SPE

SPE 21252

A Fully Coupled, Fully Implicit Reservoir Simulator for Thermal and Other Complex Reservoir Processes

R.T. Mifflin and J.W. Watts, Exxon Production Research Co., and A. Weiser, Rice U.
SPE Members

ABSTRACT

This paper describes a formulation for fully coupled, fully implicit reservoir simulation. This formulation is implemented as an option within a framework that already supports IMPES and sequential semi-implicit formulations. The resulting capability has received extensive use for the modeling of thermal processes, and has been used successfully to model coning and naturally fractured reservoirs as well.

This formulation differs from the most commonly-used approach in two ways.

(1) Its equations are derived using the volume balance approach. This gives the resulting equations physical meaning that can be helpful in understanding the simulator's behavior. Also, it makes it possible to incorporate the resulting capability into an existing simulator that is based on the volume balance equations.

(2) In isothermal cases, it uses pressures and moles as the primary variables. When the thermal option is invoked, energy becomes the additional primary variable, rather than temperature. This avoids the complication of having to change variables when a phase disappears. Saturations and temperature are treated as functions of the primary variables.

A procedure based on the Newton-Raphson method is used to solve the resulting nonlinear equations. This procedure incorporates several techniques to enable or improve convergence in difficult circumstances.

The paper includes descriptions and discussions of the resulting simulator's performance in several examples.

References and illustrations at end of paper.

INTRODUCTION

Two common approaches for deriving the fundamental reservoir simulation equations are based respectively on the Newton-Raphson method (Coats[1] and Young and Stephenson[2]) and the volume balance principle (Acs, et al.[3] and Watts[4]). Of the two, the Newton-Raphson method seems to be the more widely used. No fully implicit procedure based on the volume balance approach has been published.

Since the early 1980's, we at Exxon have used the volume balance approach. In most applications, we enhance stability by combining the volume balance approach with the total velocity sequential implicit method of Spillette, et al.[5] The resulting procedure has been quite satisfactory in many applications: full-field simulations in which there is rapid movement of gas or in which there are high flow rates through gridblocks containing wells or near wells, most single-well coning models, cross-sectional or three-dimensional models containing thin layers, etc. However, attempts to use this method to model steam processes failed. Near wells producing steam, the process exhibits extremely high volumetric flow rates, large changes in steam volume as it moves toward the producer, and strong coupling between the energy balance and fluid flow. These phenomena create stability difficulties too severe for the sequential calculation to handle effectively.

To overcome these difficulties, we developed a fully coupled, fully implicit thermal capability based on the volume balance principle. We feel that, compared to the Newton-Raphson method, the volume balance model offers the following advantages:

(1) The equations and individual terms in them have physical meanings that help in understanding the simulator and its behavior. This is a significant advantage in debugging the computer code and in analyzing situations in which the simulator is performing poorly, for example, due to stability difficulties.

(2) Phase behavior and flow are decoupled. This makes it convenient to use a single set of flow equations with multiple sets of phase behavior relationships.

(3) Many of the needed phase behavior relationships are the same as those used in the sequential implicit calculations. As a result, our existing sequential implicit capability provided a significant start in developing the fully implicit capability.

(4) The method presented in this paper, like the Newton-Raphson method, involves a nonlinear iteration at each timestep. Important to the method's success are procedures used to aid convergence of this iteration. We found the physical meaning of the equations and solution variable set to be helpful in developing these procedures.

The simulation equations are solved in terms of gridblock pressure, amount of each component in the gridblock, and amount of energy in the gridblock. Saturations are treated as auxiliary variables. This variable set is the same, regardless of which phases are present. Thus, it is a more convenient variable set than the commonly-used set of pressure, temperature, saturations, and amounts of certain components, because this latter set changes whenever a phase appears or disappears.

The next section of this paper presents an overview of the simulation equations. The appendix contains more details and derivations of the equations. The paper's third section describes the nonlinear iteration process and the procedures used to aid its convergence. The fourth section discusses a recently published application of the simulator and compares results with the three example problems from the SPE 4th Comparative Solution Project. The final section contains the conclusions we reached during this work.

FORMULATION

Conservation Equations

Before a conservation equation for a given component can be written, a unit amount of that component must be defined. This definition could be in terms of mass, mass-moles, or standard volumes. Which of these is the logical choice depends on the application. For this reason, we want to avoid being specific about the units used. Instead, we write the equations in terms of unit amounts of component, where the unit amount is understood to be defined in whatever way is convenient for the particular application. For convenience, we call the unit amount a "mole", with the understanding that this could actually

mean a pound, a pound-mole, a stock-tank barrel, or a standard cubic foot.

Consider a one-dimensional grid. The component conservation equation for a fully implicit calculation on such a grid is

$$N_{mi}^{n+1} - N_{mi}^{n} = \Delta t \left[u_{mi-1/2}^{n+1} - u_{mi+1/2}^{n+1} + q_{mi}^{n+1} \right] \quad \ldots\ldots\ldots(1)$$

This equation states that the change in the net amount of component m in gridblock i during timestep n is equal to the net amount of component m flowing into the gridblock during the timestep. The equation itself is very simple. The difficulty lies in the fact that the transport and well rates cannot be computed until the solution at time n+1 is known. The result is a nonlinear equation that must be solved iteratively.

The primary unknowns are moles of each component in the gridblock and the gridblock pressure. Thus, there are N_c+1 unknowns, where N_c is the number of components. There are N_c material balance equations, so one more equation is needed. It is obtained by using the principle of the volume balance, which states that the fluid in a gridblock should exactly fill the gridblock. In equation form this is

$$V_{Pi}^{n+1} = V_{Fi}^{n+1} \quad \ldots\ldots\ldots(2)$$

Transport Calculation

The heart of the coupled implicit method is the calculation of fluid movement between gridblocks and between gridblocks and wells. For brevity, we address only flow between gridblocks. The calculation of flow between gridblocks and wells is very similar.

The flow rate of component m from gridblock i to gridblock i+1 is given by

$$u_{mi+1/2}^{n+1} = T_{xi+1/2} \sum_{\nu} \lambda_{\nu i+1/2}^{n+1} * \left(x_{\nu m} \xi_{\nu} \right)_{i+1/2}^{n+1} \left[\Phi_{\nu i}^{n+1} - \Phi_{\nu i+1}^{n+1} \right] \quad \ldots\ldots\ldots(3)$$

The right-hand side of this equation contains quantities that have n+1 superscripts. These are not known until the solution at the new time level is known. This solution is obtained by a Newton-Raphson iteration. To write an expression for this iteration, we need to express these quantities in terms of changes in the variables that they are functions of. The mobility is a function of saturation, among other variables, so we need an expression for saturation change. We obtain this using a similar approach to that leading to the volume balance idea. The result is

$$\delta S_{\nu i} = \frac{1}{V_{Pi}^{\ell}} \left[\left(V_{\nu i}^{\ell} - V_{Pi}^{\ell} \; S_{\nu i}^{\ell} \right) \right.$$

$$- \left(\frac{V_{\nu i}^{\ell}}{V_{Pi}^{\ell}} \; V_{Pi}^{0} \; C_f - \frac{\partial V_{\nu i}}{\partial P_i} \right) \delta P_i$$

$$\left. + \sum_m \overline{V}_{\nu m i} \; \delta N_{m i} \right] \qquad \ldots \ldots \ldots \ldots (4)$$

This equation expresses the saturation change in terms of the pressure change and changes in the amount of each component in the gridblock. It is used to eliminate the saturation change from the linearized component transport equation. This leaves an expression containing changes in pressure and amount of each component, which are the unknowns that will be solved for. This expression is substituted into Equation (1) to yield the final iteration equation. There are N_C of these equations, one for each component. We need one more equation, to account for pressure. It comes from the volume balance principle and can be written

$$\left[V_{Pi}^{0} \; C_f - \frac{\partial V_{Fi}}{\partial P_i} \right] \delta P_i - \sum_m \overline{V}_{Fmi} \; \delta N_{mi}$$

$$= \left[V_{Fi}^{\ell} - V_{Pi}^{\ell} \right] \qquad \ldots \ldots \ldots \ldots (5)$$

As discussed in the Appendix, we can use this equation to reduce by one the number of unknowns to be solved for. We wind up solving for pressure and N_C-1 moles at each gridblock.

Energy Balance Equation

Now let's add another variable, E, the energy content of the gridblock. This is the sum of the internal energy contained in each of the fluid phases plus the energy contained in the reservoir rock. The quantities that were being treated as functions of pressure and moles present in the gridblock now become functions of pressure, energy in the gridblock, and moles in the gridblock. The new fundamental quantity being computed is E, and this is also the quantity being conserved. In this sense, E is analogous to N_m.

The mass transported per mole of phase ν is $x_{\nu m}$, which is moles of component m per mole of phase ν. The energy transported per mole of phase ν is H_ν, which is enthalpy of phase ν per mole of phase ν. The reason enthalpy is used, rather than internal energy, is it accounts for the pressure-volume work done by the fluid as it enters or leaves a gridblock. In the energy transport, enthalpy is analogous to mole fraction in mass transport.

Based on the preceding two paragraphs, energy is analogous to mass as far as convective transport is concerned. However, energy is also transported by conduction. This adds terms to the energy balance that are not present in the mass balance. The resulting equation is

$$E_i^{n+1} - E_i^{n} = \Delta t \sum_\nu \left[\left(H_{\nu i} \xi_\nu \right)_{i-1/2}^{n+1} \; u_{\nu i-1/2}^{n+1} \right.$$

$$- \left(H_\nu \xi_\nu \right)_{i+1/2}^{n+1} \; u_{\nu i+1/2}^{n+1} \right]$$

$$+ \Delta t \left[T_{Hxi-1/2} \left(T_{i-1}^{n+1} - T_i^{n+1} \right) \right.$$

$$\left. - T_{Hxi+1/2} \left(T_i^{n+1} - T_{i+1}^{n+1} \right) \right] \qquad \ldots \ldots \ldots (6)$$

Temperature appears explicitly in the above equation. Also, other quantities in it, and in the mass balance equation, are functions of temperature. Since temperature is not in our set of primary unknowns, we must express it in terms of them. This is done as follows.

$$T_i^{\ell+1} = T_i^{\ell} + \frac{\partial T}{\partial P_i} \; \delta P_i + \frac{\partial T}{\partial E_i} \; \delta E_i$$

$$+ \sum_\mu \frac{\partial T}{\partial N_{\mu i}} \; \delta N_{\mu i} \qquad \ldots \ldots \ldots (7)$$

Overburden and Underburden Treatment

The overburden and underburden are important in thermal simulation because they draw off energy from the reservoir. The treatment of them differs in two ways from the calculations in the reservoir. First, there is no fluid in them. This means that there are no material balances to worry about and that there is no convective energy transport. Thus, the only equation that needs to be solved is the simple heat conduction equation. The second difference is an assumption that heat conduction parallel to the reservoir can be ignored. This assumption was first made by Coats, et al.[6] One reason it is acceptable is the fact that the temperature distributions in the overburden and underburden are not of direct interest. What is important is the amount of energy lost to them, and this is little affected by horizontal conduction. With this assumption, the overburden and underburden calculations can be done as sets of decoupled one-dimensional problems. These are easily solved using finite differences.

NON-LINEAR ITERATION PROCEDURE

Thermal reservoir processes are inherently highly non-linear. Steam zone formation and collapse, particularly at low pressures, involve enormous changes in fluid volume. The hysteresis

in relative permeability associated with the reversal from injection to production can cause some problems with the iteration process; the switch from imbibition to drainage or vice versa necessarily causes a change in the slope of the mobility function.

For unconsolidated sands such as the Clearwater formation at Cold Lake, the geomechanical behavior of the reservoir can be extremely non-linear; as induced fractures open into the reservoir, large changes in permeability occur. These are particularly difficult to model. The current simulator's ability to handle large permeability changes was critical in its adoption for use in numerous reservoir studies.

The non-linear methods which have been used to adjust the linearized Newton-Raphson iterations in order to speed up convergence are based primarily upon physical principles. The volume balance formulation allows a physical interpretation to be assigned to the various equation coefficients, so that physical concepts can be applied directly to determine non-linear iteration techniques. These techniques are scaling, saturation correction, and negative mole methods. The concept of negative moles will be described later.

During the course of a typical simulation, the most frequently used technique is scaling, which is quite straightforward. Scaling requires that no value for a specified variable change more than a user-specified amount during an iteration. The program enforces this limit by scaling back changes during an iteration so that they do not exceed the limit. By doing so, it scales back all changes proportionately. The idea behind scaling is that even when an iteration goes beyond what is physically reasonable, it is still going more-or-less in the correct direction.

One way of looking at scaling is that it causes the execution of a partial time step which prevents the iteration process from getting out of hand. An example of this is the situation that occurs when pressure in a fracture block exceeds the failure pressure. Scaling brings the pressure back to just beyond the failure pressure, and a new permeability derivative with respect to pressure is calculated for the next iteration. From this point the iteration process is able to reach the correct pressure.

Saturation correction refers to the process that occurs when the saturation predicted by the linearized Equation (4) is substantially different from the value determined by flashing the contents of a block. This situation typically occurs when steam is forming in a block. The linearized saturation change continues to predict zero vapor saturation as the heat content of the block passes into the saturated zone. The flash indicates that a large amount of vapor is present, and the saturations are recalculated based on the relative volumes of the phases. Normally, saturation scaling is also activated at this point, easing the block somewhat more gently into the three-phase state.

There are a number of situations in which the non-linearity of the iteration process temporarily causes the prediction of a negative number of moles of a particular component in a block. To allow a smoother simulation, a small negative amount of moles is tolerated. Beyond this user-specified limit, action is taken. Often the problem can be corrected by appropriate use of scaling; however, there are some pathological situations in which scaling fails even as the number of moles of the offending component in the block becomes less than zero.

One special situation occurs when a column of steam develops next to a column of relatively cold blocks. Near the bottom of the column a flow reversal can occur in which at first the flow is from the oil column to the steam zone, but after an iteration the flow direction is the opposite. Upstream weighting indicates flow of dissolved gas across the boundary between the blocks, but the final upstream direction is from the steam zone, from which all dissolved gas has been distilled. The solution to this problem is to not scale the pressure change when the moles, energy, and saturation are scaled. This tends to cause the flow reversal to occur just once, after which the iteration process proceeds smoothly.

Other special situations are normally dealt with through a procedure called molar truncation. Instead of scaling the mole changes, the offending negative moles are merely thrown away. This leaves a small negative amount of moles in the block, which corrects the problem in most cases other than the one described above.

The iteration is not allowed to be considered converged when scaling or truncation takes place. Any temporary material balance errors are corrected in the succeeding iteration.

These non-linear iteration techniques have worked well in a number of isothermal process simulations as well as in heavy and light oil thermal process simulations. Should new and different iteration difficulties arise, the physical basis of the volume balance-derived equations will provide a good starting point for any new non-linear techniques which need to be developed.

EXAMPLES

This simulator has been used for a number of thermal reservoir studies since its release to the Exxon user community in 1988. It has been used extensively for examination of the recovery processes at work at Cold Lake in Alberta. There has also been some application of the simulator to studies of fields in California and in Germany.

Boberg, Rotter, and Stark[7] describe one of the Cold Lake studies. In this work, the simulator was used to history match multiwell data from a cyclic steam stimulation process. All of the most difficult-to-model non-linearities were included in this study: hysteretic pore volume, hysteretic relative permeability, and fracture permeabilities orders of magnitude larger than that of the native rock. Models that were used contained up to 4500 gridblocks and up to eight

wells, although more typically three- and four-well models were used. The multiwell nature of the model was critical for identifying the complex interwell communication behavior which occurs at these production pads.

In order to compare the simulator with industry standards, the SPE Fourth Comparative Solution Project problems[8] were run.

The oils modeled in this comparison are very light by thermal process standards; the ambient viscosity is only 510 cp in Problems 1 and 2 and a mere 15 cp in Problem 3. The simulator described in this paper, however, has been designed primarily for much heavier oils with viscosities typically greater than 100,000 cp. Another design criterion has been the ability to handle cases in which the reservoir must be fractured in order to get steam to contact the oil. The simulator has been developed to deal with hysteresis phenomena in rock properties: pore volume, absolute permeability and relative permeability. Little effort has been made to tune the simulator for light oils in unfractured reservoirs.

The participants in the SPE Comparative Solution Project all used Stone's second model for oil relative permeability. We have preferred Stone's first model, believing it to be a better representation of actual oil-phase behavior.

Problem 1A is a radial steam stimulation model with three cycles of injection and production. The results from the Comparative Solution Project were given as oil rate, cumulative oil and water production, and heat loss.

The oil rate is shown in Figure 1. Our results fall essentially on top of those of most of the participants in the Comparative Solution Project. Cumulative oil and water produced and cumulative heat loss at the end of each of the three cycles are given in Table 1. Our oil production falls more or less on ARCO's, except for the third cycle in which we produce 200-400 fewer STB. Our water production tracks closely with ARCO, Chevron, CMG, and SSI, which are tightly grouped. Our heat loss matches quite closely the curve given by Chevron.

Computer work is shown in Table 4. We are in the middle in terms of steps, but close to CMG and Chevron in terms of iterations. Only SSI did substantially better.

Problem 2A is a rectangular three-well steam stimulation model with a dead oil as in Problem 1A. Results are given in terms of the oil and water rates from each of the two producing wells, the bottom hole pressure of one of the producers, and the cumulative total oil, oil-steam ratio, and heat loss.

The oil and water rates at each of the producing wells are shown in Figures 2-5. The rates are, in general, similar to those obtained by the participants in the comparison project. Late in our simulation, the water has a greater tendency to go to the far well than in most of the other companies' simulations.

Our near-well, bottom-hole pressure tracks most closely with ARCO's, although we do not see the sharp rise at steam breakthrough that they and most of the other participants get. Our cumulative oil was 157.8 MSTB and our final OSR was .145, putting us at the upper end of the lower groupings of participants. Cumulative heat loss was 108.8 MMMBTU, which puts us at the lower end of the simulators compared.

Steam breakthrough times are given in Table 2. Our results fall essentially in the middle of the range. Computer work is shown in Table 4. Our computer cost is again in the middle.

Problem 3A has the same geometry as Problem 2A, but this time there are two lighter, distillable components in the oil. The same features are compared as in Problem 2A.

The oil and water rates at each of the producing wells are shown in Figures 6-9. The oil rates match fairly closely those of the three participants who attempted Problem 3. Our water rate for the far well matches reasonably well with the results of SSI and Chevron, but our water rate at the near well has a broader maximum and a lower minimum than any of the other simulators. It is possible that this difference is due to our use of Stone's first model.

Our near-well, bottom-hole pressure was essentially the same as for Problem 2A, except that there was even less of a rise at steam breakthrough. Our rise was of similar magnitude to that of the participants in Problem 3. Our cumulative oil was 210.4 MSTB and our final OSR was .198, in both cases marginally below the results of the other companies. Our cumulative heat loss of 114.8 MMMBTU was approximately the same as SSI's.

Steam breakthrough times are given in Table 3. Our time for breakthrough in the near well is the same as Chevron's, which is the earliest of the three, but all three times are effectively the same. Our breakthrough in the far well is about 45 days earlier than the average of the three participants in Problem 3.

Computer work is shown in Table 4. We require about ten percent more iterations than CMG, the highest of the three participants. However, the oil in Problem 3 is the lightest, with an ambient viscosity of 15 cp. These conditions are the furthest from the conditions for which we developed our simulator. This may explain why the simulator did not perform as well in this problem as it did in the first two.

This simulator has also been used in a number of isothermal reservoir models. Early uses have included coning studies, fractured reservoir models, and basin migration studies. Some laboratory analyses have also required the fully coupled, fully implicit formulation, as have certain models with very high permeabilities (greater than 100 d).

CONCLUSIONS

The volume balance method has been primarily used in IMPES and sequential formulations of the equations of reservoir flow. The current work shows that the volume balance method can be applied as well to fully coupled, fully implicit formulations.

In particular, the volume balance fully coupled formulation works well for thermal process simulation. Results are competitive with thermal simulators in use by other companies and those available commercially. The new simulator described here has already been used for a large number of thermal reservoir studies.

The fully coupled formulation has also found use in isothermal circumstances in which the sequential formulation has difficulty, such as fractured reservoirs, high-throughput coning models, and basin migration studies.

The physical basis upon which the equations have been derived has been very useful in the development of non-linear iteration techniques. Scaling, saturation correction and negative mole treatments have been critical to the rapid convergence of the iteration procedure and thus to the success of the simulator.

NOMENCLATURE

B	=	right-hand side
C_f	=	formation compressibility
E	=	total energy contained by gridblock
H	=	specific molar enthalpy of phase, enthalpy per mole of phase
M	=	matrix
N	=	amount of component expressed as "moles"
P	=	pressure of phase; without subscript ν, oil phase pressure
P_c	=	capillary pressure of phase; $P_{c\nu} = P_\nu - P$
PL, PR, NL, NR, R, EL, ER	=	groupings of terms
q	=	rate of injection
S	=	saturation of phase
T	=	temperature
T_{Hx}, T_{Hz}	=	thermal transmissibility
T_x	=	transmissibility
u	=	rate of transport of component or phase across interface in direction of increasing gridblock number
V	=	volume of pore space, phase, or total fluid
$\bar{V}$	=	partial molar volume with respect to a component
x	=	mole fraction of component in phase
δ	=	change over an iteration
Δt	=	timestep size
λ	=	effective mobility of phase; usually will be computed as upstream value
ρ	=	density of phase
Φ	=	potential of phase
ξ	=	molar density of phase

Subscripts

a	=	aqueous phase
app	=	apparent, defined in (A-24)
b	=	over/underburden unknowns
F	=	total fluid
i	=	gridblock number in x direction
$i-1/2$	=	interface between gridblock $i-1$ and gridblock i
j	=	gridblock number in y direction
k	=	gridblock number in z (vertical) direction
$k-1/2$	=	interface between gridblock $k-1$ and gridblock k
i,j,k	=	overburden block number
$i,j,k-1/2$	=	interface between overburden blocks $i,j,k-1$ and i,j,k
m,μ	=	component number
P	=	pore space
r	=	reservoir unknowns
v	=	vapor phase
ν	=	phase number

Superscripts

ℓ	=	Newton iteration level
n	=	time level; n is the old time level; n+1 is the new time level
-1	=	inverse
0	=	at time zero

REFERENCES

(1) Coats, K. H., "An Equation of State Compositional Model", Soc. Pet. Eng. J. 20 (October 1980) 363-376; Trans., AIME 269.

(2) Young, L. D., and Stephenson, R. E., "A Generalized Compositional Approach for Reservoir Simulation," Soc. Pet. Eng. J. 23 (October 1983) 727-742.

(3) Acs, G., Doleschall, S., and Farkas, E., "General Purpose Compositional Model," Soc. Pet. Eng. J. 25 (August 1985) 543-553.

(4) Watts, J. W., "A Compositional Formulation of the Pressure and Saturation Equations," SPE Reservoir Engineering 1 (May 1986) 243-252.

(5) Spillette, A. G., Hillestad, J. G., and Stone, H. L., "A High-Stability Sequential Solution Approach to Reservoir Simulation", paper 4542 presented at the 1973 SPE Annual Meeting, Las Vegas, September 30 - October 3.

(6) Coats, K. H., George, W. D., Chu, Chieh, and Marcum, B. E., "Three-Dimensional Simulation of Steamflooding", Soc. Pet. Eng. J. 14 (December 1974) 573-592; Trans., AIME 257.

(7) Boberg, T. C., Rotter, M. B., and Stark S. D., "History Match of Multiwell Simulation Models of Cyclic Steam Stimulation Process at Cold Lake", paper SPE 20743 presented at the 1990 SPE Annual Technical Conference and Exhibition, New Orleans, September 23-26.

(8) Aziz, K. A., Ramesh, A. B., and Woo, P. T., "Fourth SPE Comparative Solution Project: Comparison of Steam Injection Simulators", JPT (December 1987) 1576-1584.

(9) Coats, K. H., "A Highly Implicit Steamflood Model," Soc. Pet. Eng. J. 18 (October 1978) 369-383.

APPENDIX -- DERIVATION OF MATHEMATICAL FORMULATION

Material Balance Equation

The component conservation equation for a fully implicit calculation on a one-dimensional grid is

$$N_{mi}^{n+1} - N_{mi}^{n} = \Delta t \left[u_{mi-1/2}^{n+1} - u_{mi+1/2}^{n+1} + q_{mi}^{n+1} \right] \quad\text{.......(A-1)}$$

Volume Balance Equation

The volume balance equation is

$$V_{Pi}^{n+1} = V_{Fi}^{n+1} \qquad\text{.......(A-2)}$$

Transport Equation

The flow rate of component m from gridblock i to gridblock i+1 is given by

$$u_{mi+1/2}^{n+1} = T_{xi+1/2} \sum_{\nu} \lambda_{\nu i+1/2}^{n+1} *$$

$$\left(x_{\nu m} \xi_{\nu} \right)_{i+1/2}^{n+1} \left[\Phi_{\nu i}^{n+1} - \Phi_{\nu i+1}^{n+1} \right] \quad\text{.......(A-3)}$$

In the following, the product of $x_{\nu m}$ and ξ_{ν} is treated as a single term. Its effective value between gridblocks is normally computed upstream.

As mentioned above, quantities appearing on the right-hand side of Equation (A-3) are not known until the solution at the new time level is known. This solution is obtained by a nonlinear iteration. The following general linear approximation is used.

$$u_{m}^{\ell+1} = u_{m}^{\ell} + T_{x} \sum_{\nu} \left\{ \left[\lambda_{\nu}^{\ell} \delta(x\xi)_{\nu m} \right. \right.$$

$$+ (x\xi)_{\nu m}^{\ell} \delta\lambda_{\nu} \left] + \lambda_{\nu}^{\ell} (x\xi)_{\nu m}^{\ell} * \right.$$

$$\left[\delta \left(P_{i} - P_{i+1} \right) + \delta \left(P_{c\nu i} - P_{c\nu i+1} \right) \right] \right\} \text{....(A-4)}$$

In the above equation and in the rest of this Section, the i+1/2 subscript is dropped. Wherever no i subscript appears, i+1/2 is implied.

Equation (A-4) contains increments of certain quantities. Eventually, these need to be expressed in terms of changes in moles of each component and pressure, since these correspond to the primary variables. However, the mobilities and capillary pressures are directly functions of saturation. For this reason, we go through an intermediate step. The result is the following relationships.

$$\delta\lambda_{\nu} = \frac{\partial\lambda_{\nu}}{\partial S_{vi}} \delta S_{vi} + \frac{\partial\lambda_{\nu}}{\partial S_{vi+1}} \delta S_{vi+1}$$

$$+ \frac{\partial\lambda_{\nu}}{\partial S_{ai}} \delta S_{ai} + \frac{\partial\lambda_{\nu}}{\partial S_{ai+1}} \delta S_{ai+1} \quad\text{.....(A-5)}$$

$$\delta(x\xi)_{\nu m} = \sum_{\mu} \left[\frac{\partial(x\xi)_{\nu m}}{\partial N_{\mu i}} \delta N_{\mu i} + \frac{\partial(x\xi)_{\nu m}}{\partial N_{\mu i+1}} \delta N_{\mu i+1} \right]$$

$$+ \frac{\partial(x\xi)_{\nu m}}{\partial P_{i}} \delta P_{i} + \frac{\partial(x\xi)_{\nu m}}{\partial P_{i+1}} \delta P_{i+1} \quad\text{....(A-6)}$$

$$\delta P_{c\nu i} = \frac{\partial P_{c\nu i}}{\partial S_{\nu i}} \delta S_{\nu i} \qquad\text{........(A-7)}$$

$$\delta P_{c\nu i+1} = \frac{\partial P_{c\nu i+1}}{\partial S_{\nu i+1}} \delta S_{\nu i+1} \qquad\text{........(A-8)}$$

Here μ denotes component number, and the derivatives are evaluated at the ℓth iteration level.

Several facts should be noted. First, some of the weaker dependencies are being ignored. These include the change in viscosity during the iteration and the change in ρ_{ν} (used in the gravitational term) during the iteration. Next, most of the partial derivative quantities in the above equations are used in the sequential semi-implicit method, and they can be computed by the same routines. The one exception is $\partial(x\xi)_{\nu m}/\partial N_{\mu i}$. The sequential method uses the diagonal term (i.e., the term corresponding to $\mu = m$) but not the off-diagonal terms. Code for computing them is needed. Finally, $\delta\lambda_{\nu}$ is expressed in terms of δS_{vi} and δS_{ai}. The actual code sums over phases

rather than referring to these specific phases. This is both more compact and more general. The form given here is chosen for its greater readability.

If Equations (A-5) through (A-8) are substituted into (A-4), an equation of the following form results.

$$u_m^{\ell+1} = u_m^{\ell} + \frac{\partial u_m}{\partial S_{vi}} \delta S_{vi} + \frac{\partial u_m}{\partial S_{vi+1}} \delta S_{vi+1}$$

$$+ \frac{\partial u_m}{\partial S_{ai}} \delta S_{ai} + \frac{\partial u_m}{\partial S_{ai+1}} \delta S_{ai+1}$$

$$+ \frac{\partial u_m}{\partial P_i} \delta P_i + \frac{\partial u_m}{\partial P_{i+1}} \delta P_{i+1}$$

$$+ \sum_{\mu} \left[\frac{\partial u_m}{\partial N_{\mu i}} \delta N_{\mu i} + \frac{\partial u_m}{\partial N_{\mu i+1}} \delta N_{\mu i+1} \right] \quad \ldots \text{(A-9)}$$

Note that the form of this equation does not depend on the linearization choices made. For example, if the dependence of λ_ν on temperature were to be included, the form would not change. The equation itself is straight-forward, but it contains increments in saturation as well as in the desired primary unknowns. These saturation increments must be eliminated.

To get an expression for saturation increment, we start with the volume of phase ν. From our experience with the sequential method, we know that its value at the new iteration level can be written in terms of the pressure and molar increments as

$$V_{\nu i}^{\ell+1} = V_{\nu i} + \frac{\partial V_{\nu i}^{\ell}}{\partial P_i} \delta P_i + \sum_m \bar{V}_{\nu m i} \delta N_{m i} \quad \ldots \text{(A-10)}$$

Here $\bar{V}_{\nu m}$ is the partial volume of phase ν with respect to component m and includes the effects of mass transfer.

We define saturation as

$$S_{\nu i}^{\ell+1} = \frac{V_{\nu i}^{\ell+1}}{V_{Pi}^{\ell+1}} \quad \ldots \text{(A-11)}$$

Then we approximate

$$S_{\nu i}^{\ell+1} = \frac{V_{\nu i}^{\ell}}{V_{Pi}^{\ell}} + \frac{\delta V_{\nu i}}{V_{Pi}^{\ell}} - \frac{V_{\nu i}^{\ell}}{\left(V_{Pi}^{\ell}\right)^2} \delta V_{Pi} \quad \ldots \text{(A-12)}$$

which can be arranged to yield

$$\delta S_{\nu i} = \left[\frac{V_{\nu i}^{\ell}}{V_{Pi}^{\ell}} - S_{\nu i}^{\ell}\right] + \frac{\delta V_{\nu i}}{V_{Pi}^{\ell}} - \frac{V_{\nu i}^{\ell}}{\left(V_{Pi}^{\ell}\right)^2} \delta V_{Pi} \quad \ldots \text{(A-13)}$$

Here the term in parentheses is the phase volume discrepancy. Substituting (A-10) into (A-13), noting that

$$\delta V_{Pi} = V_{Pi}^0 C_f \delta P_i$$

and rearranging yields

$$\delta S_{\nu i} = \frac{1}{V_{Pi}^{\ell}} \left[\left(V_{\nu i}^{\ell} - V_{Pi}^{\ell} S_{\nu i}^{\ell}\right) \right.$$

$$- \left(\frac{V_{\nu i}^{\ell}}{V_{Pi}^{\ell}} V_{Pi}^0 C_f - \frac{\partial V_{\nu i}}{\partial P_i}\right) \delta P_i$$

$$+ \left. \sum_m \bar{V}_{\nu m i} \delta N_{m i} \right] \quad \ldots \text{(A-14)}$$

The term in parentheses multiplying δP_i is the total (fluid plus associated pore volume) phase compressibility.

Equation (A-14) is then substituted into (A-9) to eliminate the four saturation increments. The result is an expression for $u_m^{\ell+1}$ in terms of the primary unknowns. This expression has the following form

$$u_m^{\ell+1} = u_m^{\ell} + (PL)_m \delta P_i + (PR)_m \delta P_{i+1}$$

$$+ \sum_{\mu} \left[(NL)_{m\mu} \delta N_{\mu i} + (NR)_{m\mu} \delta N_{\mu i+1}\right] \quad \text{(A-15)}$$

Iteration Equations

To construct N_C of the equations used in the Newtonian iteration, we start with a rearranged form of the material balance equation, (A-1).

$$N_{mi}^{\ell+1} - N_{mi}^{\ell} = N_{mi}^{n} - N_{mi}^{\ell}$$

$$+ \Delta t \left[u_{mi-1/2}^{\ell+1} - u_{mi+1/2}^{\ell+1}\right] \quad \ldots \text{(A-16)}$$

For clarity we have dropped the well terms. Substituting (A-15) into this equation yields

$$\delta N_{mi} = \left(N_{mi}^{n} - N_{mi}^{\ell}\right) + \Delta t \left[u_{mi-1/2}^{\ell}\right.$$

$$\left. - u_{mi+1/2}^{\ell}\right] + (PL)_{mi-1/2} \delta P_{i-1}$$

$$+ \left[(PR)_{mi-1/2} - (PL)_{mi+1/2} \right] \delta P_i$$

$$- (PR)_{mi+1/2} \; \delta P_{i+1} + \sum_\mu \left[(NL)_{m\mu i-1/2} \; \delta N_{\mu i-1} \right.$$

$$+ \left[(NR)_{m\mu i-1/2} - (NL)_{m\mu i+1/2} \right] \delta N_{\mu i}$$

$$\left. - (NR)_{m\mu i+1/2} \; \delta N_{\mu i+1} \right] \qquad \ldots\ldots (A\text{-}17)$$

The remaining equation comes from the volume balance principle, which is given in Equation (2) and repeated below.

$$V_{Pi}^{\ell+1} = V_{Fi}^{\ell+1} \qquad \ldots\ldots (A\text{-}18)$$

The commonly-used expression for pore volume as a function of pressure is

$$V_{Pi} = V_{Pi}^0 \left[1 + C_f \left[P_i - P_i^0 \right] \right] \qquad \ldots\ldots (A\text{-}19)$$

From this,

$$V_{Pi}^{\ell+1} = V_{Pi}^\ell + V_{Pi}^0 \; C_f \; \delta P_i \qquad \ldots\ldots (A\text{-}20)$$

From experience with the sequential method, we know that we can write

$$V_{Fi}^{\ell+1} = V_{Fi}^\ell + \frac{\partial V_{Fi}}{\partial P_i} \; \delta P_i + \sum_m \bar{V}_{Fmi} \delta N_{mi} \quad \ldots (A\text{-}21)$$

Substituting (A-20) and (A-21) into (A-18) and rearranging yields

$$\left[V_{Pi}^0 \; C_f - \frac{\partial V_{Fi}}{\partial P_i} \right] \; \delta P_i - \sum_m \bar{V}_{Fmi} \; \delta N_{mi}$$

$$= \left[V_{Fi}^\ell - V_{Pi}^\ell \right] \qquad \ldots\ldots (A\text{-}22)$$

This is the pressure equation. The term multiplied by δN_{mi} is the partial volume for the total fluid.

Reduction of Number of Equations

Note that there are N_c+1 equations in N_c+1 unknowns. Others have been able to reduce the required number of equations to N_c, or one per component. Examples where this has been done are Coats' compositional[1] and steamflood[9] models.

We can accomplish the same reduction using the pressure equation, (A-22). Note that this equation contains unknowns only at gridblock i. Thus, it is what Coats would call a constraint equation[1]. Because it contains unknowns only at gridblock i, it can be solved for one of these

unknowns and used to eliminate this unknown from other equations without introducing unknowns at other gridblocks. In particular, we solve (A-22) for $\delta N_{\mu i}$, yielding

$$\delta N_{\mu i} = \frac{1}{\bar{V}_{F\mu i}} \left\{ - \left[V_{Fi}^\ell - V_{Pi}^\ell \right] \right.$$

$$+ \left[V_{Pi}^0 \; C_f - \frac{\partial V_{Fi}}{\partial P_i} \right] \; \delta P_i$$

$$\left. - \sum_{m \neq \mu} \bar{V}_{Fmi} \; \delta N_{mi} \right\} \qquad \ldots\ldots (A\text{-}23)$$

We then use this result to eliminate $\delta N_{\mu i}$ from Equations (A-17) written for all m not equal to μ and for i-1, i, and i+1. This eliminates $\delta N_{\mu i}$ as an unknown, and we drop the μth material balance equation from the set to be solved.

Some care must be taken in deciding which component change to eliminate. Obviously, the partial volume appearing in the denominator in (A-23) must be nonzero. Based on this, it might seem reasonable to choose the component with the largest partial volume. However, there might not be any of this component present. The best tactic seems to be to select the component with the largest apparent volume, which is the partial volume times the amount of the component present. Thus, we eliminate the component with the largest V_{app}, where

$$V_{app\mu i} = \bar{V}_{F\mu i} \; N_{\mu i} \qquad \ldots\ldots (A\text{-}24)$$

Our experience has shown this to work well.

The procedure has a physical interpretation. The pressure equation expresses the relationship the increments must satisfy in order for the gridblock to be filled with fluid at the end of the iteration. An obvious way to view it is as a way to determine the pressure change needed, given a set of molar changes. However, it could be viewed as a way to determine one molar change, given the other molar changes and the pressure change. In other words, if we know the pressure change and N_c-1 molar changes, we can compute how much volume must be occupied by the remaining component. Knowing this, we can compute how much of this component must be present. However, for this calculation to be accurate, the component must occupy significant volume. This leads us to choose the component with the largest apparent volume.

Energy Balance

We add a variable called E, the energy content of the gridblock. This is the sum of the internal energy contained in each of the fluid phases plus the energy contained in the reservoir rock. The quantities that were being treated as functions of P and N_m become functions of P, E,

and N_m. The new fundamental quantity being computed is E, and this is also the quantity being conserved. In this sense, E is analogous to N_m.

The mass transported per unit volume of phase ν is $(x_{\nu m}\xi_\nu)$, which is moles of component m per volume of phase m times moles of phase ν per unit reservoir volume. The energy transported per unit volume of phase ν is $(H_\nu\xi_\nu)$, which is enthalpy per mole of phase ν times moles of phase ν per unit reservoir volume. The reason enthalpy is used, rather than internal energy, is it accounts for the pressure-volume work done by fluid as it enters or leaves a gridblock.

If conduction is ignored, the energy balance can be written

$$E_i^{n+1} - E_i^n = \Delta t \sum_\nu \left[\left(H_\nu\xi_\nu\right)_{i-1/2}^{n+1} u_{\nu i-1/2}^{n+1} \right.$$

$$\left. - \left(H_\nu\xi_\nu\right)_{i+1/2}^{n+1} u_{\nu i+1/2}^{n+1} \right] \qquad \ldots\ldots\ldots(A-25)$$

Note that the form of this equation is identical to that of (A-1), the component mass balance, with E_i taking the place of N_{mi} and H_ν taking the place of $x_{\nu m}$. Well terms have been dropped for clarity. At each Newton iteration it is now necessary to solve the matrix equation for the changes over the Newton iteration δP, δE and δN_m. There is an additional unknown, but the structure is the same. It is just as if another component has been added. The resulting iteration equation for gridblock i is

$$\delta E_i = R_i^\ell + \Delta t \left\{ (PL)_{i-1/2} \; \delta P_{i-1} \right.$$

$$+ \left[(PR)_{i-1/2} - (PL)_{i+1/2} \right] \delta P_i$$

$$\left. - (PR)_{i+1/2} \; \delta P_{i+1} \right\}$$

$$+ \Delta t \sum_\mu \left\{ (NL)_{\mu i-1/2} \; \delta N_{\mu i-1} + \left[(NR)_{\mu i-1/2} \right.\right.$$

$$\left.\left. - (NL)_{\mu i+1/2} \right] \delta N_{\mu i} - (NR)_{\mu i+1/2} \; \delta N_{\mu i+1} \right\} \quad (A-26)$$

Now let's consider the effect of adding conduction to the one-dimensional energy balance equation. The result is

$$E_i^{n+1} - E_i^n = \Delta t \sum_\nu \left[\left(H_\nu\xi_\nu\right)_{i-1/2}^{n+1} u_{\nu i-1/2}^{n+1} \right.$$

$$\left. - \left(H_\nu\xi_\nu\right)_{i+1/2}^{n+1} u_{\nu i+1/2}^{n+1} \right]$$

$$+ \Delta t \left[T_{Hxi-1/2} \left(T_{i-1}^{n+1} - T_i^{n+1} \right) \right.$$

$$\left. - T_{Hxi+1/2} \left(T_i^{n+1} - T_{i+1}^{n+1} \right) \right] \qquad \ldots\ldots(A-27)$$

Since T_i is not in our set of primary unknowns, we must express it in terms of them. This is done as follows:

$$T_i^{\ell+1} = T_i^\ell + \left[\frac{\partial T}{\partial P}\right]_i \delta P_i + \left[\frac{\partial T}{\partial E}\right]_i \delta E_i$$

$$+ \sum_\mu \left[\frac{\partial T}{\partial N_\mu}\right]_i \delta N_{\mu i} \qquad \ldots\ldots\ldots(A-28)$$

If we substitute (A-28) into (A-27), the effect is to introduce terms multiplied by the primary unknowns at gridblocks i-1, i, and i+1. These unknowns also are the ones appearing in the iteration equation, (A-26). Thus, adding the effect of conduction can be accomplished by modifying the coefficients multiplying the unknowns in (A-26). This can be done in a separate step after the coefficients of the convection-only part of the energy equation have been computed.

Over/Underburden Treatment

The energy balance for gridblock i,j,k in the over/underburden can be written

$$E_{i,j,k}^{n+1} - E_{i,j,k}^n = \Delta t \left\{ T_{Hzi,j,k-1/2} \right.$$

$$* \left(T_{i,j,k-1}^{n+1} - T_{i,j,k}^{n+1} \right) - T_{Hzi,j,k+1/2}$$

$$\left. * \left(T_{i,j,k}^{n+1} - T_{i,j,k+1}^{n+1} \right) \right\} \qquad \ldots\ldots\ldots(A-29)$$

We express T as a function of E in order to obtain an expression in the desired form.

$$\delta E_{i,j,k} = R_{i,j,k}^\ell + \Delta t \left\{ (EL)_{i,j,k-1/2} \; \delta E_{i,j,k} \right.$$

$$- \left[(ER)_{i,j,k-1/2} + (EL)_{i,j,k+1/2} \right] \delta E_{i,j,k}$$

$$\left. + (ER)_{i,j,k+1/2} \; \delta E_{i,j,k+1} \right\} \ldots\ldots\ldots(A-30)$$

Inclusion of the over/underburden changes the form of the linear set of equations that must be solved. The general form becomes

$$M_{rr}x_r + M_{rb}x_b = B_r \qquad \ldots\ldots(A-31)$$

$$M_{br}x_r + M_{bb}x_b = B_b \quad \dots\dots (A\text{-}32)$$

where　x_r　=　pressure, energy, and molar changes in the reservoir

x_b　=　energy changes in the over/underburden

M_{rr}　=　entries in reservoir gridblock equations that couple x_r to itself

M_{rb}　=　entries in reservoir gridblock equations that couple x_r to x_b

M_{br}　=　entries in over/underburden gridblock equations that couple x_b to x_r

M_{bb}　=　entries in over/underburden gridblock equations that couple x_b to itself

The reduced linear system

$$\left[M_{rr} - M_{rb}M_{bb}^{-1}M_{br} \right] x_r = B_r - M_{rb}M_{bb}^{-1}B_b \quad \dots\dots (A\text{-}33)$$

is formed. Its structure is the same as it would be if the over/underburden were not present, and it can be solved by the usual methods.

TABLE 1

END-OF-CYCLE CUMULATIVES FOR PROBLEM 1A

	Cycle 1	Cycle 2	Cycle 3
Oil Produced (STB)	7156	12610	17160
Water Produced (STB)	8110	17140	26350
Heat Loss (MMMBTU)	0.654	1.306	1.971

TABLE 2

TIME FOR 10 STB/D OF STEAM RATE FOR PROBLEM 2A

	Near Producer(days)	Far Producer(days)
EXXON	392	1528
ARCO	336	2245
CHEVRON	411*	1543*
CMG	539	1398
MOBIL	257	1583
SNEA	381	1454
SSI	487*	1497*

*Estimated from adjacent time-steps.

TABLE 3

TIME FOR 10 STB/D OF STEAM RATE FOR PROBLEM 3A

	Near Producer(days)	Far Producer(days)
EXXON	557	932
CHEVRON	556*	965*
CMG	580	998
SSI	604*	966*

*Estimated from adjacent time-steps.

TABLE 4

COMPUTER WORK

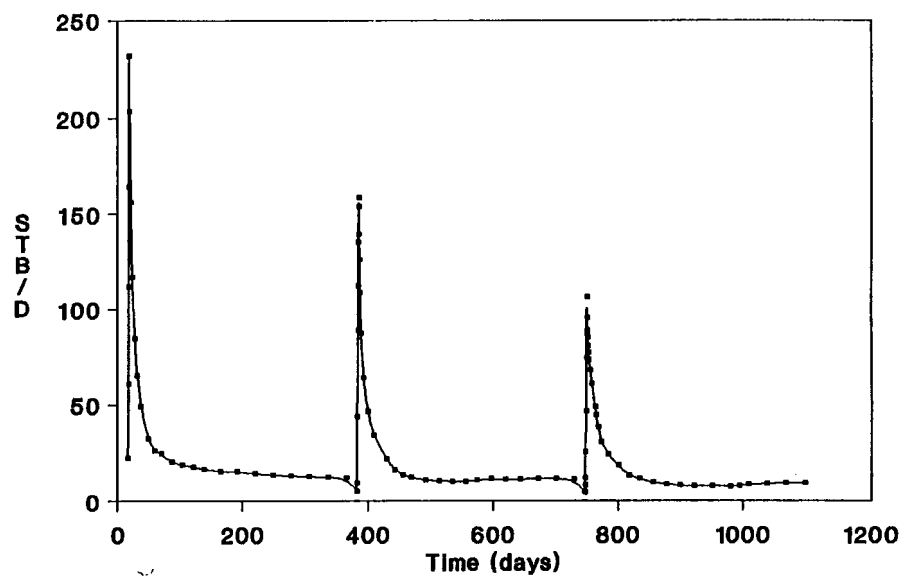|	PROBLEM 1		PROBLEM 2		PROBLEM 3	
	STEPS	ITER	STEPS	ITER	STEPS	ITER
EXXON	212	606	142	475	137	571
ARCO	414	1073	330	803	-	-
CHEVRON	132	568	60	357	54	316
CMG	124	650	89	409	98	510
MOBIL	382	1126	207	655	-	-
SNEA	297	1081	289	864	-	-
SSI	93	364	44	234	46	274

PROBLEM 1A OIL RATE

Figure 1 - Problem 1A: Oil Rate

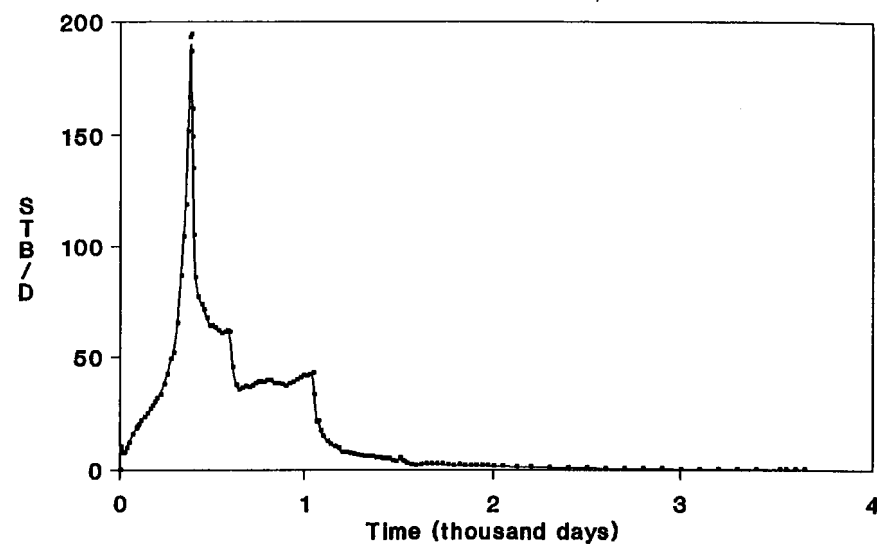## PROBLEM 2A OIL RATE NEAR WELL

Figure 2 - Problem 2A: Oil Rate for
Near Producer (full well basis)
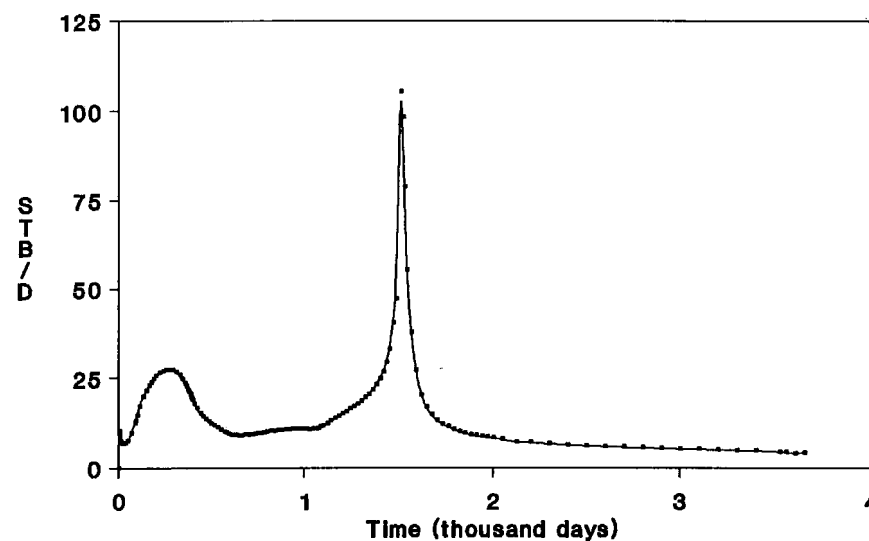
PROBLEM 2A OIL RATE FAR WELL

Figure 3 - Problem 2A: Oil Rate for
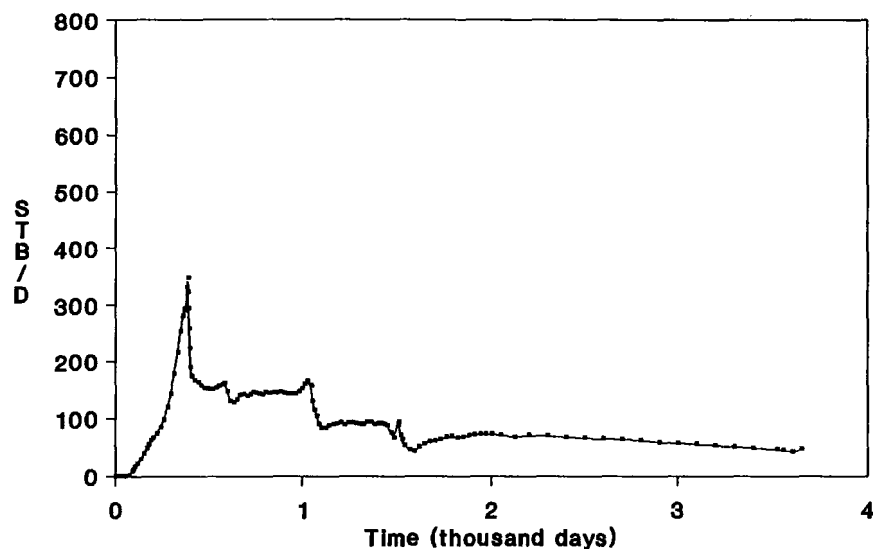Far Producer (full-well basis)

PROBLEM 2A WATER RATE NEAR WELL

Figure 4 - Problem 2A: Water Rate
For Near Producer (full-well basis)
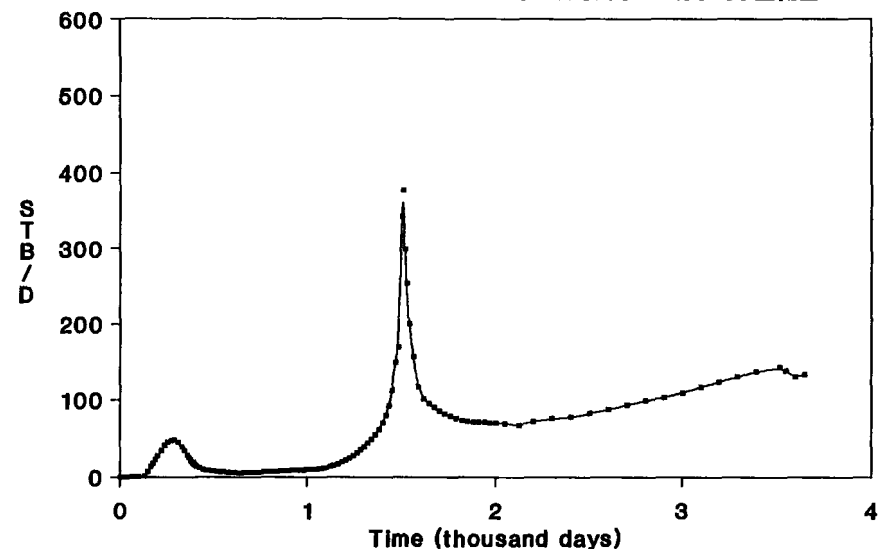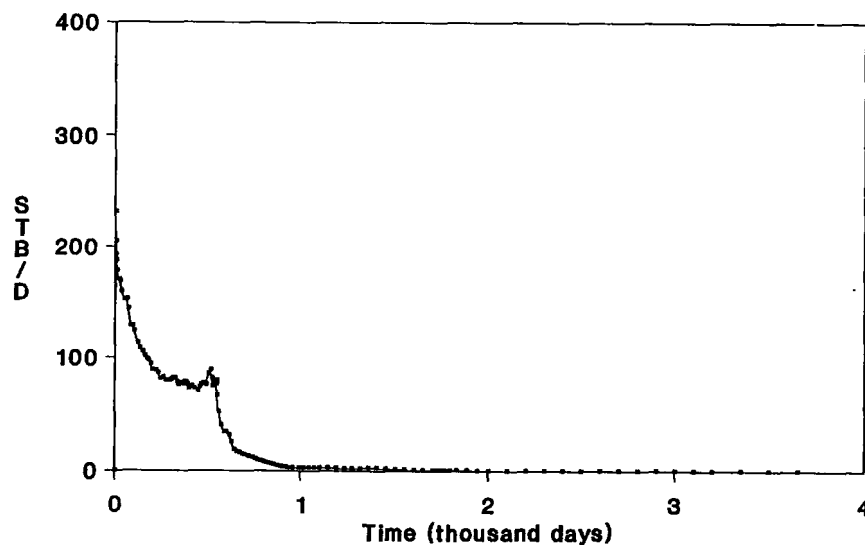
PROBLEM 2A WATER RATE FAR WELL

Figure 5 - Problem 2A: Water Rate
for Far Producer (full well basis)

PROBLEM 3A OIL RATE NEAR WELL

Figure 6 - Problem 3A: Oil Rate
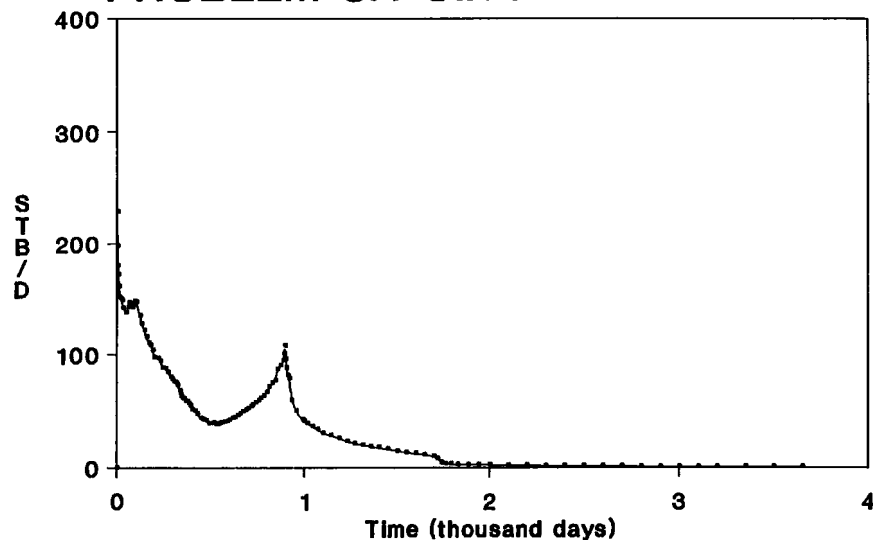for Near Producer (full well basis)

PROBLEM 3A OIL RATE FAR WELL

Figure 7 - Problem 3A: Oil Rate for
Far Producer (full well basis)
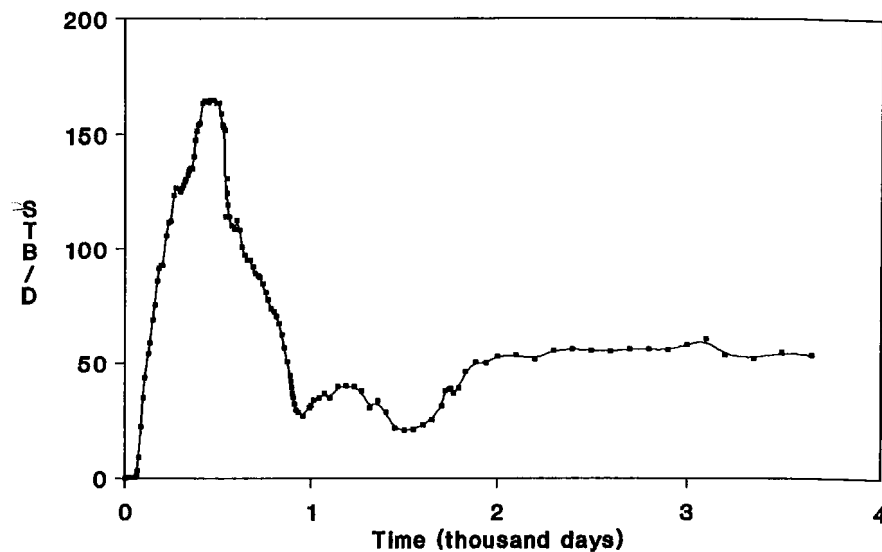
PROBLEM 3A WATER RATE NEAR WELL

Figure 8 - Problem 3A: Water Rate
for Near Producer (full well basis)
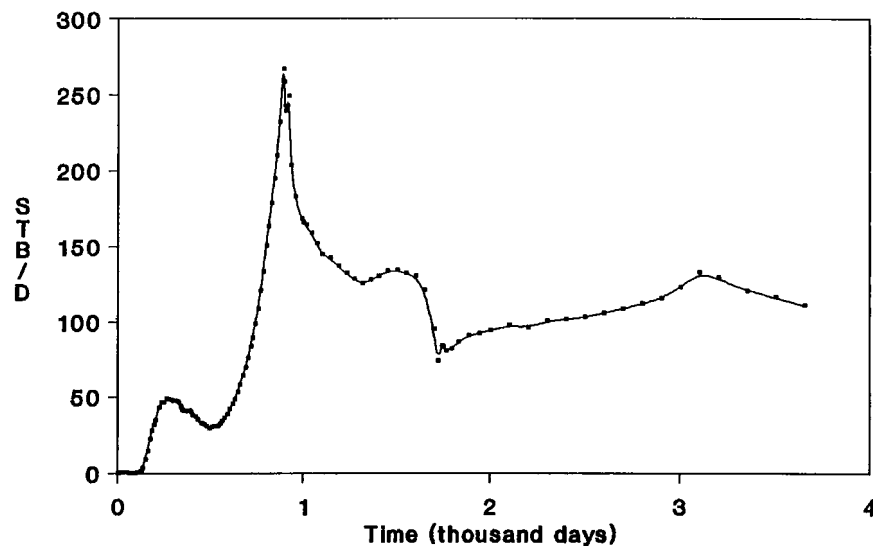
PROBLEM 3A WATER RATE FAR WELL

Figure 9 - Problem 3A: Water Rate
for Far Producer (full well basis)