

A General Unstructured-Grid, Equation-of-State-Based, Fully Implicit Thermal Simulator for Complex Reservoir Processes

K. Liu, G. Subramanian, D.I. Dratler, J.P. Lebel, and J.A. Yerian, ExxonMobil

Summary

This paper describes a general unstructured-grid, equation-of-state- (EOS) based, fully implicit thermal simulator for complex reservoir processes. Under the unstructured grid framework, the simulator uses Newton's method to solve component material-balance equations, energy-balance equation, and volume-balance equation for component moles, energy, and pressure, where chemical reactions and external heat sources/sinks are treated in source terms. Because of the similarity among component material-balance equations and the energy-balance equation, energy is treated as a "component" to achieve a uniform formulation with common code for all simulations (black-oil, compositional, and thermal).

The thermal simulator was validated using analytical models and other thermal simulators. The thermal simulator is used to study grid-orientation problems and to design and optimize Cold Lake heavy-oil development.

Introduction

Modern reservoir management requires a simulator to represent reservoir details accurately using fine-scale geologic features, complex well paths, and modeling of large-scale interactions among multiple fields. Unstructured gridding makes it possible to capture and honor more geologic and engineering detail in reservoir-simulation models with greater exactness than Cartesian-based reservoir grids. However, industry generally has been reluctant to apply this capability to practical reservoir simulation partly because of concerns about potential loss in computational efficiency. Many papers have been published under Cartesian-based framework (Mifflin et al. 1991; Watts 1986; Coats 1980; Watts et al. 2005). Few papers are available to address reservoir simulation issues under general unstructured-grid framework (Naccache 1997; Beckner et al. 2001, 2006; Heinemann et al. 1991; Usadi et al. 2007; Karypis and Kumar 1998).

Naccache (1997) presented a 3D thermal reservoir simulator that models the injection of steam into heavy oil. Pressure, component molar densities, and bulk internal energy density were chosen as primary variables to be solved from volume-balance, component, and energy-conservation equations. Because mass/energy densities (Naccache 1997) are not state variables, the total energy and component masses of a node would be more physically meaningful and more easily interpreted by a user/developer. In addition, changes of component masses and energy are symmetric between adjacent nodes. As a result of these issues, we have chosen the node pressure, energy, and component moles as primary variables in this simulator, rather than pressure, component molar density, and bulk internal energy density as chosen by Naccache (1997). Furthermore, these primary variables fit naturally in the single-value decomposition (SVD) solver (Watts 2005), which has proved to be very efficient for thermal simulation. More discussions on variable selections will be given later.

Dead-oil examples are given in Naccache's paper (1997), which is only a special case of the generalized thermodynamic

treatment in this paper when all phase-component K -values are pressure- and temperature-dependent. Also, Naccache's (1997) treatment needs to predetermine the phase state by calculating three temperatures at which gas appears, oil disappears, and water disappears, which compares to a simple summation of missing phase compositions in this paper. More discussions will be given in Appendix A.

In 2001, Beckner et al. (2001) presented ExxonMobil's new unstructured-grid reservoir-simulation system, which discussed field examples involving complex geologic features (e.g., nonvertical faults and stratigraphic pinchouts) and multiple reservoirs connected to a common production infrastructure. It was reported that the simulator significantly reduces simulation cycle time through ease of use and integration with geologic models. One example indicated that approximately 100,000 blocks can represent the equivalent of 1.6 million rectangular gridblocks for achieving accurate geologic features.

One of the most important aspects for unstructured reservoir simulator development is the linear solver for solving large linear systems created by an unstructured grid that cannot be efficiently solved by conventional solution methods normally applied to simulators using rectangular gridding. Beckner et al. (2006) reported their collaborative effort on developing an unstructured linear-solver library, called SparSol, which includes a numerical library of scaling and reordering methods, preconditioners, and iterative methods. Results show that SparSol is faster than several popular, freely available packages for the set of matrices tested.

Usadi et al. (2007) reported their experiences with parallelizing an unstructured reservoir simulator on symmetric multiprocessing machines. Their paper includes how parallelization is performed at a high level through several variants of data partitioning adapted to the specific algorithmic needs, that solver-convergence rate can be strongly dependent on simulator-determined data partitioning, and that well-management performance can be strongly dependent on the way reservoir engineers have applied their constraints and field production analysis.

The next few sections of this paper present an overview of the simulation equations, solution procedures, and some discussions. Examples are given to illustrate simulator results, to demonstrate how the simulator can reduce grid-orientation problems and how the EOS method can be used in thermal simulation. The final section contains the conclusions resulting from this work.

Governing Equations

The governing equations that will be solved in thermal simulations include a volume-balance equation and N_c+1 conservation equations (N_c mass-balance equations for each material component and an energy-balance equation). Assume that there are N_{conn} connections connecting to the given node i . The component mass-balance equation for component m can be written as

$$N_{m,i}^{n+1} - N_{m,i}^n = -\Delta t \left(\sum_j^{N_{\text{conn}}} U_{m,i \rightarrow j}^{n+1} + q_{m,i}^{n+1} \right), \dots \dots \dots (1)$$

where $q_{m,i}^{n+1}$ represents the sources/sinks, including injection, production, and/or reactions. $U_{m,i \rightarrow j}^{n+1}$ is the mass flow rate of component m across a connection of nodes i and j (positive from node i to node j). $U_{m,i \rightarrow j}^{n+1}$ is calculated as

$$U_{m,i \rightarrow j}^{n+1} = \tau_{ij} \sum_v^{N_p} (x_{v,m,i,j}^{n+1} \lambda_{v,i,j}^{n+1} \Delta \Phi_{v,i \rightarrow j}^{n+1}) \dots (2)$$

Eq. 1 states that the net mole change of component m in node i during a timestep is equal to the net amount of component m flowing into the node during the timestep.

The energy-balance equation can be written as

$$E_i^{n+1} - E_i^n = -\Delta t \left(\sum_j^{N_{\text{conn}}} U_{E,i \rightarrow j}^{n+1} + q_{E,i}^{n+1} \right), \dots (3)$$

where $q_{E,i}^{n+1}$ represents the energy sources/sinks. $U_{E,i \rightarrow j}^{n+1}$ is the energy flow rate across a connection of nodes i and j . $U_{E,i \rightarrow j}^{n+1}$ is calculated as

$$U_{E,i \rightarrow j}^{n+1} = \tau_{ij} \sum_v^{N_p} (h_{v,i,j}^{n+1} \lambda_{v,i,j}^{n+1} \Delta \Phi_{v,i \rightarrow j}^{n+1} + \tau_{h,ij} (\Delta T_{i \rightarrow j}^{n+1})) \dots (4)$$

For the connection between rock-only nodes or connection between rock-only and rock/fluid nodes, the energy flow rate is calculated as

$$U_{E,i \rightarrow j}^{n+1} = \tau_{h,ij} (\Delta T_{i \rightarrow j}^{n+1}) \dots (5)$$

Eq. 3 states that the net energy change in node i during a timestep is equal to the net amount of energy flowing into the node during the timestep.

Note that the form of Eq. 3, the energy-balance equation, is identical to that of Eq. 1, the component mass-balance equation, with E_i taking the place of $N_{m,i}$, U_E taking the place of U_m , and q_E taking the place of q_m . Also note that, if conduction is ignored, the form of Eq. 4, the energy flow rate, is identical to that of Eq. 2, the component mass flow rate, with phase molar enthalpy h taking the place of phase composition x . Therefore, energy is analogous to mass as far as convective transport is concerned.

The volume balance equation can be written as

$$\sum_v^{N_p} V_v = V_p \dots (6)$$

Eq. 6 simply states that the fluid volume in a node should exactly fill its pore space.

The N_c+2 equations of Eqs. 1, 3, and 6 are used to solve for N_c+2 primary variables (e.g., N_c component moles, one energy, and one pressure).

To solve these N_c+2 equations, all terms must be expressed as linear combinations of N_c+2 primary variables. Especially, the node temperature in the conduction term of the energy-balance equation must be expressed in terms of the changes of N_c+2 primary variables for rock/fluid node:

$$T_i^{\ell+1} = T_i^\ell + \frac{\partial T_i}{\partial p_i} \delta p_i + \sum_k^{N_c+1} \frac{\partial T_i}{\partial M_{ki}} \delta M_{ki}, \dots (7)$$

where M_{ki} represents both masses and energy of node i , and $k = 1, 2, \dots, N_c$, and energy. For the rock-only node, temperature is a function of energy only:

$$T_i^{\ell+1} = T_i^\ell + \frac{\partial T_i}{\partial E_i} \delta E_i \dots (8)$$

The linearized component mass-balance equations and energy-balance equation have the following form:

$$\delta M + F_M \delta M + F_p \delta p = r_M, \dots (9)$$

where M at each node is a vector of masses and energy, p is the vector of pressure, and r_M is the vector of residuals. The matrix F_M and F_p relate to flow between nodes. This form enables us to apply the SVD method (Watts and Shaw 2005) to component mass-balance equations as well as energy-balance equation.

The linearized volume-balance equation of node i in rock/fluid regions is

$$\frac{\partial \left(V_p - \sum_v^{N_p} V_v \right)}{\partial p} \delta p + \sum_{k=1}^{N_c+1} \frac{\partial \left(V_p - \sum_v^{N_p} V_v \right)}{\partial M_k} \delta M_k = r_V \dots (10)$$

Eq. 10 is used to eliminate one of the variables in the linear solver.

Constant Energy Flash Calculation

The Newton solution from governing equations gives updated pressure, component moles, and energy for each node. The constant-energy-flash-calculation procedure provides node temperature, phase compositions, phase fractions, all physical properties, and all partial derivatives needed for solving node pressure, energy, and component moles from governing equations.

Assume that there are N_p phases and N_c components for a given node. At equilibrium, the sum of the phase compositions of phase v must be equal to 1:

$$\sum_m^{N_c} \frac{K_{vm} z_m}{\sum_{k=1}^{N_p} f_k K_{km}} = 1, \dots (11)$$

where equilibrium K -value for a component m in phase v , K_{vm} , is defined as the ratio of the composition of component m in phase v , x_{vm} , to the master phase composition of the same component m , x_{Mm} :

$$K_{vm} = \frac{x_{vm}}{x_{Mm}} \dots (12)$$

An individual equilibrium phase-component K -value may be specified by the user or calculated from phase-equilibrium principles as

$$f_{vm} = f_{pm}, \dots (13)$$

where subscripts $v, p = 1, 2, \dots, N_p$. The phase-component fugacity may be calculated based on the Peng-Robinson EOS (Peng and Robinson 1976).

The updated energy E from governing equations should be absorbed by rock and fluid within a node:

$$E = \sum_{v=1}^{N_p} E_v + E_{\text{rock}} \dots (14)$$

For an N_p -phase and N_c -component system, there are $(N_p-1)N_c+N_p+1$ unknowns [i.e., $(N_p-1)N_c$ phase-component K -values, N_p phase fractions, and 1 temperature]. Eqs. 11, 13, and 14 provide $(N_p-1)N_c+N_p$ equations. The phase fraction constraint is used to close the set:

$$\sum_{v=1}^{N_p} f_v = 1. \dots (15)$$

Newton's method is used to solve these nonlinear equations simultaneously. After convergence, all physical properties and all partial derivatives needed for solving the governing equations are calculated accordingly. For a rock-only node, the node energy-balance equation is used to solve for temperature:

$$E = E_{\text{rock}} \dots (16)$$

Timestep Solution Procedure

For a given timestep size, simulation involves solving for primary variables (pressure, energy, and component moles) from governing equations and secondary variables (temperature, phase fractions, and phase-component equilibrium K -values) from constant-energy flash calculations. The solution procedure is outlined as follows.

1. Initialize reservoir at time zero.
2. For a given timestep:
 - a. All physical properties and all partial derivatives are obtained from corresponding packages.
 - b. Jacobian matrix is formed from coefficient-generation package.
 - c. Globally solve for changes of pressure, energy and component moles.
 - d. Update pressure, energy, and component moles.
 - e. Constant-energy flash to calculate all physical properties and all partial derivatives needed for solving governing equations.
 - f. Repeat Steps a through e until global Newton convergence.
3. Proceed to the next timestep and repeat Step 2.

Discussion

- When steam is injected into a reservoir in thermal reservoir processes, some node temperatures may be several hundred degrees higher than normal reservoir temperature for a given timestep, which results in extremely large changes in fluid volume and saturations. The reversal from injection to production or vice versa requires modeling hysteresis in relative permeability. The QUAD model (Lebel 2002) for modeling the geomechanical behavior of the unconsolidated sands also can be extremely nonlinear. When steam is injected into heavy-oil reservoirs, the original water, gas, and oil phases are redistributed into emulsion water and gas phases. The emulsion model, which was developed to handle the emulsion phenomena, makes phase densities and viscosities very complicated and nonlinear. Therefore, thermal process simulation is usually much more time-consuming than isothermal process simulations. Fully implicit schemes and iterative procedures are developed for efficient thermal simulation.

- Equations to be solved are divided into two categories: governing equations that must be solved simultaneously for the entire model and constituent equations, which are solved node by node. Because thermal simulation involves significant changes of pressure, temperature, and saturations, a large number of global Newton iterations would be required if all governing and constituent equations were solved simultaneously. The iterative procedure described in the previous section enables us to focus on nodes that require more Newton iterations to converge the constant-energy flash calculations. Because only a very small number of nodes experience significant changes for a given timestep, the overall computing time is saved.

- Selection of primary variables plays an important role in thermal simulation. For a bitumen/water two-component system, it is possible to have bitumen/water/steam three phases. Phase rule indicates that pressure and temperature are dependent on each other in a two-component/three-phase system and cannot be treated as independent variables simultaneously. Phase compositions, phase fraction, and saturations are not considered primary variables because a phase may appear/disappear in simulation processes. A technique of variable substitution may be applied to solve those problems, but it complicates the software design and makes simulator development and maintenance very costly. Variable substitution also makes it more difficult to apply the SVD method (Watts and Shaw 2005) to solve the linear matrix system.

The selection of pressure, energy, and component moles as primary variables helps to avoid these problems. Especially because energy is treated as a component, a uniform formulation with common code for all simulations (black-oil, compositional, and thermal) can be achieved, and the SVD method is applied easily to solve the linear matrix system. A uniform formulation helps simulator design, development, and maintenance.

The problem associated with the selection of pressure, energy, and component moles as primary variables is that we need to solve a constant-energy flash problem. On the other hand, the cost associated with a constant-energy flash is very small because the calculations are node-based, and just a small number of nodes require a large number of Newton iterations to converge the solution.

- The overburden and underburden draw off energy from the reservoir, which must be included in thermal simulation. The treatment of overburden and underburden is different from the calculations in the reservoir. There are no material balance and volume balance, which leaves one equation (energy-balance equation) and one unknown (energy) per node. The heat conduction parallel to reservoir can be included or ignored. If it is ignored, the linearized overburden and underburden energy-balance equations are decoupled from reservoir equations and the resulting linear matrix structure is the same as it would be if the overburden and underburden were not present, which also serves as the preconditioner if the heat conduction parallel to reservoir is included.

- The packages for calculating fluid properties, rock properties, reaction properties, displacement properties, and well/surface facility calculations are completely separated from the rest of the simulator, which enables us to rapidly develop and verify various models for business needs. For example, the EOS-based constant-energy fluid-phase equilibrium package was developed for modeling the various solvent-assisted thermal processes, where fluid-phase equilibrium principles and energy-balance equation are used to solve for K -values and temperature. The reaction package was developed to handle Cold Lake CO₂ generation during the thermal process.

Examples

Except for the recently developed thermal EOS, the simulator has been validated against analytical models, cases of SPE 4 (Aziz et al. 1987), and other simulators (Mifflin et al. 1991). This section gives examples to show that the simulator developed can be used to reduce grid orientation problems and that the thermal EOS capability can be used in Cold Lake cyclic-steam stimulation (CSS) process.

Grid Orientation. Grid orientation effects in rectangular grids are well known and have been demonstrated by Todd et al. (1972). Yanosik and McCracken (1979) reported results for five- and nine-point Cartesian grids, and five-point grids can predict completely unphysical erroneous results.

Fig. 1 shows a grid-orientation problem when using five-point rectangular grids in a steamdrive recovery process. The steam reaches the far producer before reaching the near producer because of the zigzag path dictated by the five-point finite-difference formulation.

To get comparable results with an unstructured hexagonal perpendicular-bisector (pebi) grid, no refinement was done around the wells, and the number of gridpoints is very similar. **Fig. 2** shows that the hexagonal pebi grid yields much better predictions of steam breakthrough. This shows that the unstructured grid can

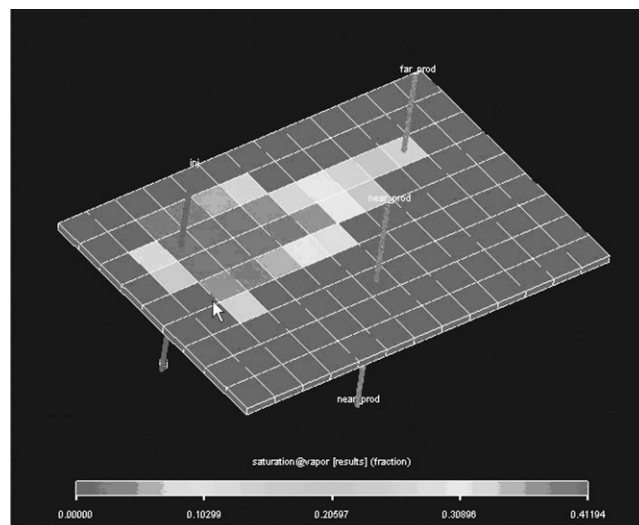


Fig. 1—Grid orientation: Steam reaches the far producer before reaching the near producer when using five-point rectangular grids.

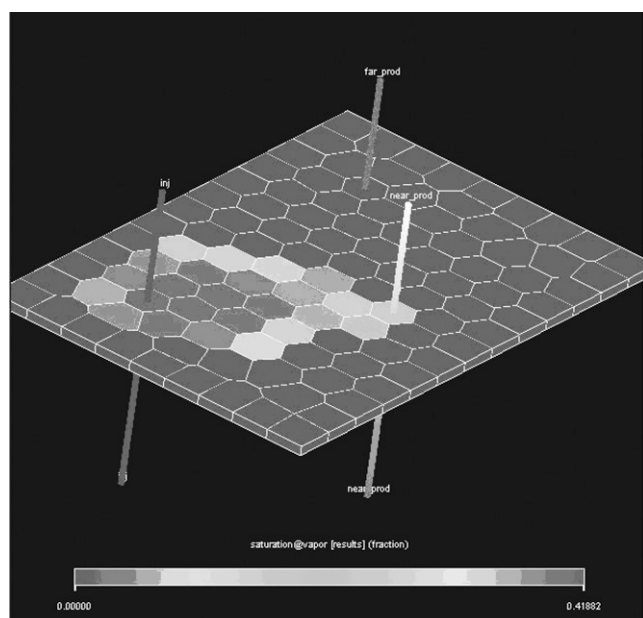


Fig. 2—Steam reaches the near producer before reaching the far producer when using unstructured hexagonal pebi grids.

be used for flood patterns, and the results are similar to what has been reported by Heinemann et al. (1991). The unstructured grids are flexible in that it is easy to refine the grid near the wells if one needs more accuracy. The change in block size near the wells is much smoother than when using Cartesian grids and, consequently, is less prone to discretization error.

Thermal EOS in Cold Lake CSS Process. This example illustrates modeling a Cold Lake CSS process with the simulator's thermal EOS capability and is intended to show that equivalent results can be achieved using the EOS approach vs. an equilibrium K -value table approach. We compare a CSS case that does not use the EOS formulation to one that does. Fluid properties of each case are the same, except that EOS parameters (Table 1) are used in the EOS case. The CSS models use four components: bitumen, water, methane, and CO_2 . The heptane component listed in the table is used only in the "liquid addition to steam for enhancing recovery" (LASER) case described later. Other simulation parameters are similar to previous Cold Lake CSS models (Lebel 2002).

As described later, the EOS approach gives roughly the same results as the K -value table method. In principle, the EOS approach more easily and correctly represents component interactions and is inherently consistent with the use of EOS determination of phase densities. We expect that, as the complexity of the system increases, so will the importance of component interactions. Further work is needed to demonstrate this.

A second case compares results using solvent (heptane) coinjection with the steam starting in Cycle 7 as in Imperial Oil's ongoing LASER process (Leaute 2002; Laute and Carey 2005) to illustrate a situation in which a volatile solvent is employed. The EOS approach used allows accurate representation of fluid properties in this case without the use of cumbersome, composition-dependent fluid property and K -value tables.

Cumulative bitumen volumes are shown for the two CSS cases in Fig 3. The CSS cases, with and without the EOS formulation, compare to within 0.8 percent after 10 cycles. The case with solvent coinjection illustrates a successful run using a vaporizing solvent. As can be seen in Fig. 4, this case shows recovery uplift over either of the base CSS cases in Cycles 7 and 8 shown in the figure.

The use of EOS does slow down the simulation because the EOS approach involves more calculations. When all phase-component K -values are in table format, the pressure-volume-temperature/displacement package takes approximately 15% of the total computing time, which compares to approximately 25% of the total computing time when all nonwater component K -values are determined from the Peng-Robinson EOS (Peng and Robinson 1976).

Summary

A general unstructured-grid, EOS-based, fully implicit thermal simulator has been developed for complex reservoir processes. An iterative procedure has been developed to solve nonlinear equations, in which pressure, energy, and component moles are solved simultaneously from mass-/energy-/volume-balance equations, but temperature, phase fractions, and phase-component K -values are solved node by node from constant-energy flash calculations.

The selection of pressure, energy, and component moles as primary variables helps us to achieve a uniform formulation with common code for all simulations (black-oil, compositional, and thermal), design unstructured-grid linear solvers, and reduce the cost for simulator design, development, and maintenance.

Examples show that the simulator developed can be used to reduce grid-orientation problems and that the thermal EOS capability can be used in Cold Lake CSS-process modeling. Further details regarding the examples can be obtained from the authors—Subramanian for Example 1, Grid Orientation, and Lebel for Example 2, Thermal EOS in Cold Lake CSS Process.

Nomenclature

E	= energy, BTU
F	= flow between nodes, RB/D
f	= phase-component fugacity in Eq. 13, psi, or phase fraction in Eqs. 11 and 15
h	= phase molar enthalpy, BTU/lbm mole
K	= phase-component K -value
M	= vector of masses and energy, lbm moles or BTU
N	= component moles, lbm moles
N_c	= number of components
N_{conn}	= number of connections
N_p	= number of phases
q	= sources/sinks, including injection, production, and reactions
r	= vector of residuals
T	= temperature, °F
T_h	= thermal transmissibility
U	= flow rate, moles/day
V	= volume, barrels
x	= phase composition

TABLE 1—EOS PARAMETERS FOR FLUID PROPERTIES

Component	Critical Temperature (°C)	Critical Pressure (kPa)	Accentric Factor	Molecular Weight
Bitumen	931.00	743.0	0.9930	487.0
Water	374.00	22,106.0	0.8600	18.0
Methane	−82.55	4,604.3	0.0104	16.0
CO_2	31.05	7,384.0	0.2250	44.0
Heptane	267.05	2,735.8	0.3494	100.2

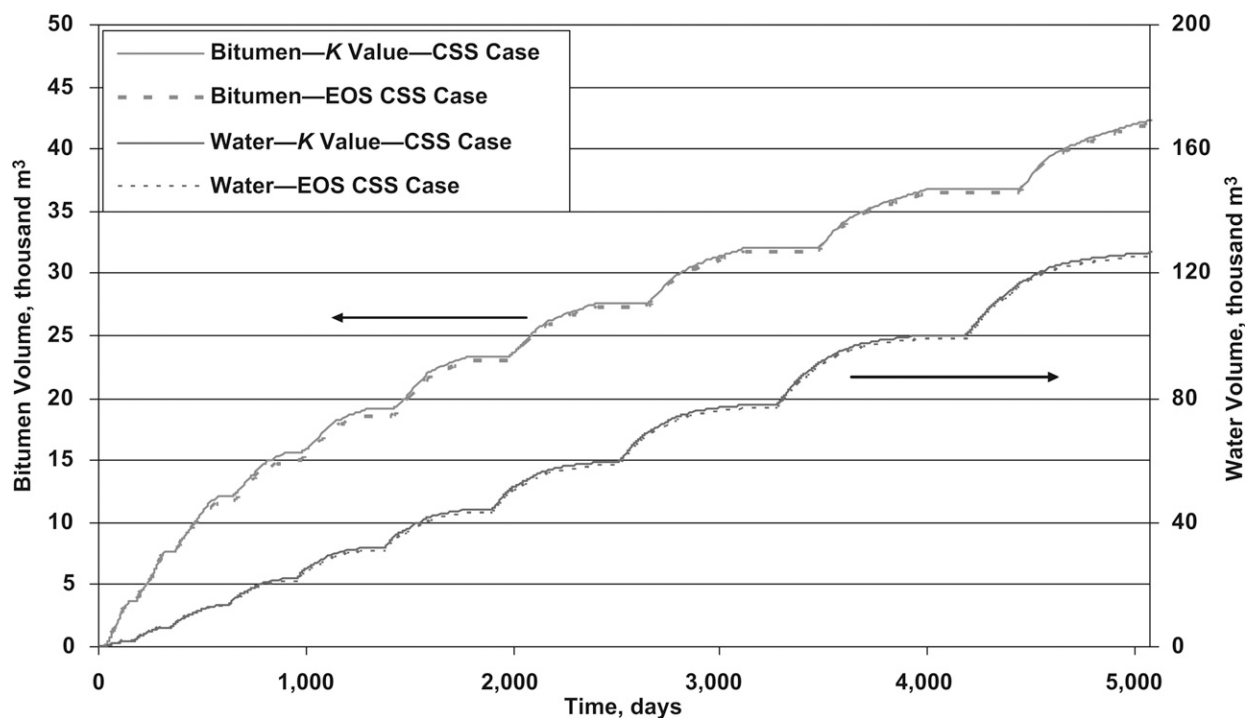


Fig. 3—Cumulative oil and water showing good agreement.

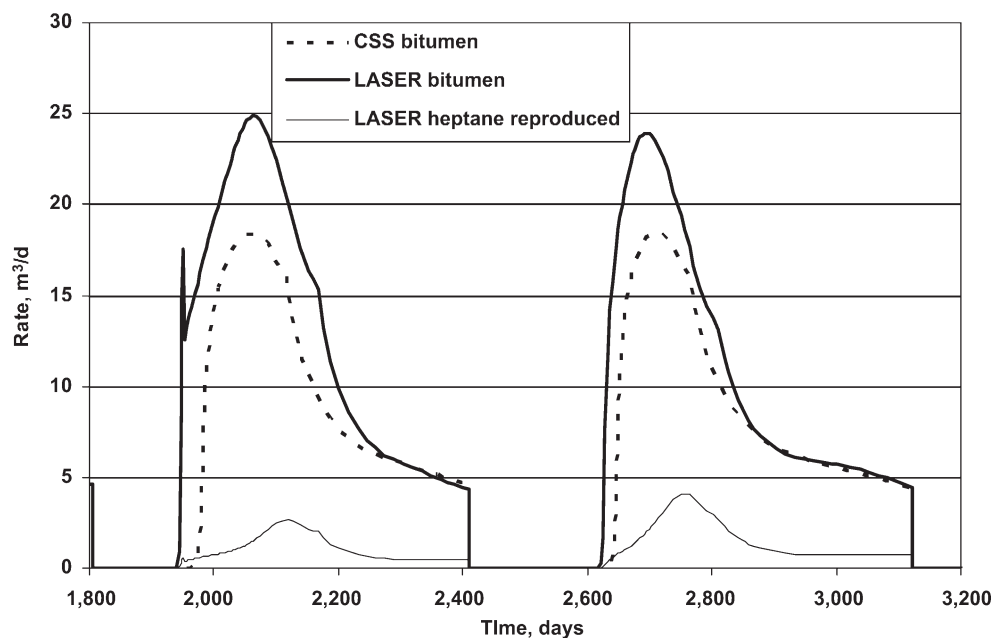


Fig. 4—Performance of CSS vs. LASER in Cycles 7 and 8 shows that the EOS approach handles the solvent case.

z = overall composition
 Δt = timestep size, day
 δ = change over an iteration
 λ = mobility, 1/cp
 ξ = molar density, lbm moles/bbl
 τ = transmissibility, bbl-cp/day-psi
 τ_h = thermal transmissibility, BTU/day-°F
 Φ = potential, psi

Subscripts

E = energy
 i = node index

ij = connection property between nodes i and j (upstream weighted)
 $i \rightarrow j$ = flow across a connection of nodes i and j (positive as going from node i to node j)
 j = node index
 M = master component in Eq. 12
 m = component index
 p = pore volume in Eq. 6 or phase index in Eq. 13
 v = phase index

Superscripts

n = timestep number
 ℓ = Newton iteration level

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Appendix A—More on Constant-Energy Flash Calculation

Eqs. 11 through 16 are used to solve the constant-energy flash problem in a thermal-process simulation. This appendix describes related model variations.

An individual equilibrium phase-component K -value, K_{vm} , may be specified by the user or calculated from phase-equilibrium principles. Several options are available in our simulator, including

- Pressure/temperature-dependent analytical model:

$$K_{vm} = \left(K_{1vm} + \frac{K_{2vm}}{P} + K_{3vm}P \right) e^{\frac{-K_{4vm}}{T - K_{5vm}}}, \dots \dots \dots (A-1)$$

where K_{1vm} , K_{2vm} , K_{3vm} , K_{4vm} , and K_{5vm} are called first, second, third, fourth, and fifth K -value coefficients for component m in phase v , which are user-input constants from matching pressure/volume/temperature laboratory data.

- Pressure/temperature-dependent table.
- Pressure/temperature/composition-dependent table.
- EOS:

$$K_{vm} = \frac{\phi_{Mm}}{\phi_{vm}}, \dots \dots \dots (A-2)$$

where ϕ_{Mm} and ϕ_{vm} are fugacity coefficients of component m in master phase M and phase v , $v = 1, 2, \dots, N_p$. The phase-component fugacity coefficients may be calculated on the basis of the Peng-Robinson EOS (Peng and Robinson 1976).

The user also can specify a particular phase-component K -value to zero, which means no solubility of the specified component in the specified phase. For example, the user may specify zero K -values for bitumen component in an aqueous phase or for water component in an oleic phase.

The number of simultaneous nonlinear equations to be solved in constant-energy flash calculations depends on the number of phase-component K -values that are EOS-dependent or not. When all K -values are only pressure/temperature-dependent, the number of simultaneous nonlinear equations equals the number of phases. Solution variables include temperature and $N_p - 1$ phase fractions when Eq. 15 is used to eliminate one of the phase fraction unknowns. The number of simultaneous nonlinear equations is increased as more EOS-dependent phase-component K -values are present.

Both phase-stability analysis and negative flash are used to handle the phase appearance and disappearance problem when EOS is involved. When all K -values are only pressure/temperature-dependent, the sum of the missing phase compositions is used to determine whether a phase should be added during the flash process.

Models are needed to calculate phase volumes, phase densities, phase viscosities, phase heat capacities, rock heat capacity, etc. Many options are available to model rock and fluid properties. For estimation of viscosity of multicomponent mixtures, we can use combinations of table formats, correlations, and mixing rules [Linear, Koval (1963), and Log mixing rules] to handle phase viscosities. If a mixing rule is chosen, there are options for component viscosity calculations. These are incidental to our paper and are not included.

Temperature-dependent relative permeability or capillary-pressure curves are not considered at this time.

Kai Liu is a senior engineering specialist at ExxonMobil's Upstream Research Center in Houston. He holds a PhD degree in petroleum engineering from Texas A&M University. Liu's main research interests are reservoir-simulator development, reservoir simulation, and EOS modeling. He is also a technical reviewer for the *SPE Reservoir Evaluation & Engineering*. **Ganesan Subramanian** is an engineering associate at ExxonMobil's Upstream Research Center in Houston. He specializes in simulation studies and has been involved in the development and support of ExxonMobil's reservoir simulation software for several years. Subramanian holds a PhD degree in chemical engineering from the University of Minnesota. **David Dratler** is the supervisor of reservoir technology with ExxonMobil's

Technical Computing Company. Dratler has worked for ExxonMobil for 13 years. He holds a PhD in aerospace engineering from The University of Arizona and a BS degree in aeronautical and astronautical engineering from The Ohio State University. Dratler is a technical reviewer for the *SPE Reservoir Evaluation & Engineering* journal. **Jean-Pierre Lebel** holds a BS degree in mechanical engineering from the University of Calgary. Currently with Imperial Oil Limited, he has more than 30 years of experience in production and reservoir engineering. As a research advisor with Imperial, his reservoir engineering skills included design, evaluation, and monitoring of secondary and

tertiary conventional-oil-recovery schemes as well as heavy oil and bitumen thermal, nonthermal, and hybrid recovery schemes. In reservoir simulation, his responsibilities included development, utilization, training, and advisory roles with Imperial and ExxonMobil. He has also led research teams responsible for implementing six new heavy-oil recovery technology pilots. **Jeff Yerian** works as a reservoir engineer in heavy-oil research at ExxonMobil Upstream Research Company. His main research interests are reservoir simulation of steam and solvent processes. Yerian holds a PhD degree in chemical engineering from North Carolina State University.