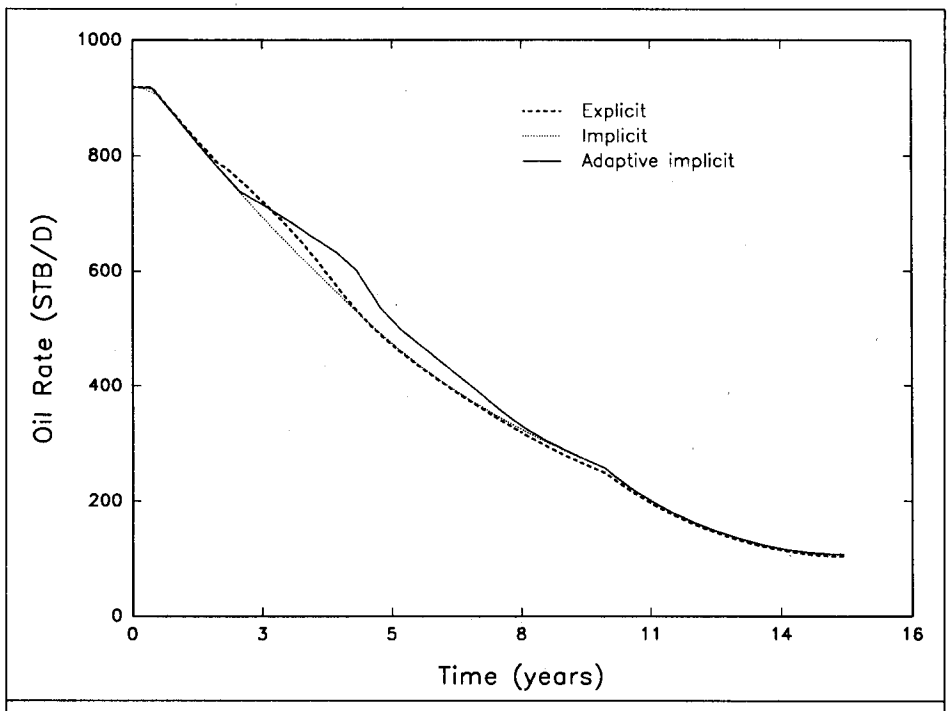

Fig. 2—Stock-tank oil rate.

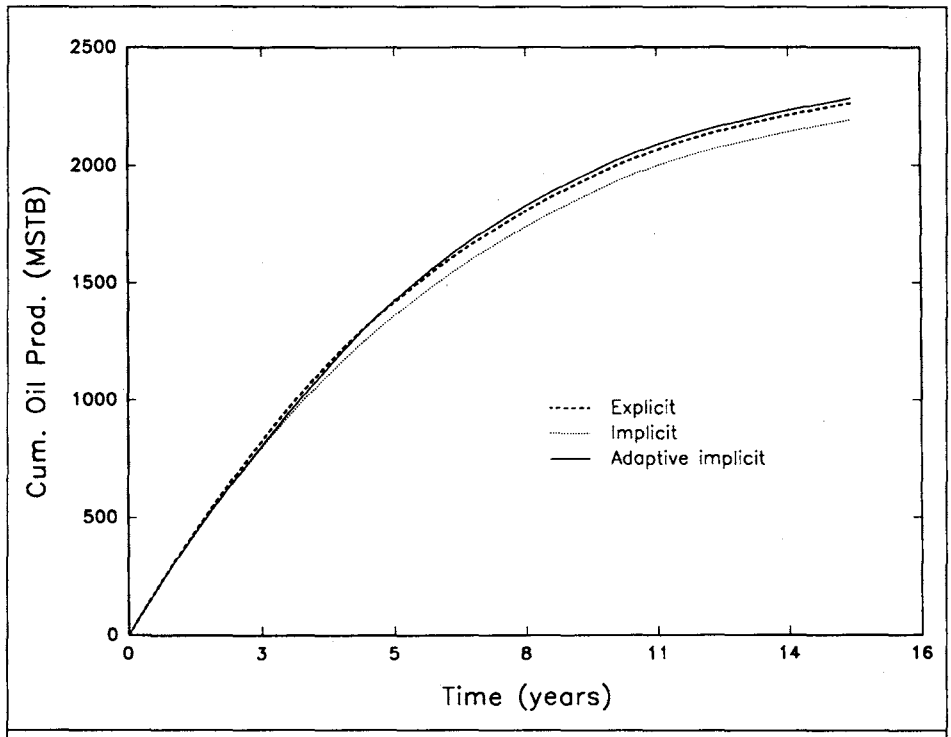

Fig. 3—Stock-tank oil produced.

The cycling is stopped after 10 years. The gas condensate is modeled with 10 components with the composition shown in **Table 1**.

Results. Table 2 shows the performance of the three methods for the 15-year simulation. The total number of iterations corresponds to the number of Newtonian iterations for the whole run. The numbers in Table 2 clearly demonstrate the efficiency of the adaptive-implicit method. This method is two to three times faster than the fully implicit or explicit-transmissibility approaches. The adaptive-implicit run took an average of 92.5% of the fully implicit timestep size with only 7.8% of the gridblocks implicit. The reduction in total computing time of the adaptive-implicit approach compared with the fully implicit approach is consistent with the observations of Forsyth and Sammon,[9] who reported at least a 40% improvement for a variety of black-oil simulations.

The results of the three approaches are quite similar, as demonstrated by **Figs. 2 through 4**. Figs. 2 and 3 depict the oil rate and cumulative oil produced, respectively. Fig. 4 shows the oil saturation in Gridblock (7,7,4), which corresponds to the bottom block of the production completion. This saturation is representative of the near-well liquid accumulation.

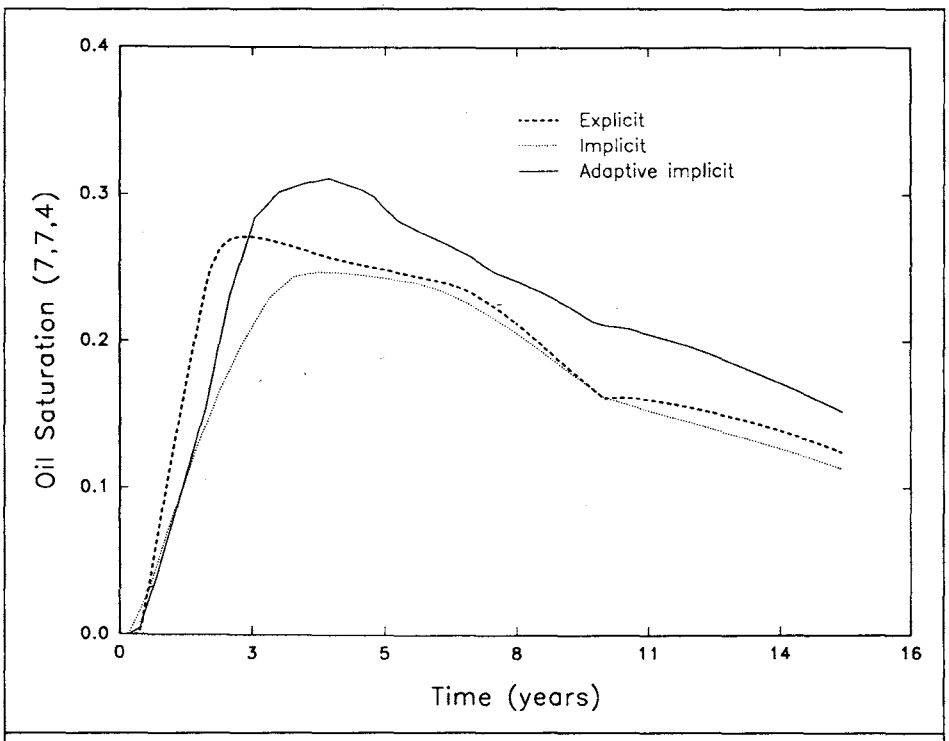

Fig. 4—Oil saturation in Gridblock (7,7,4).

Conclusions

This paper discusses a robust and efficient approach for adaptive-implicit compositional simulation. The salient features of the approach are the selection of equations and primary variables and decoupling of the flash calculations from the solution of the flow equations. This allows the flexibility of implementing powerful flash-calculation methods developed elsewhere into the simulator.

A comparison of the adaptive-implicit, fully implicit, and explicit-transmissibility approaches was carried out with the Third SPE Comparative Solution Project as the test example. Results show that the adaptive-implicit method is two to three times faster than the other two approaches. This demonstrates that the adaptive-implicit concept can efficiently be used to solve discretized equations with a large number of unknowns per gridblock.

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Nomenclature

D = depth
f_{im} = fugacity of Component i in Phase m ($m=o,g$)
F = function defined in Eq. 8
g = phase-equilibrium equation
n_b = number of gridblocks
N = defined in Eq. 12
N_g = moles of gas per unit of gridblock volume
N_i = moles of Component i per unit of gridblock volume ($i=1 \ldots n_c+1$)
N_{im} = moles of Component i in Phase m ($m=o,g$) per unit of gridblock volume
N_o = moles of oil per unit of gridblock volume
p = oil-phase pressure
P_{cog} = gas/oil capillary pressure
P_{cwo} = oil/water capillary pressure
q_i = molar injection/production rate of Component i
S_m = saturation of Phase m ($m=o,g,w$)
t = time
T = temperature
T_m = molar transmissibility of Phase m ($m=o,g,w$)
V = gridblock volume
x = primary variable defined in Eq. 9
y_{im} = mole fraction of Component i in Phase m ($m=o,g$)
z_i = global mole fraction of Component i ($i=1 \ldots n_c$)
γ_m = gradient of Phase m ($m=o,g,w$)
Δ = difference operator
ρ_m = molar density of Phase m ($m=o,g,w$)
ϕ = porosity
Ψ_i = material-balance or volume-consistency equation

Subscripts

g = gas phase
i,j,s = subscripts for components
k = subscripts for components or gridblocks
m,q = phase subscripts
n_c+1 = water component
o = oil phase
w = aqueous phase

Superscripts

(k) = iteration level
m = old or new time level
n = old time level
$n+1$ = new time level

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Appendix—Analytical Differentiation of the Thermodynamic Equilibrium Equations

The thermodynamic equilibrium equations are

$$g_i=\ln f_{ig}(p,y_g)-\ln f_{io}(p,y_o)=0,\ i=1 \ldots n_c. \quad \ldots\ldots\ldots (A\text{-}1)$$

The mole fractions y_{io} and y_{ig} are related to the moles N_{io} and N_{ig} through the expression

$$y_{im}=N_{im}/\sum_{g=1}^{n_c} N_{sm}\, i=1 \ldots n_c; m=o,g. \quad \ldots\ldots\ldots\ldots (A\text{-}2)$$

The moles N_{ic} and N_{ig} also satisfy

$$N_{io}=N_i-N_{ig}. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (A\text{-}3)$$

By treating the N_{io} as the dependent variables from Eq. A-3, the required derivatives in Eq. 13 are

$$(\partial g_i/\partial p)_{N,N_g}=(\partial \ln f_{ig}/\partial p)_{y_g}-(\partial \ln f_{io}/\partial p)_{y_o}, \quad \ldots\ldots\ldots (A\text{-}4)$$

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$$(\partial g_i/\partial N_{jg})_{p,N,N_{kg\neq j}}=(\partial \ln f_{ig}/\partial N_{jg})_{p,N_{kg\neq j}}, \quad \ldots\ldots\ldots\ldots (A\text{-}5)$$

and $(\partial g_i/\partial N_j)_{p,N_g,N_{k,k\neq j}}=-(\partial \ln f_{io}/\partial N_{jo})_{p,N_{ko,k\neq j}}$

$$\times(\partial N_{jo}/\partial N_j)_{p,N_g,N_{k,k\neq j}}=-(\partial \ln f_{io}/\partial N_{jo})_{p,N_{ko,k\neq j}}. \quad \ldots\ldots (A\text{-}6)$$

To evaluate the derivatives of fugacities with respect to mole numbers, the following chain rule for $m=o,g$ is required.[22]

$$(\partial \ln f_{im}/\partial N_{jm})_{p,N_{km,k\neq j}}=\Big[(\partial \ln f_{im}/\partial y_{jm})_{p,y_{km,k\neq j}}$$

$$-\sum_{s=1}^{n_c} y_{sm}(\partial \ln f_{im}/\partial y_{sm})_{p,y_{km,k\neq s}}\Big]/N_m, \quad \ldots\ldots\ldots\ldots (A\text{-}7)$$

where all $y_{sm}(s=1\ldots n_c)$ are treated as independent variables.

SI Metric Conversion Factors

bbl	× 1.589 873	E−01	= m^3
ft^3	× 2.831 685	E−02	= m^3

*Conversion factor is exact.

SPERE

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