



## Reservoir Simulation: State of the Art

by Keith H. Coats, SPE

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### Introduction

The purpose of this paper is to describe the current level of development in reservoir simulation. This requires some discussion of what a simulation model is and why it is needed or used. Following a brief history of simulation and a general description of a simulation model, two sections describe the reservoir simulator through discussions of recovery mechanisms and model methodology. The second of these sections discusses past and recent developments and summarizes the technology currently used in simulation models. The two descriptive sections are followed by a discussion of why simulation is used (i.e., typical reservoir performance questions addressed by computer simulation), a section with examples pertinent to simulation today, and a summary.

### A Brief History

In a broad sense, reservoir simulation has been practiced since the beginning of petroleum engineering in the 1930's. Simulation is simply the use of calculations to predict reservoir performance (to forecast recovery or compare economics of alternative recovery methods). Before 1960, these calculations consisted largely of analytical methods,<sup>1,2</sup> zero-dimensional material balances,<sup>3,4</sup> and one-dimensional (1D) Buckley-Leverett<sup>5,6</sup> calculations.

The term "simulation" became common in the early 1960's, as predictive methods evolved into relatively sophisticated computer programs. These programs represented a major advancement because they allowed solution of large sets of finite-difference equations describing two- and three-dimensional (2- and 3D), transient, multiphase flow in heterogeneous porous media. This advancement was made possible by the rapid evolution of large-scale, high-speed digital computers and development of numerical mathematical methods for solving large systems of finite-difference equations.

During the 1960's, reservoir simulation efforts were devoted largely to two-phase gas/water and three-phase black-oil reservoir problems. Recovery methods simulated essentially were limited to depletion or

pressure maintenance. It was possible to develop a single simulation model capable of addressing most reservoir problems encountered. This concept of a single, general model always has appealed to operating companies because it significantly reduces the cost of training and usage, and, potentially, the cost of model development and maintenance.

During the 1970's, the picture changed markedly. The sharp rise in oil prices and governmental trends toward deregulation and partial funding of field pilot projects led to a proliferation of enhanced-recovery processes. This led to simulation of new processes that extended beyond conventional depletion and pressure maintenance to miscible flooding, chemical flooding, CO<sub>2</sub> injection, steam or hot water stimulation/flooding, and in-situ combustion. A relatively comfortable understanding of two-component (gas and oil) hydrocarbon behavior in simple immiscible flow was replaced by a struggle to unravel and characterize the physics of oil displacement under the influence of temperature, chemical agents, and complex multicomponent phase behavior. In addition to simple multiphase flow in porous media, simulators had to reflect chemical adsorption and degradation, emulsifying and interfacial tension (IFT) reduction effects, reaction kinetics, and other thermal effects and complex equilibrium phase behavior.

The proliferation of recovery methods in the 1970's caused a departure from the single-model concept as individual models were developed to represent each of these new recovery schemes. Thus, the emphasis today is on examining and fine tuning the equations and related assumptions pertinent to these techniques.

Research during the 1970's resulted in many significant advances in simulation model formulations and numerical solution methods. These advances allowed simulation of more complex recovery processes and/or reduced computing costs through increased stability of the formulations and efficiency of the numerical solution methods.

### Simulation Models—A Brief Description

Odeh<sup>7</sup> gives an excellent description of the conceptual simplicity of a simulation model. He illustrates the subdivision of a reservoir into a 2- or 3D network of grid blocks. He then shows that the simulation model

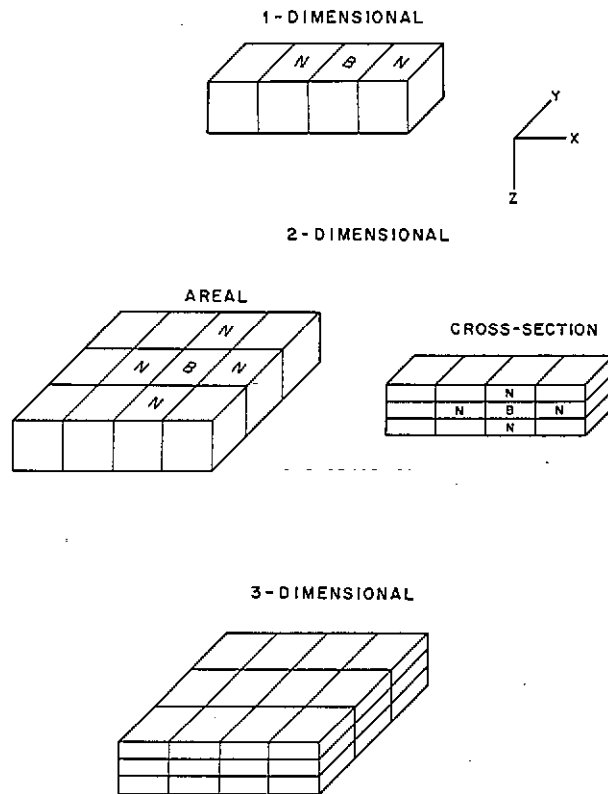


Fig. 1—1-, 2-, and 3D grids.

equations are basically the familiar volumetric material balance equation<sup>3,4</sup> written for each phase for each grid block. The phase flow rates between each grid block and its two, four, or six (in 1-, 2-, or 3D cases, respectively) adjacent blocks are represented by Darcy's law modified by the relative permeability concept. Fig. 1 illustrates 1-, 2-, and 3D grids representing a portion of a reservoir. The block and its two or four neighbors are denoted by B and N in the 1- and 2D grids. One can visualize an interior block of the 3D grid with its six neighbors, two on either side of the block in the x, y, and z directions. In practice, the subsea depths to the top surface of each grid vary with areal position, reflecting reservoir formation dip.

Reservoir properties such as permeability and porosity, and fluid properties such as pressure, temperature, and composition, are assumed uniform throughout a given grid block. However, reservoir and fluid properties vary from one block to another; fluid properties for each grid block also vary with time during the simulation period.

A simulation model is a set of partial-difference equations requiring numerical solution as opposed to a set of partial differential equations amenable to analytical solution. The reasons for this are: (1) reservoir heterogeneity—variable permeability and porosity and irregular geometry; (2) nonlinearity of relative permeability and capillary pressure vs.

saturation relationship; and (3) nonlinearity of fluid PVT properties as functions of pressure, composition, and temperature. The models require high-speed digital computers because of the amount of arithmetic associated with the solutions.

A simulation model requires three types of input data. First, reservoir description data include (1) overall geometry, (2) grid size specification, (3) permeability, porosity, and elevation for each grid block, and (4) relative permeability and capillary pressure vs. saturation functions or tables. Geological and petrophysical work involving logs and core analyses is necessary for items 1 and 3. Laboratory tests on core samples yield estimates of relative permeability and capillary pressure relationships. Second, fluid PVT properties, such as formation volume factors, solution gas, and viscosities are obtained by laboratory tests. Finally, well locations, perforated intervals, productivity indices (PI's), and rate schedules must be specified.

Model output or calculated results include spatial fluid pressure and saturation distributions, and producing GOR and WOR and injection/production rate (for wells on injectivity/productivity) for each well at the end of each time step of the computations. Internal manipulation of these results gives average reservoir pressure and instantaneous rates and cumulative injection/production of oil, gas, and water by well and total field vs. time.

#### Simulation Models and Oil-Recovery Mechanisms

Different types of simulation models are used to describe different oil-recovery mechanisms. The most widely used types are black oil, compositional, thermal, and chemical flood. The four basic recovery mechanisms for recovering oil from reservoirs are: (1) fluid expansion, (2) displacement, (3) gravity drainage, and (4) capillary imbibition. Simple fluid expansion with pressure decline results in oil expulsion from and subsequent flow through the porous matrix. Oil is displaced by gas and injected or naturally encroaching water. Gravity drainage, caused by positive (water/oil and oil/gas) density differences, aids oil recovery by causing upward drainage of oil from below an advancing bottomwater drive and downward drainage from above a declining gas/oil contact. Finally, imbibition, generally normal to the flow direction, can be an important recovery mechanism in lateral waterfloods in heterogeneous sands with large vertical variation of permeability.

To accommodate compositional and the enhanced-recovery processes in this discussion, we add a fifth mechanism, oil *mobilization*. This loosely defined term includes widely different phenomena that create or mobilize recoverable oil. Some of these phenomena are not really distinct from the first four.

The black oil model accounts for the four basic mechanisms in simulation of oil recovery by natural depletion or pressure maintenance (e.g.,

waterflooding). This isothermal model applies to reservoirs containing immiscible water, oil, and gas phases with a simple pressure-dependent solubility of gas in the oil phase. This two-component representation of the hydrocarbon content presumes constant (pressure-independent) oil and gas phase compositions, no volatility of oil in the gas phase, and zero solubility of gas and oil in the water.

The remaining model types discussed here account for some mobilization mechanisms in addition to the four basic recovery mechanisms. Compositional models are used to simulate recovery processes for which the black oil assumption of constant-composition, immiscible gas and oil phases is invalid. Some examples are: (1) depletion of a volatile oil or gas condensate reservoir where phase compositions and properties vary significantly with pressure below bubble- or dewpoint; (2) injection of nonequilibrium gas (dry or enriched) into a black-oil reservoir to mobilize oil by vaporization into the more mobile gas phase or by attainment of outright (single-contact) or dynamic (multiple-contact) miscibility; and (3) injection of CO<sub>2</sub> into an oil reservoir to mobilize oil by Mechanism 2 and by oil viscosity reduction and oil swelling. Holm<sup>8</sup> gives an excellent description of mechanisms active in CO<sub>2</sub> and miscible flooding.

The compositional model describes reservoir hydrocarbon content as an *N*-component mixture. Gas/oil phase properties and equilibrium (*K*-values) are calculated from pressure- and composition-dependent correlations or, more recently, from equations of state (EOS).

Thermal simulators are applied to steam injection or in-situ combustion processes in heavy-oil reservoirs where oil is mobilized primarily by (1) reduction of oil viscosity with increased temperature, (2) distillation of intermediate hydrocarbon components from the oil phase to the more mobile gas phase, and (3) cracking of the oil phase [usually above 500°F (260°C)] with subsequent distillation. Thermal models include PVT correlations to describe *N*-component oil and gas phase properties as functions of pressure, temperature, and composition.

Chemical flood models include polymer, micellar (surfactant), and alkaline (caustic). Polymer waterflooding improves oil recovery by lowering the oil/water mobility ratio by reducing the effective permeability to water and/or by increasing water viscosity. In micellar flooding, surfactants greatly reduce oil/water IFT, thereby solubilizing oil into the micelles and forming an oil bank.<sup>9</sup> The surfactant slug and mobilized oil normally are propelled toward the production well by a graded bank of polymer-thickened water. The mechanisms responsible for improved oil recovery in alkaline flooding are not understood clearly but are thought to include low IFT, wettability alteration, and emulsification.<sup>10</sup> Chemical flooding processes involve complicated fluid/fluid and rock/fluid interactions such as adsorption, ion

exchange, viscous shear, and three- (or more) phase flow.

### Why Simulation Models Are Used

Reservoir simulation is used to estimate recovery for a given existing producing scheme (forecasting), to evaluate the effects on recovery of altered operating conditions, and to compare economics of different recovery methods. Staggs and Herbeck<sup>11</sup> give an excellent discussion of the uses of simulation with examples. Coats<sup>12</sup> gives a general discussion of simulation use and misuse. McCulloch *et al.*<sup>13</sup> and a number of papers in Ref. 14 describe field applications of simulation models. Harpole and Hearn<sup>15</sup> and Killough *et al.*<sup>16</sup> describe recent black-oil models of rather complex reservoirs.

Black-oil models frequently are used to estimate the effect of these parameters on oil recovery: (1) well pattern and spacing, (2) well completion intervals, (3) gas and/or water coning as a function of rate, (4) producing rate, (5) augmenting a natural water drive by water injection and desirability of flank or peripheral as opposed to pattern waterflooding, (6) infill drilling, and (7) gas vs. water vs. gas plus water injection.

Compositional models also are used for most of these purposes but, as stated previously, only in cases where the black-oil two-component, fixed-composition PVT representation is invalid. They are applied in reservoir studies to estimate (1) loss of recovery caused by liquid dropout during depletion of condensate reservoirs and the reduction of this loss by full or partial cycling (re injection of gas from surface facilities), and (2) effects of pressure level, injected gas composition, and CO<sub>2</sub> or N<sub>2</sub> injection on oil recovery by vaporization or miscibility. Graue and Zana<sup>17</sup> describe application of a compositional model in estimating Rangely field oil recovery by CO<sub>2</sub> injection as a function of injected composition and pressure level.

Results of compositional simulation of a CO<sub>2</sub> project include CO<sub>2</sub> breakthrough time and rate and composition of produced fluids. These are required to design production facilities and CO<sub>2</sub> recycling strategies.<sup>18</sup> Modeling is also useful to optimize pattern size and CO<sub>2</sub>/water injection rates to overcome the effects of reservoir heterogeneity.<sup>19</sup>

Thermal models are applied in reservoir studies of in-situ combustion and are used to simulate performance of cyclic steam stimulation and steamflooding. In steam injection, questions addressed by simulation relate to effects of injected steam quality and injection rate, operating pressure level, and inclusion of gas with the injected steam. One question in cyclic stimulation concerns the optimal time periods per cycle for steam injection, soak, and production. The flooding case introduces the issues of well pattern and spacing. A number of steam-injection field studies using models have been published. Herrera and

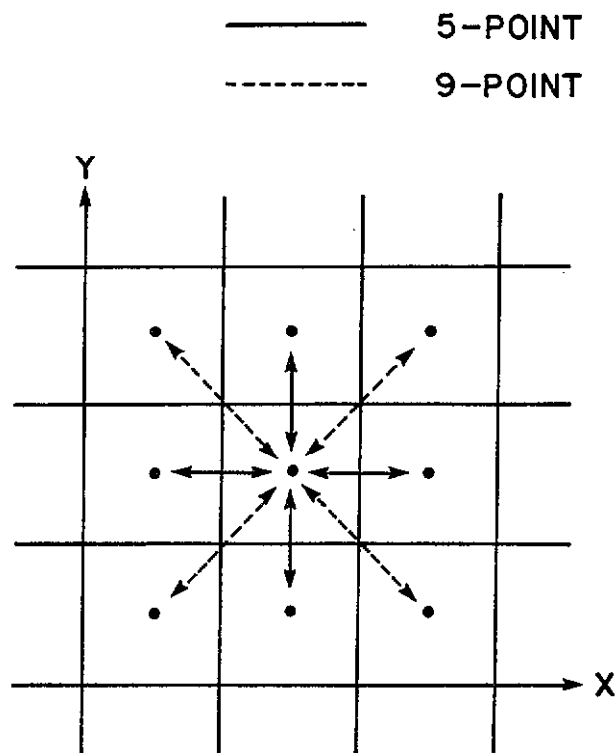


Fig. 2—Five- and nine-point difference schemes.

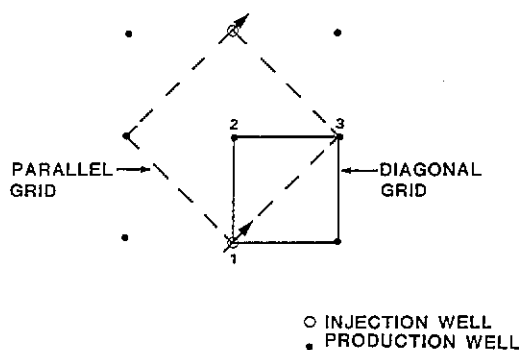


Fig. 3—Nine-spot grids.

Hanzlik<sup>20</sup> compare field data and model results for a cyclic stimulation operation, Williams<sup>21</sup> discusses field performance and model results for stimulation and flooding, and Meldau<sup>22</sup> discusses field and model results related to addition of gas to the injected steam.

Numerical simulation provides a reliable means to predict chemical flood performance in a reservoir environment, because the processes are very complex and many reservoir parameters affect the results. Consequently, chemical flood simulation has been used to construct a screening algorithm for the selection of reservoirs suitable for micellar/polymer flooding<sup>23</sup> and to examine competing EOR strategies—e.g., CO<sub>2</sub> vs. surfactant flooding.<sup>24</sup> For caustic<sup>25</sup> and polymer<sup>26</sup> applications, as well as for the micellar process, chemical flood modeling is useful to discern controlling process mechanisms and to identify laboratory data required for process description.

In recent years, simulation has been used increasingly to estimate and compare recoveries from a given reservoir under alternative enhanced-recovery processes, such as CO<sub>2</sub> injection, thermal methods (steam injection and in-situ combustion), and several types of chemical flooding.

#### Simulation Models—Methodology

In the interest of brevity and with some oversimplification, the discussion of formulations currently used in simulation models uses a concept of a single, general model. The general model is a set of  $N$  partial difference equations written for each grid block comprising the reservoir. Each equation is simply a mathematical statement of conservation of mass of a specified substance or of conservation of energy. Each substance or component may be present in all phases, distributed according to  $K$ -values or distribution coefficients obtained from correlations or an equation of state. With allowance for rock adsorption isotherms, chemical reactions, temperature-, pressure-, and composition-dependence of viscosity, relative permeabilities, and capillary pressure, each of the previously described model types is a subset of the single, general model.

Note that *components* (and *energy*), not phases, are the conserved substances requiring equations in the simulation model. Thus, the number of phases is unrelated to the number of model equations.

Until recently, simulation models made use of the common five-point difference scheme for areal ( $x$ - $y$ ) interblock, Darcy flow terms in each of the conservation equations. Fig. 2 illustrates this flow between a grid block and each of its four neighbors. A strong grid-orientation effect was reported by Todd *et al.*<sup>27</sup> for highly adverse mobility waterfloods and later observed by Coats *et al.*<sup>28</sup> for pattern steamfloods. An areal grid with the usual perpendicular  $x$  and  $y$  axes may be placed over a five-spot pattern with the  $x$  axis either parallel to or at a 45° angle to the line

connecting the injector to a producer (Fig. 3). These parallel and diagonal grids<sup>27</sup> can result in markedly different calculated shapes of the water or steam front and the breakthrough times. This difference was reduced by the nine-point finite difference formulation described by Yanosik and McCracken<sup>29</sup> and is illustrated by the four extra diagonal flow terms in Fig. 2. Their technique is being programmed rapidly into simulators treating steamflooding and miscible CO<sub>2</sub> injection where adverse mobility pattern floods commonly are encountered.

The formulation terms described here apply within the context of either the conventional five- or nine-point finite-difference scheme. The IMPES™ formulation denotes implicit pressure, explicit saturation. Sheldon *et al.*,<sup>30</sup> Stone *et al.*,<sup>31</sup> and Fagin *et al.*<sup>32</sup> describe the IMPES method for black-oil (three-equation) problems, and Coats<sup>33</sup> gives an obvious extension to the *N*-equation case. This method is explicit in saturation in that it uses old time-level values of relative permeabilities in the interblock flow terms. Solution of a single pressure equation is followed by an explicit updating of fluid saturations and compositions in each grid block.

MacDonald<sup>34</sup> improved the stability of the IMPES method for the two-phase water/oil case by following the pressure equation solution with solution of a water-saturation equation over the grid using implicit (new-time-level or end-of-time-step) values of relative permeabilities in the interblock flow terms. Spillette *et al.*<sup>35</sup> extended this concept to the three-phase case and called the formulation *sequential*.

The *implicit* formulation makes use of end-of-time-step values of relative permeabilities (and densities, viscosities) in the interblock flow term transmissibilities. This requires simultaneous solution of all *N* equations. Blair and Weinaug<sup>36</sup> first published this fully implicit formulation. Implementation of implicit or highly implicit formulations in black-oil, geothermal, steamflood, compositional, and combustion models is described in a number of papers.<sup>33,37-44</sup>

The IMPES formulation can become unstable if the volumetric flow through a grid block in a time step exceeds a small fraction of the block PV. The more stable sequential formulation remains stable to much larger ratios of grid block volumetric throughput/PV. The tolerable throughput ratio for the implicit formulation is significantly larger than that of the sequential method.

Arithmetic (or computing cost) per time step and time-step size both increase from IMPES to sequential to implicit formulations. Since the total cost of simulating a given time period is proportional to the product of arithmetic per time step and time-step size, all three formulations are used widely today.

Single-well coning studies generally involve radial grid spacings, resulting in very small grid blocks near the well and large throughput ratios. For these studies, the IMPES formulation is unsuitable, and the implicit

formulation is generally the most efficient.

For field-scale, 3D black-oil studies, the overall computing time is frequently less with the sequential than with the IMPES or implicit formulation. The typical black-oil simulator applied today in 1,000- or more grid-block, field-scale studies is an IMPES model with a user-specified option of sequential solution. Smaller black-oil studies and preliminary cross-sectional, coning, and sensitivity studies associated with the large problems are using the implicit formulation more and more frequently.

Thermal models<sup>39,43,45-47</sup> generally involve implicit formulations. The emerging compositional model involves an equation of state, with options of IMPES or implicit formulations. One difficulty here is that the IMPES formulation lacks sufficient stability for some field-scale problems, while the implicit formulation requires too much machine storage capacity (associated with solution of *N<sub>c</sub>* simultaneous equations) to handle problems larger than, say, 2,000 grid blocks. This dilemma is absent for black-oil models because the sequential formulation fills the gap. However, the sequential formulation does not preserve material balances in compositional problems for which adjacent grid block compositions differ greatly.<sup>39</sup>

Meijerink<sup>48</sup> wrote a revised stabilized IMPES formulation that has potential for filling this compositional model gap between IMPES and implicit methods. Meijerink's scheme improves the stability of IMPES, as does the sequential method, without resulting in material balance error in regions of steep composition gradients.

### Numerical Dispersion

The term *numerical dispersion* refers to spatial truncation error in finite-difference simulator results. In physical terms, this error generally appears as falsely smeared spatial gradients of water saturation in waterflooding, temperature in steamflooding, solvent in miscible flooding, and chemical agent in chemical flooding. This excessive smearing occurs primarily in the areal (*x* or *y*) directions and, if uncontrolled, results in too early calculated breakthrough times of water (heat, solvent, etc.) at production wells.

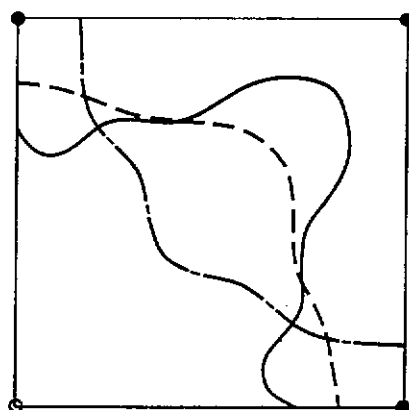
This numerical dispersion generally increases with increasing areal grid block size ( $\Delta x$  and  $\Delta y$ ). Thus, one remedy is use of a finer areal grid. However, a prohibitive increase in required computer time and storage frequently results from use of a grid sufficiently fine to eliminate numerical dispersion.

Kyte and Berry<sup>49</sup> describe control of numerical dispersion in simulation of waterflooding through large areal grid blocks. They use pseudorelative permeability curves obtained from detailed (fine-grid) cross-sectional simulations. Harpole and Hearn<sup>15</sup> used their method in a 3D black-oil study. To date, steamflood simulation generally has been confined to pattern studies for which a sufficient number of grid blocks between unlike wells is used to minimize numerical

TABLE 1—CALCULATED STEAM BREAKTHROUGH TIMES (days) FOR A NINE-SPOT PATTERN

Difference Scheme	Well 2		Well 3	
	Diagonal	Parallel	Diagonal	Parallel
five-point	47.8	204	1,400	117
nine-point	87.7	75.5	900	1,000

GRID	DIFFERENCE-SCHEME
———— PARALLEL	5-POINT
- - - - DIAGONAL	5-POINT
- - - - EITHER	9-POINT



TIME = 80 DAYS

- INJECTOR
- PRODUCER

Fig. 4—Calculated shape of steamflood front in a nine-spot pattern.

dispersion effects.

Gas fingering in black-oil reservoirs, and unstable viscous fingering of solvent in adverse-viscosity-ratio miscible floods, can result in simulation results with too little smearing of saturation and concentration gradients. Remedies in these two cases are beyond the scope of this discussion. Killough *et al.*<sup>16</sup> describe alteration of a black-oil formulation to force additional dispersion into the gas saturation profile. Koval<sup>50</sup> and Todd and Longstaff<sup>51</sup> describe methods of forcing additional dispersion to represent viscous fingering in simulation of miscible displacements.

#### Impact of Hardware Advances on Simulation Practice

The computational speed, storage, and vectorization capabilities of computer hardware have increased sharply in the past few years. As an example, the Cray-1S™ computer provides up to 4,000,000 decimal-words of storage, compared with a typically available

100,000 words on most machines used until 1975. Recently introduced computers offer sharp increases in computational speeds and speed/cost ratios. In addition, vector processing capabilities of Control Data Corp. and Cray computers allow significantly greater efficiency of simulators coded to use this vectorization. Nolen *et al.*<sup>52</sup> found that vectorization of code in the solution technique subroutine of a simulator can reduce solution computing time by factors as large as 40.

This vectorization together with increased machine size and speed contributes strongly to the feasibility of larger reservoir studies. Until recently, most black-oil studies used up to about 3,000 grid blocks. We currently are performing an 11,000-grid-block study; Mrosovsky *et al.*<sup>53</sup> describe a 3D black-oil model study of Prudhoe Bay field using more than 16,000 active grid blocks, and larger studies than this undoubtedly are under way elsewhere.

#### Examples and Discussion

This section illustrates the grid-orientation effect for a pattern steamflood. Fig. 3 shows a 3-acre ( $12 \times 10^3\text{-m}^2$ ) nine-spot pattern with the diagonal grid and 45°-shifted parallel grid. This pattern has three types of wells—labeled 1 (injector), 2 (near producer), and 3 (far producer).

The isotropic homogeneous formation has permeability of 4,000 md, porosity of 0.36, thickness of 20 ft (6.1 m) and rock-specific heat of 35 Btu/cu ft rock-°F. Oil viscosity is 6,750 cp (6.75 Pa·s) at initial reservoir temperature and 45 cp (0.045 Pa·s) at 500°F (260°C). Initial pressure is 200 psia (1.4 MPa), initial saturations are  $S_{wi}=0.19$ ,  $S_{or}=0.81$ , and irreducible water saturation is 0.17.

Specified rate for each injection well is 1,000 B/D ( $159\text{ m}^3/\text{d}$ ) of 80% quality steam at 800 psia (5.5 MPa) and 517°F (269°C). All production wells are produced on deliverability against a constant bottomhole pressure (BHP) of 200 psia (1.4 MPa).

The calculated results in Table 1 show the pronounced effect of grid orientation on steam breakthrough times through use of the five-point difference scheme. Obviously, steam should arrive at the near Producer 2 before it reaches the far producer, Well 3. The parallel grid with the five-point scheme actually gives breakthrough at Well 3 at 117 days, before breakthrough at Well 2 (204 days).

Table 1 shows that the nine-point difference scheme virtually eliminates the effect of grid orientation for this problem. Fig. 4 shows calculated steam front shapes at 80 days for the two different schemes using parallel and diagonal grids. The difference between the nine-point fronts for the two grids is small and about equal to the error of manual interpolation.

Recent compositional models<sup>42,54</sup> use an EOS as opposed to separate correlations for oil density, gas density, and equilibrium  $K$ -values. These papers emphasize that the EOS offers the advantage of

consistency in that phase densities and  $K$ -values are obtained from a single source. This consistency results in smooth and differentiable convergence of separate phase densities and compositions to identical values as computations approach a critical point. Phase viscosities based on a correlation<sup>55</sup> using EOS densities also converge smoothly to a single value at a critical point.

The EOS's most widely used in reservoir calculations today are Redlich-Kwong<sup>56-58</sup> and Peng-Robinson<sup>59</sup> equations. Martin<sup>60</sup> shows that all cubic EOS's can be obtained from a single, general EOS form. Yarborough<sup>61</sup> describes applications of a modified Redlich-Kwong EOS to reservoir fluids; Katz *et al.*<sup>62</sup> give applications of the Peng-Robinson EOS.

In our compositional work, we have found that nonlinear regression on EOR parameters is necessary. Frequently, prohibitive time requirements result from trial-and-error efforts to match laboratory test data. We generally have found some adjustment of EOS parameters necessary to match laboratory PVT data.

Table 2 compares EOS calculated results with laboratory PVT data reported by Simon *et al.*<sup>63</sup> for mixtures of CO<sub>2</sub> and a SACROC oil sample at 130°F (54°C). Simon *et al.* presented the crude oil sample analysis through C<sub>13</sub><sup>+</sup>. We performed regressions, using all the data listed, with 14 components (C<sub>1</sub> through C<sub>13</sub><sup>+</sup> and CO<sub>2</sub>) and with five components after pseudoizing (lumping components) the crude to four components. The calculated results correspond to use of the four pseudocomponents. These results used a modified Redlich-Kwong EOS<sup>57</sup>, but very similar results were obtained with the Peng-Robinson EOS. Baker and Luks<sup>64</sup> calculated an equally good saturation pressure match of these data using 39 components, without regression, using a modified

Redlich-Kwong EOS.

The predicted values in Table 2 were calculated with no regression using 14 components in the Peng-Robinson EOS. We used binary interaction coefficients given by Katz *et al.*,<sup>62</sup> except that CO<sub>2</sub>/hydrocarbon values were 0.10 and the C<sub>1</sub> through C<sub>13</sub><sup>+</sup> binary was adjusted to 0.1298 to match the crude bubble-point pressure of 1,660 psia (11.4 MPa). Without the latter adjustment, the Peng-Robinson EOS calculated a bubble-point pressure of 1,469 psia (10.1 MPa). All the predicted saturation pressures are bubble points, while the last three observed and last two pressures, calculated through regression, are dewpoints.

Our compositional simulation of CO<sub>2</sub> injection, using the previously discussed EOS match, indicated completely immiscible displacement at all pressures. The simulations showed pronounced vaporization of light and intermediate oil components into the CO<sub>2</sub>, increasing with increasing flood pressure level. Dicharry *et al.*<sup>65</sup> discuss design-stage tests indicating multiple-contact miscibility for CO<sub>2</sub> injection at pressures as low as 1,800 psia (12.4 MPa) for SACROC Unit. Kane<sup>66</sup> reports subsequent work indicating higher pressures necessary for miscibility.

Simulation frequently is employed to study rate sensitivity. We define rate sensitivity as an adverse relationship between ultimate oil recovery and production or reservoir voidage rate. Ref. 67 describes a simulation study of rate sensitivity in different types of reservoirs in Alberta. This study was restricted to pressure-maintained, water/oil displacements and included coning and 2- and 3D calculations in formations ranging from moderate to severe heterogeneity.

The conclusion of that rather lengthy reference is simple and brief: Water/oil displacements are rate-

TABLE 2—SACROC OIL/CO<sub>2</sub> PVT DATA

	Observed <sup>62</sup>	Calculated (after regression)	Predicted
Saturation pressure, psia	1,660	1,660	1,660
Saturation pressure, psia	1,920	1,870	1,792
Saturation pressure, psia	2,160	2,079	1,947
Saturation pressure, psia	2,420	2,344	2,118
Saturation pressure, psia	2,570*	2,589	2,215
Saturation pressure, psia	3,000	3,000*	2,352
Saturation pressure, psia	3,740	3,724	2,534
Volume ratio	1.0	1.0	1.0
Volume ratio	1.1016	1.1123	1.2385
Volume ratio	1.2791	1.3043	1.4336
Volume ratio	1.5234	1.5562	1.6970
Volume ratio	1.6443	1.6694	1.8270
Volume % liquid	73	73	82
Volume % liquid	59	57	68
Volume % liquid	50	51	62
Volume % liquid	40	39	47
Volume % liquid	7	7	11
Volume % liquid of crude at 610 psia	40	39	—
Crude gas, mol wt	20.3	21.2	20.9
Crude gas, Z	0.776	0.781	0.758
ZCO <sub>2</sub> at 2,000 psia	0.38	0.38	—

\*Critical point

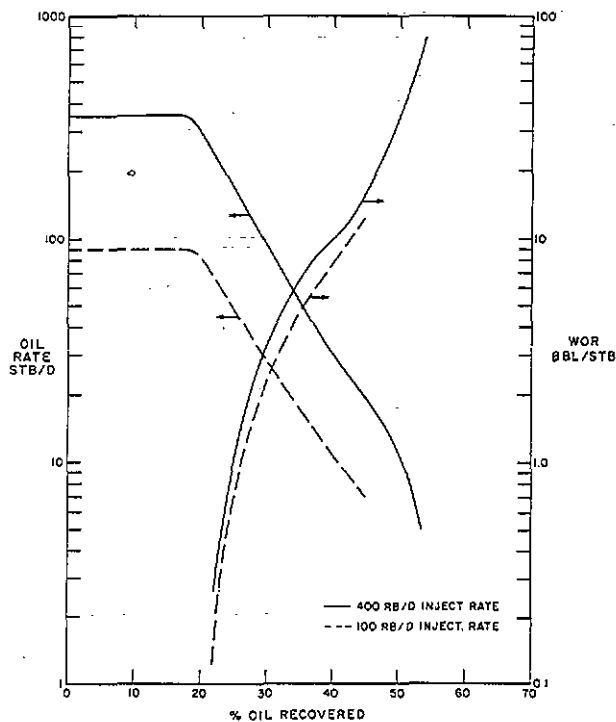


Fig. 5—Belly River B pool, cross section.<sup>67</sup>

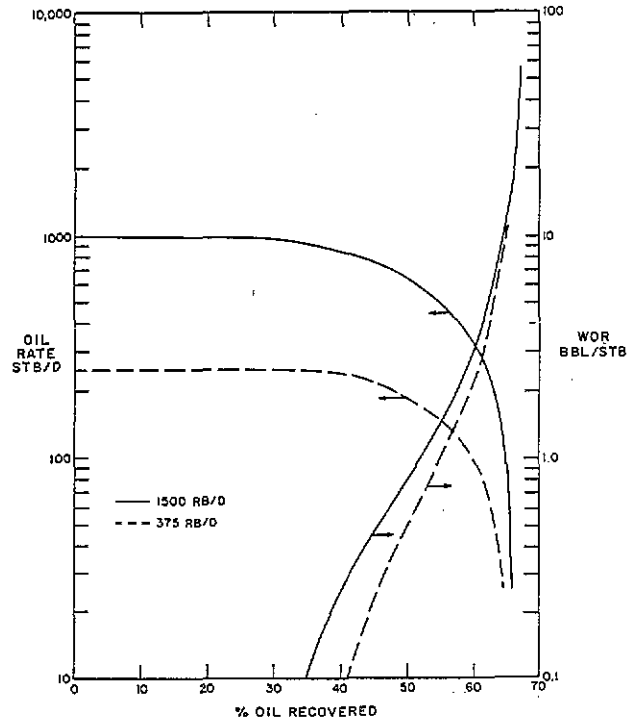


Fig. 6—Sturgeon Lake D-3 pool, Run 1.<sup>67</sup>

sensitive if an economic limit of maximum water cut is used, and are not rate-sensitive if an economic limit of a minimum oil rate is used. Thus, the existence of rate sensitivity in any particular case depends on the relative weights given those two economic limits in the definition of economic limit adopted.

Figs. 5, 6, and 7 illustrate this conclusion. Selecting a fixed oil rate as an economic limit and reading across the figure, we find ultimate oil recovery higher at a higher rate. Selecting a fixed water/oil ratio as the limit and reading across the figure, we find ultimate recovery lower at the higher rate.

Coats *et al.*<sup>68,69</sup> discuss the concept of pseudo capillary pressure curves, which should be used in place of rock or laboratory curves to initialize fluid-saturation distributions correctly. The pseudocurve definition<sup>68</sup> is fairly straightforward if the grid blocks representing the reservoir are viewed as a set of horizontal blocks at staggered depth values representing reservoir structure (dip). The definition becomes more complex as the grid blocks are viewed as inclined in both  $x$  and  $y$  directions. In practice, the pseudo capillary pressure definition is unimportant if the water/oil and gas/oil transition-zone lengths significantly exceed grid block thickness (horizontal block case) or overall elevation difference (inclined block case).

Where rock and pseudo capillary pressure curves give significantly different initial fluid-saturation distributions, the latter should be used irrespective of arguments about the existence of phase segregation or vertical equilibrium during dynamic reservoir

depletion. Strictly speaking, if pseudocurves are not used, the initialized distributions will not reflect horizontal water/oil and gas/oil contacts. In addition, if the reservoir were shut-in, the calculations would not yield (in time) equilibrium distributions corresponding to level contacts. In a sense, the pseudo capillary pressure curves give the background equilibrium condition from which dynamic viscous and gravity forces act in distorting contact shapes (overrides, underrunning).

Several authors, including Jacks *et al.*<sup>70</sup> and Kyte and Berry,<sup>49</sup> discuss the use of pseudo relative permeability curves obtained from comparing detailed cross-sectional results with results using fewer layers.

#### The Future of Simulation

Within 1 to 2 years, we will be using strongly vectorized black-oil, and perhaps compositional, models on very high-speed, large-capacity machines. The computing cost savings on small studies will be offset by a trend toward larger studies—i.e., use of more grid blocks or reservoir definition.

Research under way now will continue toward the goal of a single, general simulator capable of simulating all or most recovery processes of interest. Ref. 33 is an example of a small step in that direction. Success of this research will depend in part on improved understanding and extension of equations of state to represent the PVT behavior of multicomponent fluid systems in three or more phases over wide ranges of pressure and temperature.

Until this goal is reached, we will witness a



continued development and increasing application of a variety of types of simulation models for different processes.

### Conclusions

A reservoir simulation model is a set of partial, finite-difference material balance equations. For each grid block, one equation is written for each component or substance comprising the reservoir fluid description. The model is described here in terms of the various formulations used. Current models generally employ an IMPES formulation with options of increased stability provided by sequential and implicit formulations.

Examples of recent significant advances include (1) a nine-point difference formulation which reduces grid-orientation effects; (2) equation-of-state usage, which promises improvements in compositional simulation and may aid development of a generalized simulator; and (3) increased computer speeds, storage capacities, and vectorization capabilities, which contribute to the feasibility of larger, more detailed field studies.

Current research may lead away from the present proliferation of models of different processes toward a single, generalized model applicable to all or most recovery processes of interest.

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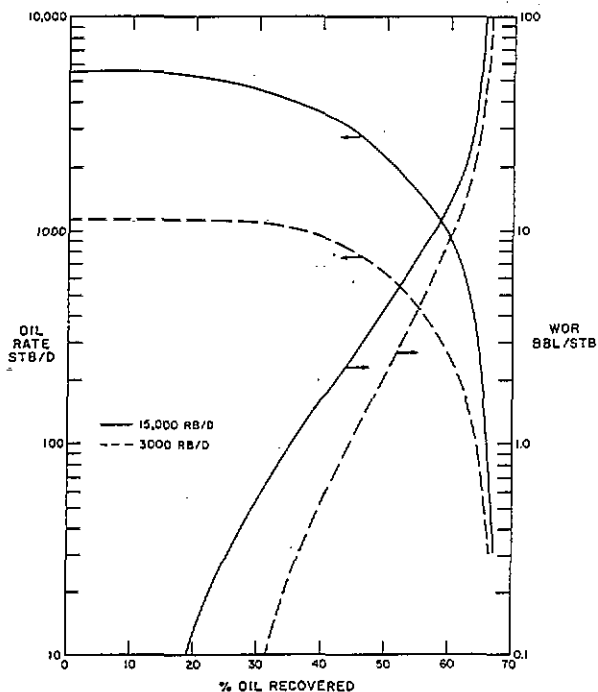


Fig. 7—Simonette D-3 pool, Run 2.<sup>67</sup>

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#### SI Metric Conversion Factors

$$\begin{array}{l} \text{bbl} \times 1.589\ 873 \quad \text{E-01} = \text{m}^3/\text{d} \\ \text{psi} \times 6.894\ 757 \quad \text{E-03} = \text{MPa} \end{array}$$

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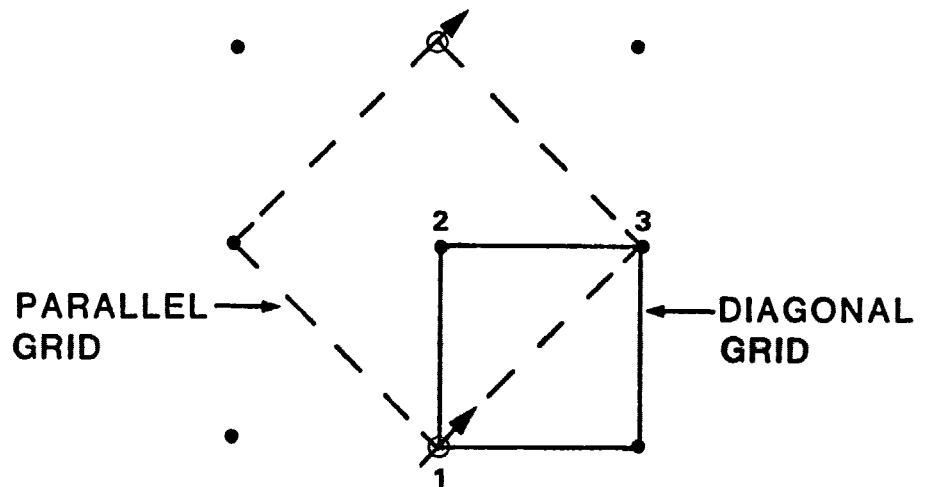
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**TABLE 1**  
**CALCULATED STEAM BREAKTHROUGH TIMES (DAYS)**  
**FOR A NINE-SPOT PATTERN**

DIFFERENCE SCHEME	WELL 2		WELL 3	
	DIAGONAL	PARALLEL	DIAGONAL	PARALLEL
5-POINT	47.8	204	1400	117
9-POINT	87.7	75.5	900	1000



○ INJECTION WELL  
 • PRODUCTION WELL

TABLE 2  
SACROC OIL-CO<sub>2</sub> PVT DATA

<u>QUANTITY</u>	<u>OBSERVED</u> <sup>68</sup>	<u>CALCULATED</u> <u>(AFTER REGRESSION)</u>	<u>PREDICTED</u>
SATURATION PRESSURE, PSIA	1660	1660	1660
SATURATION PRESSURE, PSIA	1920	1870	1792
SATURATION PRESSURE, PSIA	2160	2079	1947
SATURATION PRESSURE, PSIA	2420	2344	2118
SATURATION PRESSURE, PSIA	2570*	2589*	2215
SATURATION PRESSURE, PSIA	3000	3000	2352
SATURATION PRESSURE, PSIA	3740	3724	2534
VOLUME RATIO	1.0	1.0	1.0
VOLUME RATIO	1.1016	1.1123	1.2385
VOLUME RATIO	1.2791	1.3043	1.4336
VOLUME RATIO	1.5234	1.5562	1.6970
VOLUME RATIO	1.6443	1.6694	1.8270
VOLUME % LIQUID	73	73	82
VOLUME % LIQUID	59	57	68
VOLUME % LIQUID	50	51	62
VOLUME % LIQUID	40	39	47
VOLUME % LIQUID	7	7	11
VOLUME % LIQUID OF CRUDE AT 610 PSIA	40	39	-
CRUDE GAS M.W.	20.3	21.2	20.9
CRUDE GAS Z	.776	.781	.758
ZCO <sub>2</sub> AT 2000 PSIA	.38	.38	

\* CRITICAL POINT

TABLE 3  
ILLUSTRATIVE RELATIVE PERMEABILITY AND  
CAPILLARY PRESSURE DATA

<u>WATER-OIL TABLE</u>				<u>GAS-OIL TABLE</u>			
<u>S<sub>w</sub></u>	<u>P<sub>cwo</sub></u>	<u>k<sub>rw</sub></u>	<u>k<sub>row</sub></u>	<u>S<sub>w</sub> + S<sub>o</sub></u>	<u>P<sub>cgo</sub></u>	<u>k<sub>rog</sub></u>	<u>k<sub>rg</sub></u>
.2	P <sub>cwo1</sub>	0.	.8	.2	P <sub>cgo1</sub>	0.	.7
.22		0.		.3		0.	
.3		.03		.4		.05	
.4				.6			
.6			.05	.8			.02
.7		.45	0.	.95			0.
1.0	P <sub>cwo7</sub>	1.0	0.	1.0	P <sub>cgo7</sub>	.8	0.

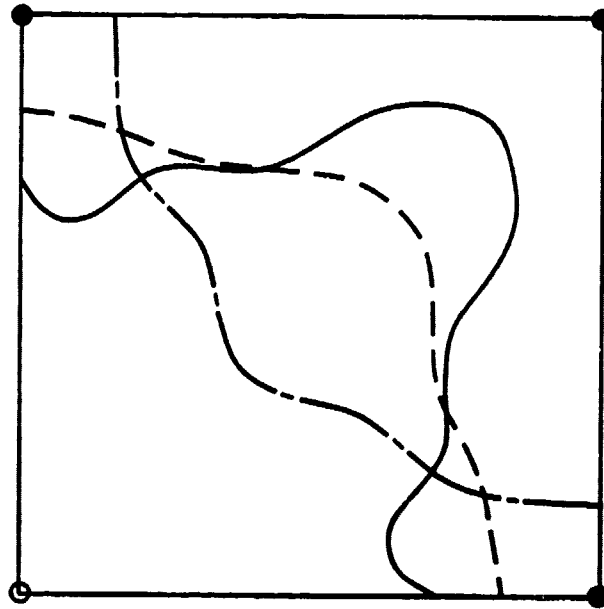
**TABLE 4**  
**INITIAL VALUES OF PHASE PRESSURES AND SATURATIONS**

CASE	$P_{cwo}$	$P_{cgo}$	MOBILE PHASES	SATURATION S			PRESSURES		
				$S_w$	$S_o$	$S_g$	$P_w$	$P_o$	$P_g$
1	$P_{cgo} < P_{cwo7}$	$P_{cgo} < P_{cgo7}$	W	1.0	0	0	Eq(1b)	$P_w + P_{cwo7}$	$P_o + P_{cgo7}$
2	$P_{cwo1} > P_{cwo} > P_{cwo7}$	$P_{cgo} < P_{cgo7}$	W, O	$S_w$	$S_o$	0	(1b)	(1a)	$P_o + P_{cgo7}$
3	$P_{cwo1} > P_{cwo} > P_{cwo7}$	$P_{cgo1} > P_{cgo} > P_{cgo7}$	W, O, G	$S_w$	$S_o$	$S_g$	(1b)	(1a)	(1c)
4	$P_{cwo} > P_{cwo1}$	$P_{cgo1} > P_{cgo} > P_{cgo7}$	O, G	$S_{wc}$	$S_o$	$S_g$	$P_o - P_{cwo1}$	(1a)	(1c)
5	$P_{cwo} > P_{cwo1}$	$P_{cgo} > P_{cgo1}$	G	$S_{wc}$	$S_{or}$	$S_g$	$P_o - P_{cwo1}$	$P_g - P_{cgo1}$	(1c)
6	$P_{cwo1} > P_{cwo} > P_{cwo7}$	$P_{cgo1} > P_{cgo} > P_{cgo7}$	W, G	$S_w$	$S_{or}$	$S_g$	(1b)	*	(1c)

\* SEE DISCUSSION



	<u>GRID</u>	<u>DIFFERENCE-SCHEME</u>
————	PARALLEL	5-POINT
-----	DIAGONAL	5-POINT
-----	EITHER	9-POINT



TIME = 80 DAYS

- INJECTOR
- PRODUCER

FIGURE 1  
CALCULATED SHAPE OF STEAMFLOOD  
FRONT IN A NINE-SPOT PATTERN

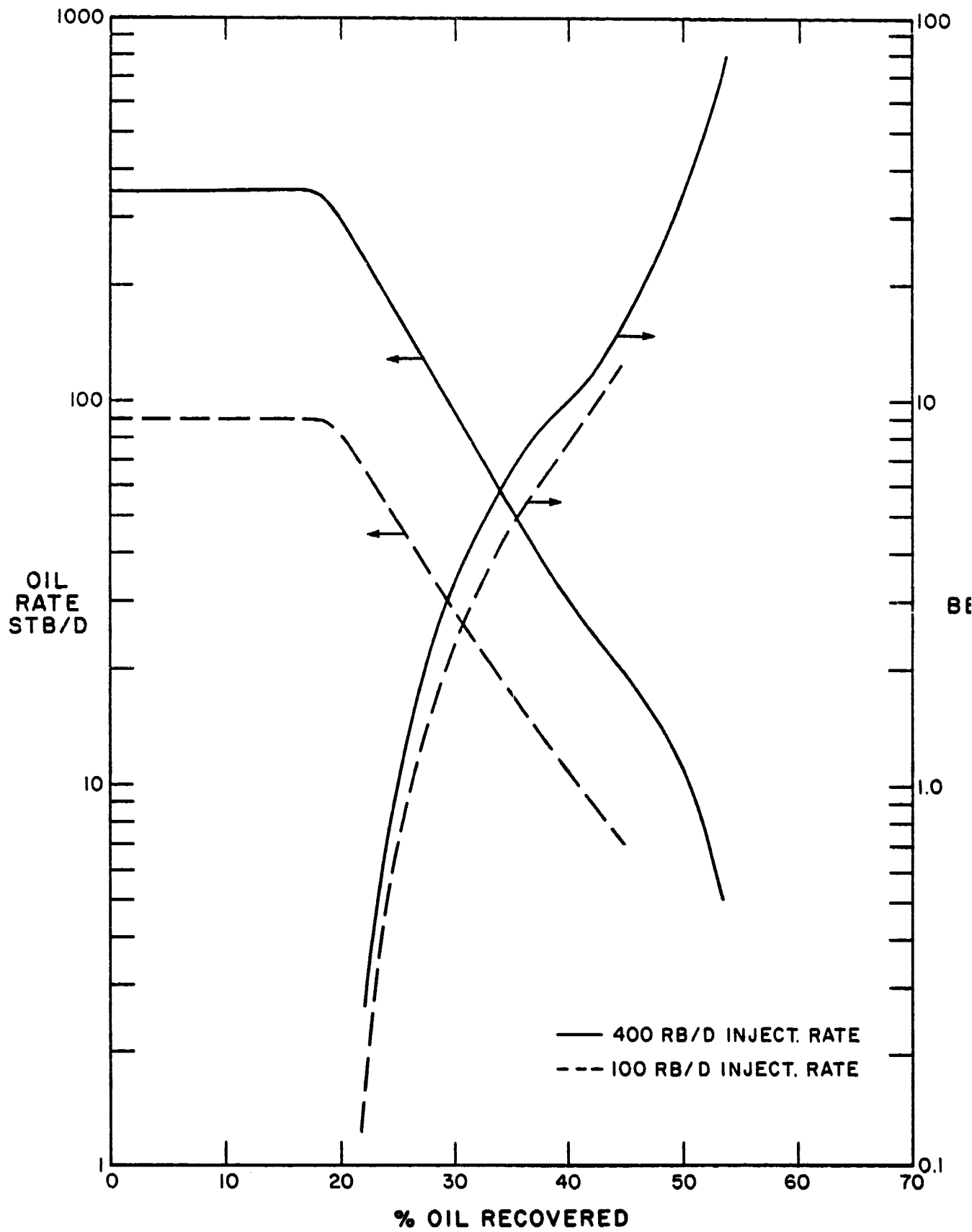


FIGURE 2  
 BELLY RIVER B POOL-CROSS SECTION  
 (Figure 39 of Reference 72)

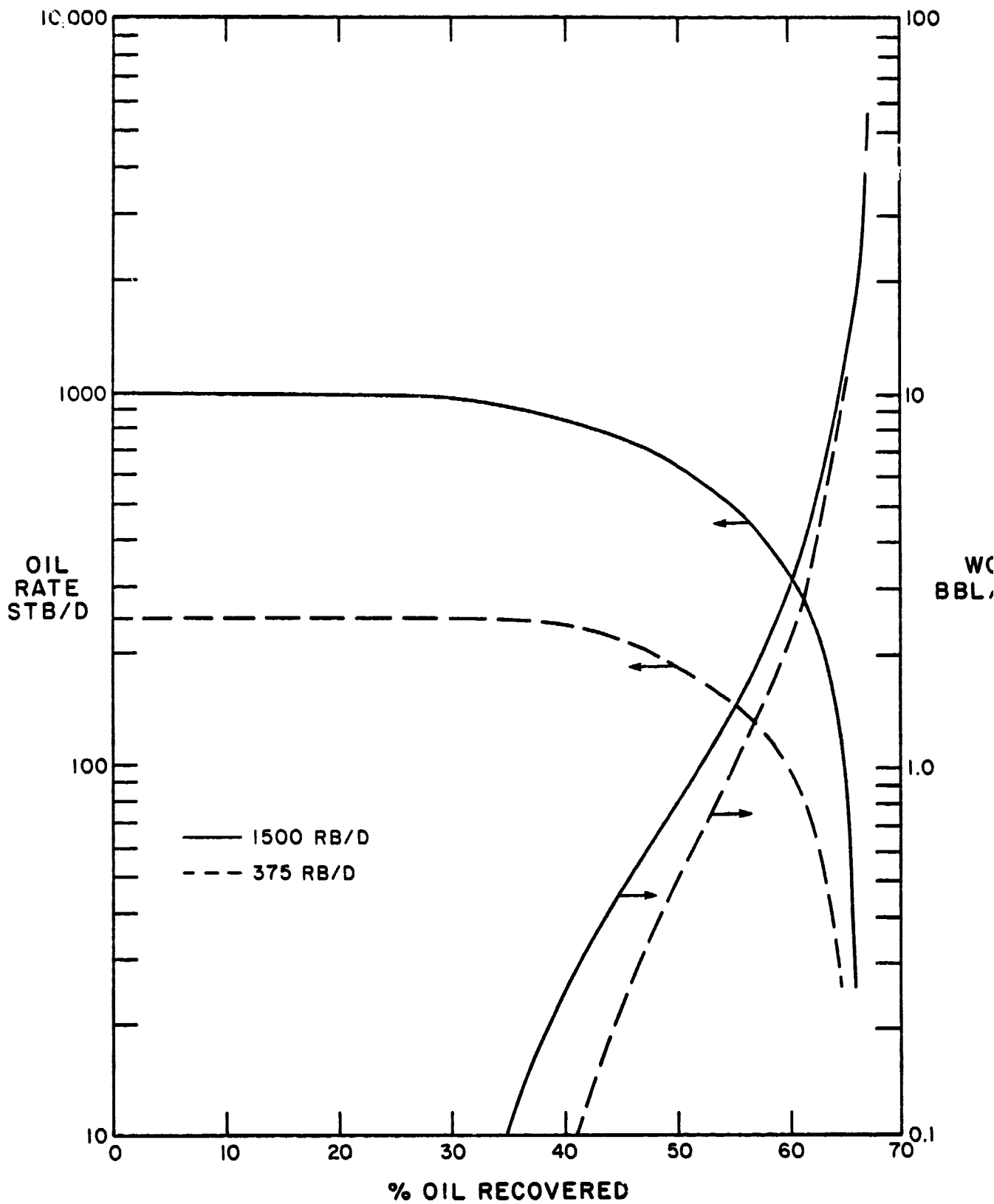


FIGURE 3  
 STURGEON LAKE D-3 POOL, RUN 1  
 (Figure 34 of Reference 72)

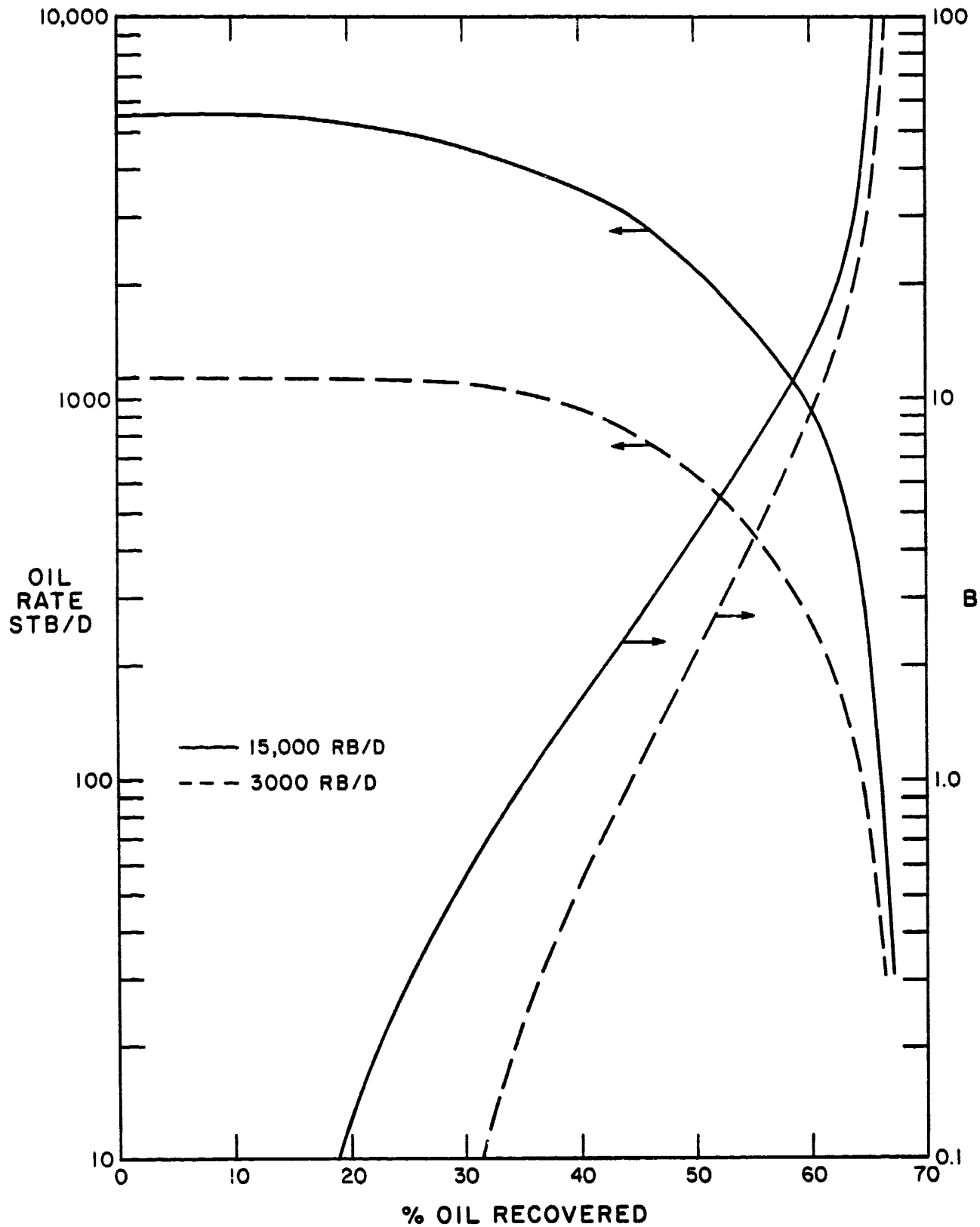


FIGURE 4  
 SIMONETTE D-3 POOL, RUN 2  
 (Figure 28 of Reference 72)