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NUMERICAL SIMULATION OF COMPOSITIONAL  
PHENOMENA IN PETROLEUM RESERVOIRS

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ABSTRACT

The only fundamental difference between compositional reservoir simulators and simulators of the black-oil type lies in their treatment of fluid properties and phase behavior. Since compositional simulation is necessarily a more expensive proposition than black-oil simulation, the only justification for a compositional study is the increased accuracy that can be obtained by a more realistic description of the fluid.

This paper focuses on the consistent and accurate treatment of fluid properties in describing a three dimensional compositional simulator. It describes the methods used to calculate densities, viscosities, and

equilibrium K-values, presenting comparisons between calculated values and experimental data.

Another subject of discussion in the paper is the problem of numerical dispersion. An example simulation illustrates the magnitude of the problem and demonstrates that the method-of-characteristics provides a practical means of eliminating numerical dispersion in multicomponent miscible displacement problems.

INTRODUCTION

Most numerical simulations of petroleum reservoirs are performed with "black-oil" type simulators. The validity of these black-oil models rests on the assumption that the reservoir fluid consists of only two components, denoted oil and gas. The gas is said to be dissolved in the oil, the amount of dissolved gas decreasing with pres-

References and illustrations at end of paper.

sure below the bubble point.

One variation on this approach is to treat the reservoir fluid as a gas condensate, consisting of a gas component and vaporized oil. The amount of oil carried in the gas phase is a function of pressure below the dew point.

In contrast to the two component fluid representations described above, a compositional reservoir simulator represents the hydrocarbon phases as N-component mixtures. It computes the changing compositions of liquid and gaseous phases using the principles of mass conservation and phase equilibrium.

By virtue of its multicomponent treatment of the reservoir fluid, a compositional simulator can more accurately simulate reservoir processes that are sensitive to fluid composition. This includes the following:

- (1) Miscible flooding by enriched gas or LPG injection.
- (2) The cycling of gas-condensate reservoirs with dry gas.
- (3) The injection of gas into volatile oil reservoirs.
- (4) Natural depletion of volatile oil or gas condensate reservoirs.

In some cases a compositional model may also be required to accurately simulate immiscible gas injection in a black-oil reservoir. For example, a very lean gas may cause significant vaporization of residual oil, resulting in higher recoveries than a black-oil model would predict. On the other hand, pressure maintenance by water injection can usually be simulated with a black-oil model, even for very volatile oils.

This paper describes some of the methods that have been used in developing a three dimensional, compositional reservoir simulator. The major focus of the paper is the consistent and accurate treatment of fluid properties and phase behavior.

#### SOLUTION OF THE COMPOSITIONAL MATERIAL BALANCE EQUATIONS

By combining Darcy's law with the continuity equation one can derive differential equations that conserve the

mass of water and of each constituent in the oil and gas phases:

$$V \cdot \left[ \frac{k_{rw}}{B_w \mu_w} \left( \nabla p_w - \frac{\rho_w g}{144 g_c} \nabla h \right) \right] - q_{wv} = \frac{\partial}{\partial t} \left( \frac{\phi S_w}{B_w} \right) \dots \dots \dots (1)$$

$$V \cdot \left[ \frac{k_{ro}}{\mu_o} C_o x_i \left( \nabla p_o - \frac{\rho_o g}{144 g_c} \nabla h \right) + \frac{k_{rg}}{\mu_g} C_g y_i \left( \nabla p_g - \frac{\rho_g g}{144 g_c} \nabla h \right) \right] - (x_i q_{ov} + y_i q_{gv}) = \frac{\partial}{\partial t} [\phi (S_o C_o x_i + S_g C_g y_i)], i=1, N. (2)$$

Constraints which must be satisfied are

$$\sum_{i=1}^N x_i = 1 \quad \sum_{i=1}^N y_i = 1$$

$$S_w + S_o + S_g = 1. \dots \dots \dots (3)$$

The pressures of the three fluid phases are related by capillary pressure

$$p_w = p_o - p_{cwo}$$

$$p_g = p_o + p_{cgo} \dots \dots \dots (4)$$

Finally, if it is assumed that mass transfer in the reservoir is rapid relative to fluid movement, then the oil and gas are everywhere in phase equilibrium. This assumption leads to the following equation:

$$y_i = K_i x_i, i=1, N \dots \dots \dots (5)$$

Equations 1 through 5 are 2N+6 equations in the 2N+6 unknowns:  $p_w, p_o, p_g, S_w, S_o, S_g, x_1, x_2, \dots, x_N, y_1, y_2, \dots, y_N$ . The fluid properties appearing in the equations are, in the general case, nonlinear functions of the pressures and compositions:

$$\rho_o = \rho_o(p_o, x_1, x_2, \dots, x_N)$$

$$\rho_g = \rho_g(p_o, y_1, y_2, \dots, y_N)$$

$$\rho_w = \rho_w(p_o)$$

$$\mu_o = \mu_o(p_o, x_1, x_2, \dots, x_N)$$

$$\mu_g = \mu_g(p_o, y_1, y_2, \dots, y_N)$$

$$\mu_w = \text{constant}$$

$$K_i = K_i(p_o, x_1, x_2, \dots, x_N, y_1, y_2, \dots, y_N) \dots \dots \dots (6)$$

In the compositional simulator these equations are solved by an implicit pressure, explicit saturation method. Equations (1) and (2) are differenced and then combined in a fashion that eliminates the implicit (n+1) time level saturations, yielding a single finite difference equation for each grid block. The only unknowns in these equations are oil pressures, although the coefficients are nonlinear functions of composition and pressure.

The equations then are solved in an iterative fashion as outlined below:

- (1) Perform one or more iterations on the pressure equation holding the nonlinear coefficients constant.
- (2) Using the latest pressure iterates, explicitly solve for water saturation and calculate the number of moles of each component present in each grid block.
- (3) Flash the hydrocarbon mixture to obtain the compositions and saturations of the oil and gas phases.
- (4) If convergence has not been achieved, recalculate the nonlinear pressure coefficients and return to step 1.

When convergence is achieved, densities and K-values correspond to the compositions and pressures at time level n+1. Viscosities, capillary pressures, and relative permeabilities are evaluated at time level n.

#### CONSISTENCY OF FLUID PROPERTIES

In early versions of the compositional simulator separate correlations were used to calculate oil densities,

gas densities, oil viscosities, and gas viscosities. For example, one version of the program used the Alani-Kennedy method to calculate liquid densities, generalized compressibility factors for gas densities, the Little-Kennedy method for oil viscosities, and tables of gas viscosity versus gravity and pressure.<sup>16,17</sup>

The first attempt to use the above approach on a miscible displacement problem met with disaster. Pressures and saturations began to oscillate badly as miscible conditions were approached, eventually causing the program to blowup. Analysis of the oscillatory behavior traced the source of the problem to inconsistencies between the densities of the gas and the liquid. The large saturation changes that accompany the approach to miscibility produced large changes in density, causing what amounted to small explosions in the grid blocks.

In a real fluid system the approach to miscibility is accompanied by a growing equivalence between properties of the oil and the gas. Finally, at a point infinitesimally removed from the critical, all of their physical properties are identical. Failure to simulate this behavior lead to the computational problems cited above.

A similar problem is encountered in the single-phase region above the critical point. Consider the case of an oil progressively mixed with a gas that is miscible in all proportions. The density of the oil should originally be calculated with the liquid density correlation, and the gas density should similarly be calculated with the gas correlation. The problem encountered is how to smoothly switch from the liquid correlation to the gas correlation as the series of mixtures passes around the critical point. Unless something is done, there will be a discrete discontinuity in density that will lead to computational errors.

The obvious solution to these problems, and in our view the only practical one, is to use the same correlation to calculate the densities of both phases. The same arguments apply to the viscosities of the two phases.

There is one other point of consistency that must be satisfied for realistic calculations in the vicinity of a critical point. This is the

requirement that the fluid compositions become equal as the critical is approached. This is equivalent to requiring the equilibrium K-values to approach 1.0 as pressure approaches convergence pressure.

The present version of the compositional simulator satisfies all of the above requirements; however, one point of inconsistency remains in the simulator at this time. This is the possible lack of agreement between the critical point predicted by the K-value correlations and the one that is implied by the density predictions of an equation-of-state. This has been a source of minor trouble in several cases.

The only way to eliminate this last inconsistency is to calculate K-values from the same equation-of-state used to calculate densities. This approach has not yet been adopted because of the expense of detecting single-phase mixtures and the difficulty of adjusting properties to match experimental data.

#### DENSITIES OF OIL AND GAS

The compositional simulator provides a choice of two density options. One option is simply to tabulate oil densities and gas Z-factors against pressure. This treatment ignores compositional effects, so its application is limited. The other option is to calculate both oil and gas densities from the Lee and Edmister modification of the Redlich-Kwong equation-of-state.<sup>1</sup>

This equation has the following general form:

$$P = \frac{RT}{V-b} - \frac{a}{V(V-b)} + \frac{c}{V(V-b)(V+b)} \quad (7)$$

The equation is solved for molar volume,  $V$ , by means of a Newton-Raphson iteration. The coefficients  $a$ ,  $b$ , and  $c$  are related to the reservoir temperature and to the critical temperatures, critical pressures, acentric factors, and mole fractions of the individual components.

Our experience with this form of the R-K equation has shown that "a priori" predictions of oil densities are generally unreliable, but by adjusting the critical properties and acentric factors of the heavy fractions ( $C_7+$ ,  $C_{10}-C_{12}$ ,  $C_{15}+$ , etc.) we have succeeded in accurately duplicating both

oil and gas densities over a wide range of conditions. Examples appear in a later section of this paper.

#### VISCOSITIES OF OIL AND GAS

The compositional simulator allows its user to choose between two methods of calculating viscosities. One choice is to tabulate oil and gas viscosities against pressure. The other is to calculate both oil and gas viscosities from the Lohrenz, Bray, and Clark correlation.<sup>2</sup>

The form of the correlation is

$$\mu = \mu^* + [(0.1023 + a_1 \rho_r + a_2 \rho_r^2 + a_3 \rho_r^3 + a_4 \rho_r^4) - 0.0001] / \zeta \quad (8)$$

where

$$\rho_r = \frac{\rho}{\rho_c} \quad (9)$$

$$\rho_c = \frac{1}{V_c} = \frac{1}{\sum_{i=1}^N (z_i V_{ci})} \quad (10)$$

$$\zeta = \frac{\left[ \sum_{i=1}^N (z_i T_{ci}) \right]^{1/6}}{\left[ \sum_{i=1}^N (z_i M_i) \right]^{1/2} \left[ \sum_{i=1}^N (z_i P_{ci}) \right]^{2/3}} \quad (11)$$

This correlation was developed for oils, but the authors suggested that it might also be suitable for gases. Our experience supports their contention. Once a good set of densities is found, it is usually easy to fit liquid viscosity data by adjusting the critical volumes of the heavy fractions. Gas viscosities can be readily adjusted by modifying the critical volume of methane or other abundant light components. In some cases it is also necessary to adjust the coefficients  $a_1$ - $a_4$  of equation (2) to obtain the correct variation of viscosity with pressure.

#### EQUILIBRIUM K-VALUES

The K-values used in phase equilibrium calculations are calculated from a series of empirical equations

approximating the graphs presented in the NGPSA Engineering Data Book.<sup>5</sup> These equations interpolate smoothly in temperature, pressure, and convergence pressure and satisfy the condition that all K-values equal 1.0 for pressure equal to convergence pressure. They are described in more detail in the Appendix.

In order to accurately match the laboratory - measured phase behavior of reservoir fluids, it is usually necessary to modify the K-value correlations of selected components. Normally, it is the correlations of methane and the heavy petroleum fractions that are modified, but carbon dioxide and hydrogen sulfide are also candidates if present in sufficient quantity. The K-values are modified by changing the values of empirical parameters appearing in the correlations. This is done automatically with a nonlinear regression procedure, as described in a subsequent section.

#### CONVERGENCE PRESSURE

In order to use K-value correlations of the NGPSA type it is necessary to calculate convergence pressure. Convergence pressure, as used in the compositional simulator, is defined as the critical pressure of a critical mixture. This critical mixture is related in the following way to the mixture whose convergence pressure is sought:

- (1) Its composition is a linear combination of the compositions of the liquid and equilibrium vapor in the original mixture. (Its composition lies on an equilibrium tie-line.)
- (2) Its critical temperature equals the operating temperature of the original mixture.

This concept of convergence pressure was originally advanced by Rowe and Silberberg.<sup>3</sup>

Once the critical mixture is found, its critical pressure is calculated by either of two correlations, Simon and Yarborough or Etter and Kay.<sup>7,8</sup> The Etter and Kay correlation was developed for mixtures of pure hydrocarbons, but MacDonald has shown that it can be extended to mixtures containing heptanes-plus fractions.<sup>4</sup>

#### ADJUSTMENT OF FLUID PROPERTIES

Reservoir oils and gases are such complex mixtures that no known correlations can be expected to accurately predict their fluid properties and phase behavior "a priori." The available correlations are particularly unreliable near the critical point, where compositional reservoir simulators must be able to operate. For this reason it is necessary to adjust or "tune-up" the simulator's fluid property correlations before reservoir calculations are begun.

A companion program to the compositional simulator, called the fluid property package, simulates four standard laboratory procedures, constant composition expansions, constant volume depletions, differential liberations, and swelling tests. Comparing the simulated results of these experiments with actual laboratory data, the fluid property package adjusts user-selected empirical parameters until a least-squares fit of the data is obtained. The program can simulate several different sets of data for each laboratory procedure simultaneously, determining one set of parameters that best fits all of the available data.

The fluid property package consists of a nonlinear regression program coupled directly to subroutines that simulate the laboratory experiments. The regression program minimizes a sum-of-squares function,  $Q$ , where

$$Q = \sum_{j=1}^M R_j^2 \dots \dots \dots (12)$$

$$R_j = s_j (\psi_j^{\text{obs}} - \psi_j^{\text{calc}}) \dots \dots \dots (13)$$

The constant  $s_j$  is a scale factor used to weight individual pieces of data.  $\psi_j^{\text{obs}}$  and  $\psi_j^{\text{calc}}$  are the measured and the simulated values of physical measurement  $\psi$ .  $\psi$  may be a density, a gas compressibility factor, viscosity, saturation pressure, liquid saturation, volume factor, etc. The program can use as data most of the properties commonly measured in the laboratory experiments.

It is not possible to generalize the procedure followed in matching a given set of fluid property data since

The quantity and type of data varies from one application to another; however the following approach is used when sufficient data is available:

- (1) All of the density data for which the composition of the fluid is known is used to tune the Redlich-Kwong equation. These data may include relative volumes and compressibility factors as well as densities. The regression variables used to adjust the densities normally include the critical temperature, critical pressure, and acentric factor of the  $C_7^+$  fraction(s). (Oftentimes the  $C_7^+$  is split into two or three separate components. In this case the above properties are adjusted for each of these components.) If the fluid contains enough  $CO_2$  or  $H_2S$  to warrant treatment as a separate component, then the critical temperature, critical pressure, and acentric factor of this component are also adjusted.
- (2) All of the data, excluding viscosities, are used to adjust the K-value correlations of methane, carbon-dioxide, and the  $C_7^+$  fractions. These data ideally include saturation pressures, liquid saturation versus pressure, oil densities in the two-phase region, gas compositions, and gas withdrawal. The regression variables include  $m$ ,  $b_0$  and  $b_1$  in equation A.1,  $M$  in equation A.4, and  $b$  in equation A.5.
- (3) Once all of the density and K-value parameters are set, the viscosity data is matched by adjusting the critical volumes of the  $C_7^+$  fractions and sometimes methane or carbon dioxide. If this provides insufficient flexibility, then parameters  $a_1$ - $a_4$  of equation (8) are added as regression variables.

#### THE PROBLEM OF NUMERICAL DISPERSION

Both spatial and time truncation errors are introduced into the numerical solutions of differential equations. When equations like (1) and (2) are

solved by finite differences, these errors tend to smear, or smooth, sharp gradients of saturation or composition. Since this smearing has the same general effect that second-order spatial derivatives would have on the exact solutions to the differential equations, it is commonly called "numerical diffusion" or "numerical dispersion."

Numerous authors have addressed the problem of eliminating numerical dispersion, primarily with a view toward solving miscible displacement problems<sup>10-15</sup>. The methods proposed by Lantz, Chaudhari, and Laumbach take the approach of cancelling spatial truncation error with time truncation error. This can be very effective for one-dimensional flow, but it has limitations in multidimensional flow with irregular grids. Price et al used the Galerkin method to reduce spatial truncation error. The Galerkin method and other methods of the weighted residual and variational type offer great potential for future development, but as yet they have not been applied to multidimensional reservoir flow problems with great success. In our estimation the method of characteristics, described by Gardner et al, is the most practical approach to the numerical dispersion problem at the present time.

Simply stated, the method is to inject discrete points that carry the composition of the injected fluid and move with the local fluid velocity. By tracking these points it is possible to determine the location of fronts dividing fluids of different composition. Real dispersion, as opposed to numerical dispersion, can be included in the calculations by modifying the compositions of the moving points.

This method has been included as an option in the compositional simulator. Experience with it is limited at this point, but results have been promising. It completely eliminates numerical dispersion without serious increases in computer time. A simple illustration of the method appears in the examples that follow.

#### EXAMPLES

##### Example 1: Oil and Gas Densities

A recently studied reservoir produces large quantities of carbon dioxide. A large number of gas

compressibility factors had been measured for samples of CO<sub>2</sub>-rich gas taken from two compressor stations serving the reservoir. In addition there were data on the volume of gas relative to the volume at 3000 psia for a series of isothermal, constant composition expansions. The above data covered a temperature range of 100-300°F. and a pressure range of 400-3000 psia. The CO<sub>2</sub> content of the gas samples averaged about 0.75 mole fraction.

Modifying only the critical temperature, critical pressure, and acentric factor of carbon dioxide, the fluid property package succeeded in fitting all of this data with the Lee and Edmister version of the Redlich-Kwong equation. Fig. 1 compares compressibility factors calculated with the R-K equation with a portion of the experimental data. Fig. 2 provides a similar comparison of relative volume calculations. (The data for 150, 200, and 300°F are not shown in Fig. 2 because of their proximity to the 250° curve.)

In general the calculated compressibility factors agree with the data within 2%, the exception being the 100° data. There the errors get as large as 6%. The shapes of the Z-factor curves are very similar to the experimental data over the entire range of temperature. This is reflected in the excellent agreement of relative volumes, which depend strongly upon compressibility. (Gas compressibility is a function of  $dz/dp$ .) A closer match of the Z-factors could be obtained by weighting them more heavily in the sum-of-squares function, but the match of relative volumes would suffer as a result.

The same CO<sub>2</sub> density parameters that matched the gas data discussed above were subsequently used in calculating the densities of two oils sampled from this same reservoir. These oils contained 0.171 and 0.357 mole fraction of CO<sub>2</sub>, respectively. Fig. 3 compares calculated densities for the oils to experimental ones over pressure ranges of 3900 and 3300 psi, respectively. The lowest pressure point on each curve corresponds to the bubble point. All of the densities are within 4% of the measured values, and the compressibilities are virtually exact.

Both sets of data were matched with the same set of density parameters. The match resulted from a nonlinear

regression run in which critical temperature, critical pressure, and acentric factor were modified for each of the two heavy components. (The C<sub>7</sub><sup>+</sup> fraction was split into two components having molecular weights of 140 and 447, respectively. A better fit might have resulted from a different C<sub>7</sub><sup>+</sup> split.)

#### Example 2: Phase Behavior

The circles in Fig. 4 show the liquid saturations measured in a constant volume depletion experiment performed on a rich condensate. The solid line in the figure shows the liquid dropout calculated in a numerical simulation of the experiment. The simulation was performed with eight components including two pseudo components that together represented the C<sub>7</sub><sup>+</sup> fraction. The calculated dew point in the simulation is in error by only 10 psi, and the largest error in liquid saturation is 1.3 volume percent.

This experiment was matched by simultaneously regressing on the K-values of methane and the two heavy components. The methane K-values were modified by adjusting the values of the constants  $m$ ,  $b_0$ , and  $b_2$  in equation A.1. The heavy components were adjusted by modifying their  $b$  parameters in equation A.5. The C<sub>7</sub><sup>+</sup> density parameters had already been adjusted to fit some relative volume data measured in a constant composition expansion. Published values were used for all other density parameters.

Fig. 5 summarizes the results obtained in simulating a swelling test using fluids from the same reservoir that provided the data in Example 1. In this experiment saturation pressures were measured for six mixtures. These were prepared by combining a rather volatile oil and a gas condensate in proportions that varied from pure oil to pure gas. The circles in Fig. 5 represent the saturation pressures measured for the six mixtures. The solid line connects the saturation pressures calculated in a simulation of the experiment. The maximum error incurred was 140 psi, but five of the six calculated values lay within 60 psi of the experimental values. This is a reasonably good fit since the saturation pressures vary over a range of 990 psi.



This fit was obtained by modifying the K-values of CO<sub>2</sub> and the two heavy components.

#### Example 3: Oil and Gas Viscosities

Fig. 5 shows a comparison between calculated and experimental values of oil viscosity for the two oils used in the liquid density comparison of Example 1. A single set of viscosity parameters and critical volumes was used to match the data. The fit was obtained by modifying the critical volumes of the two heavy fractions and the parameters  $a_1$ - $a_4$  of equation (8). The maximum error is less than 1%.

Fig. 6 shows the results of an attempt to fit some viscosity data reported for the rich condensate discussed in Example 2. (See Fig. 4.) The solid lines show the viscosities calculated by the Lohrenz, Bray, and Clark correlation after modification of the critical volumes of the two heavy components and the parameters  $a_1$ - $a_4$  of equation (8). The viscosities calculated for both the oil and the gas agree reasonably well with the reported values. Excluding the 700 psia values, the maximum errors are 3% for the liquid and 10% for the gas. A single set of viscosity parameters was used for both phases.

#### Example 4: Numerical Dispersion

This example involves miscible displacement calculations in a hypothetical reservoir. The reservoir is modeled by three layers of 20 grid blocks, inclined at an angle of 30° relative to horizontal. A schematic diagram of the reservoir is shown in Fig. 8. (The horizontal and vertical axes are skewed because the diagram exaggerates the thickness of the grid blocks.) Tables 1-3 summarize some of the characteristics of the problem.

Beginning at time = 0, the reservoir is produced from all three layers at the downdip end. The production rate is held at approximately 630 res. bbl./day. For the first 360 days of production, an enriched gas, immediately miscible with the oil, is injected at the updip end of the reservoir. Beginning at 360 days, the composition of the injection gas is changed to 97% methane and 3% ethane. The gas injection rate changes with time since it is controlled by bottomhole pressure, but the average rate is about 740 mcf/day.

This problem was simulated to a time of 1440 days, using 30-day time steps and the point-tracking option of the compositional simulator. Flow was entirely convective, i.e. no dispersion was included in the calculations. Nine movable points were initially placed in each of the six grid blocks closest to the injection well.

Additional points carrying the composition of the injection gas were injected at a rate of one point for every 10000 moles of gas.

At the end of 1440 days the gas bank had moved to the location shown in Fig. 8. The contact between the rich gas and the oil was essentially horizontal with a small amount of override, and there was no evidence of the dry gas overriding the rich gas. (Notice the orientation of the horizontal axis in the figure.)

In order to assess the severity of the numerical dispersion problem in this application, the same simulation was repeated without use of the point-tracking feature.

At the end of only 570 days the dry gas had mixed sufficiently with the enriched gas to cause loss of miscibility. The displacement was immiscible from that point on. Fig. 9 compares the composition profile of the method-of-characteristics solution (point-tracking) with that of the finite difference solution at a time of 480 days. As expected, the composition profile calculated by finite differences is badly smeared.

Some critics of the method of characteristics have claimed that it consumes too much computer time to be of value in practical miscible displacement applications. It is interesting to note that there was no significant difference in the average computer time per time step for the two runs described above. (The point-tracking run was actually somewhat faster due to differences in the number of iterations required for convergence.)

#### CONCLUSIONS

- 1) Consistent fluid properties are required in order to perform accurate compositional simulations on fluids that are near their critical state.



- 2) Minimum consistency requirements are:
- Gas density must equal oil density at the critical point.
  - Gas viscosity must equal oil viscosity at the critical point.
  - K-value correlations should interpolate smoothly in pressure and convergence pressure and must yield  $K_i = 1.0$  when pressure equals convergence pressure.
- 3) The Lee and Edmister form of the Redlich-Kwong equation of state can accurately predict both oil and gas densities under reservoir conditions, provided that the critical properties and acentric factors of the components are properly adjusted.
- 4) The Lohrenz, Bray, and Clark correlation can accurately predict both oil and gas viscosities under reservoir conditions with appropriate adjustment of critical volumes and the empirical constants in the basic L-B-C equation.
- 5) The K-value correlations of MacDonald are readily adjusted to fit phase behavior data for both oils and gas condensates.
- 6) The method of characteristics provides a practical means of eliminating numerical dispersion in multicomponent simulations of miscible displacement processes.
- h • depth (measured positive down), ft.  
 k • permeability  
 $k_r$  • relative permeability  
 K • equilibrium phase constant ( $y_i/x_i$ )  
 L • moles of liquid per mole of hydrocarbon  
 M • molecular weight  
 N • total number of hydrocarbon components  
 p • pressure, psi  
 $P_c$  • capillary pressure or critical pressure, psia  
 $q_v$  • production rate per unit volume  
 R • universal gas constant  
 S • saturation  
 t • time  
 T • temperature  
 $x_i$  • mole fraction of component "i" in oil  
 $y_i$  • mole fraction of component "i" in gas  
 $z_i$  • mole fraction of component "i" in total hydrocarbon  
 $\mu$  • viscosity, cp.  
 $\rho$  • density, lb./ft.<sup>3</sup>  
 $\phi$  • porosity  
 $\omega$  • acentric factor

#### NOMENCLATURE

##### Variables:

- a • an empirical constant  
 B • formation volume factor, res.bbl./STB  
 b • an empirical constant  
 c • compressibility, psi<sup>-1</sup>, or an empirical constant  
 C • molar concentration, lb. moles/bbl.  
 g • acceleration of gravity, ft./sec.<sup>2</sup>  
 $g_c$  • gravity conversion constant, 32.17 lb.<sub>m</sub>-ft./lb.<sub>f</sub>-sec.<sup>2</sup>

##### Subscripts:

- i • component number  
 c • critical properties or capillary pressure  
 g • gas  
 o • oil

##### Superscripts:

- \* • atmospheric pressure

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Dr. K. H. Coats developed major portions of the compositional reservoir simulator. Among other things, his contributions include the primary iteration segment of the program, which numerically solves the differential material balance equations.

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## APPENDIX

## Correlations for Equilibrium K-Values

Methane, CO<sub>2</sub>, H<sub>2</sub>S, and Nitrogen:

The NGPA K-values of methane, carbon dioxide, hydrogen sulfide, and nitrogen are approximated by the following equation:

$$\ln K = (1 - \frac{p}{p_k})^m [b_0 + b_1 \ln p + b_2 (\ln p)^2] \quad \dots \dots \dots (A.1)$$

where  $m$  is constant and  $b_0$ ,  $b_1$ , and  $b_2$  are functions of temperature. For methane,  $b_1$  is -1. For CO<sub>2</sub>, H<sub>2</sub>S, and nitrogen,  $b_2$  is zero. Otherwise the coefficients are polynomials in temperature that are automatically calculated within the program. The methane correlation was developed by MacDonald, the others by Lohrenz, Clark, and Francis.<sup>5,9</sup>

## Ethane through Decane:

The K-value curves for the components ethane through decane are all similar in appearance. Typical curves are illustrated in Figure 10 for two convergence pressures at a common temperature. Each curve is divided into three regions. The first region is identical for both convergence pressures and encompasses all pressures for which the K-value exceeds one. Regions II and III, which include all K-values smaller than 1.0, are separated by the pressure at which the minimum K-value occurs. MacDonald presented correlations that fit these regions independently, subject to the constraint that the two correlations tie together with a zero derivative at the boundary.<sup>4</sup>

In Region I the form of the correlating equation is

$$\ln K = c_0 - \ln p + c_1 (\ln p)^2 \quad \dots \dots (A.2)$$

where  $c_0$  and  $c_1$  are cubic polynomials in temperature.

In Region II the correlating equation is

$$\ln K = X \left\{ S_x + \frac{X}{X_m} \left[ -2S_x + \frac{3 \ln K_m}{X_m} + \left( S_x - \frac{2 \ln K_m}{X_m} \right) \frac{X}{X_m} \right] \right\} \quad \dots \dots (A.3)$$

$$\text{where } \ln \left( \frac{p}{p_{vp}} \right) \dots \dots \dots (A.3)$$

$$X = \frac{p_k}{p_{vp}} \dots \dots \dots$$

$K_m$ , the minimum K-value at a given temperature and convergence pressure, occurs at a pressure of  $p_m$ .  $p_{vp}$  is the pressure at which the K-value equals unity.  $K_m$ ,  $p_m$ , and  $p_{vp}$  are all correlated versus temperature and convergence pressure.  $S_x$  is  $\partial \ln K / \partial X$  at the boundary of Region I.

The K-values in Region III are calculated from

$$\ln k = \ln K_m \left[ 1 - \left( \frac{X - X_m}{1 - X_m} \right)^M \right] \dots \dots \dots (A.4)$$

This equation is a generalization of the one proposed by MacDonald. This adjustable power  $M$  was always 2 in the original equation.

## Heavy Fractions:

The K-values of heavy petroleum fractions (C<sub>7</sub><sup>+</sup>, C<sub>10-15</sub>, C<sub>20</sub><sup>+</sup>, etc.) can be calculated two different ways. If the average boiling point of the fraction is lower than that of decane (345°F.), the K-values can be interpolated from the K-values of the normal paraffins having boiling points above and below that of the fraction. If the boiling point is higher than decane, then the following equation is used:

$$K_i = \frac{K_7}{(K_2/K_7)^b} \dots \dots \dots (A.5)$$

where  $K_7$  is the K-value of heptane,  $K_2$  is the K-value of ethane, and  $b$  is an empirical constant.<sup>6</sup> This approach can also be used for petroleum fractions whose average boiling points lie between heptane and decane.

TABLE 1 - RESERVOIR PROPERTIES FOR THE  
MISCIBLE SLUG EXAMPLE

Reservoir Pressure, psia (at highest point)	4029
Reservoir Temperature, °F.	259
Reservoir Dimensions, ft.	
Length	1320
Width	1320
Thickness	30
Grid Increments	
x-direction	20
z-direction	3
Dip, degrees	30°
Porosity	0.15
Permeability, md.	
x-direction	50.
z-direction	5.
Injection Well Location	
x-index	1
z-index	1-3
Production Well Location	
x-index	20
z-index	1-3
Oil Viscosity, cp. (at reservoir pressure)	0.458
Oil Density, g./cc. " " "	0.695

TABLE 2 - PHYSICAL PROPERTIES OF THE COMPONENTS  
FOR THE MISCIBLE SLUG EXAMPLE

<u>Component</u>	<u>Mol. Wt.</u>	<u>T<sub>c</sub>, °F.</u>	<u>P<sub>c</sub>, psia</u>	<u>V<sub>c</sub>, ft.<sup>3</sup>/lb.</u>	<u>ω</u>
C <sub>1</sub>	16.	-157.	606.	.063	.013
C <sub>2</sub>	30.	90.	710.	.079	.105
C <sub>3</sub>	44.	204.	617.	.073	.152
C <sub>4</sub>	58.	304.	551.	.070	.198
C <sub>5</sub> -C <sub>6</sub>	79.	424.	460.	.069	.260
A	132.	631.	523.	.066	.333
C <sub>7</sub> + B	217.	847.	354.	.066	.388
C	366.	1098.	258.	.066	.444

TABLE 3 - FLUID COMPOSITIONS FOR THE  
MISCIBLE SLUG EXAMPLE

<u>Component</u>	<u>Mole Fraction</u>		
	<u>Oil</u>	<u>Rich Gas</u>	<u>Dry Gas</u>
C <sub>1</sub>	.396	.664	.97
C <sub>2</sub>	.107	.150	.03
C <sub>3</sub>	.074	.085	0
C <sub>4</sub>	.076	.067	0
C <sub>5</sub> -C <sub>6</sub>	.126	.025	0
A	.110	.010	0
C <sub>7</sub> + B	.070	0	0
C	.041	0	0

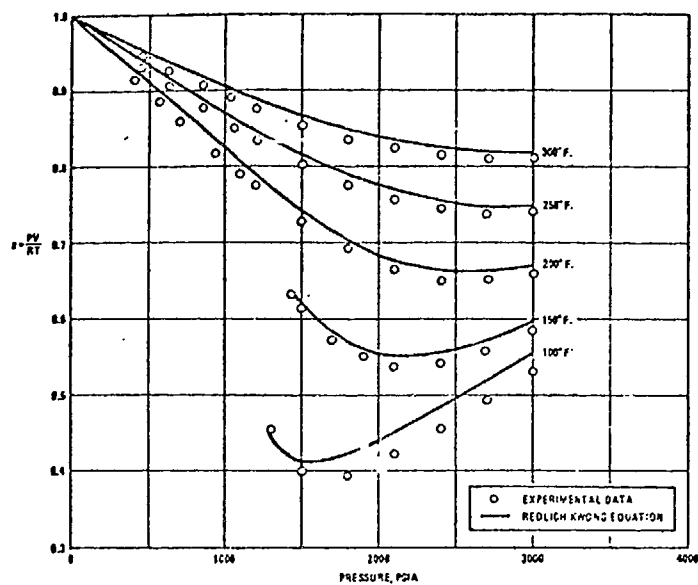


Fig. 1 - Comparison of calculated gas compressibility factors with experimental data. (Example 1)

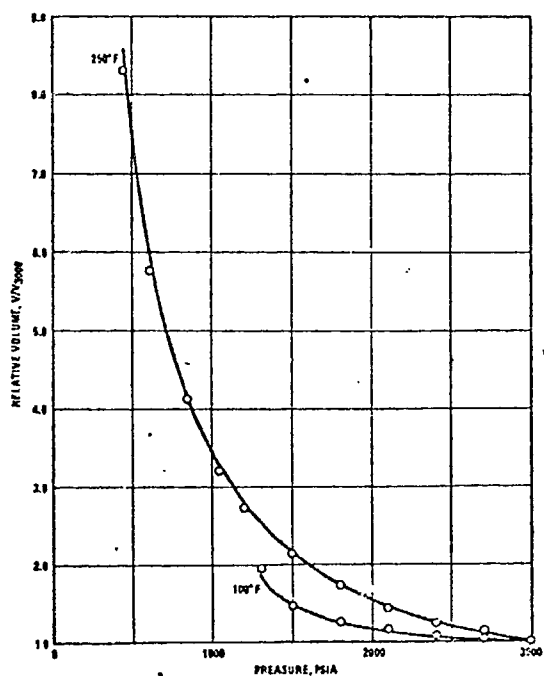


Fig. 2 - Comparison of calculated relative volumes with experimental data. (Example 1)

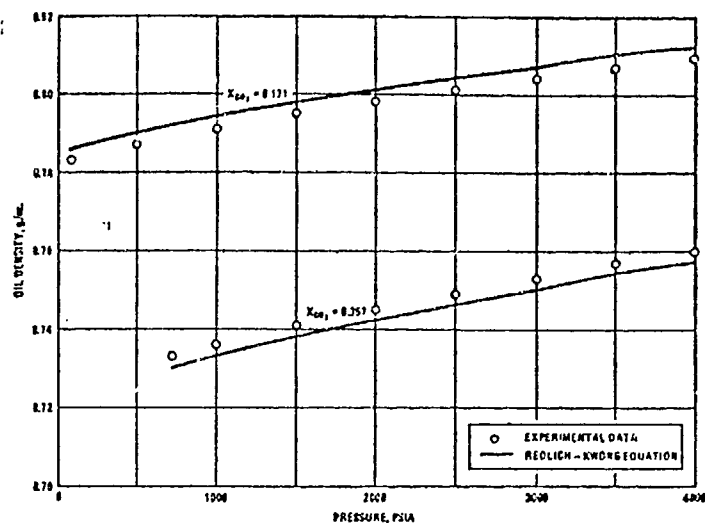


Fig. 3 - Comparison of calculated liquid densities with experimental data. (Example 1)

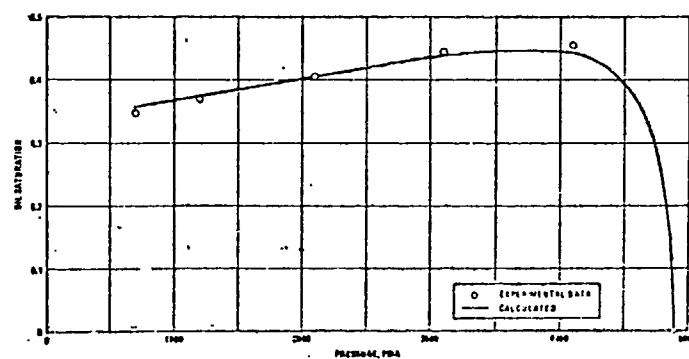


Fig. 4 - Comparison of simulated liquid dropout with experimental data for a constant volume depletion experiment. (Example 2)

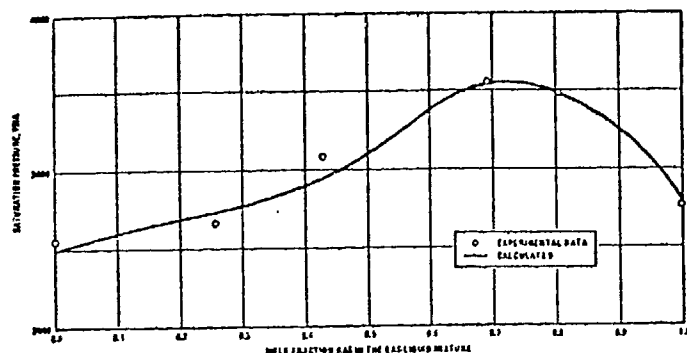


Fig. 5 - Comparison of calculated saturation pressures with experimental data from a swelling test. (Example 2)

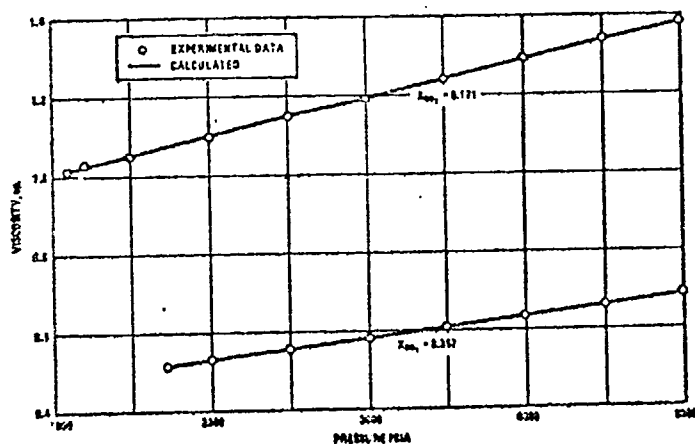


Fig. 6 - Comparison of calculated liquid viscosities with experimental data. (Example 3)

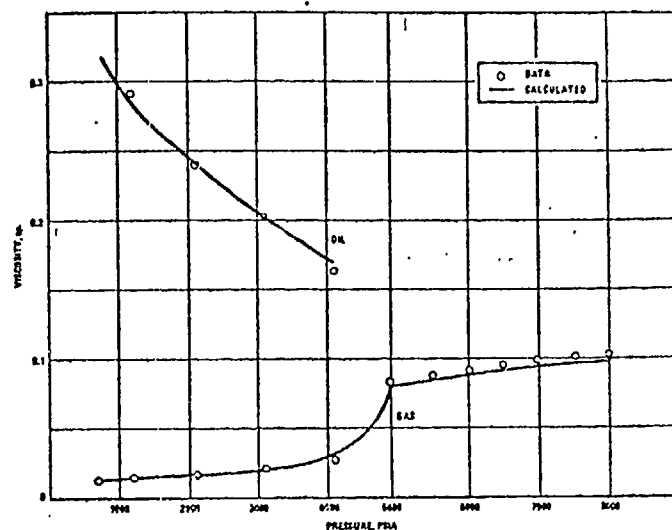


Fig. 7 - Comparison of calculated viscosities with values reported for a constant volume depletion experiment. (Example 3)

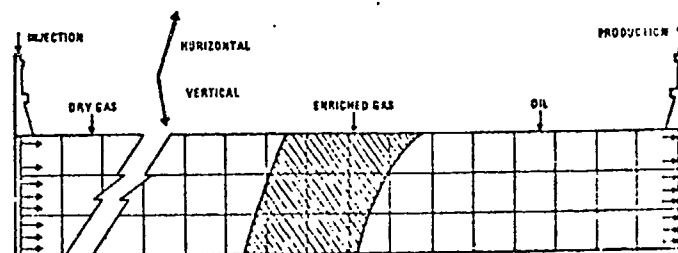


Fig. 8 - Position of the enriched gas slug after 1440 days. (Example 4)



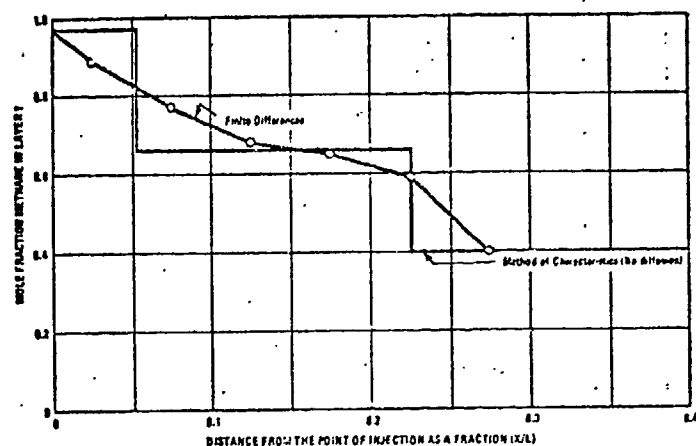


Fig. 9 - Comparison of the composition profile calculated in layer 1 by finite differences with that calculated by the method of characteristics. Time equals 480 days. (Example 4)

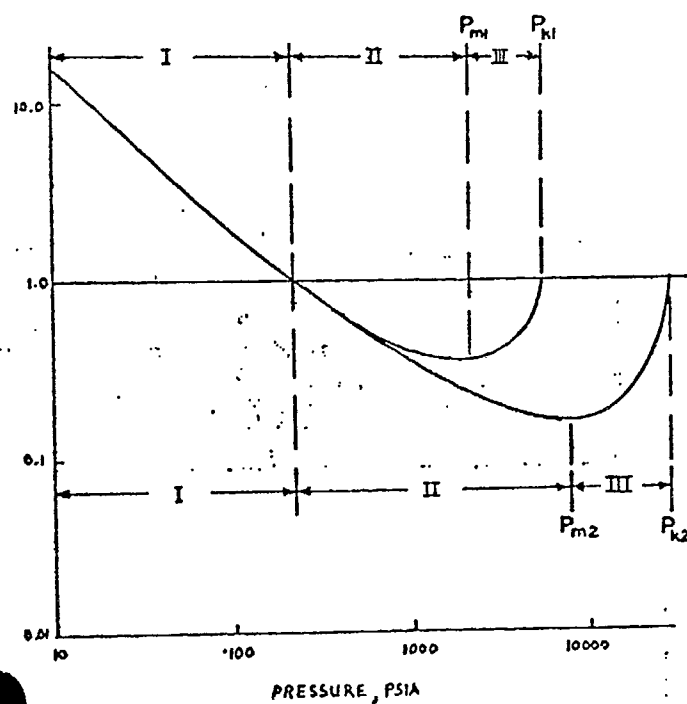


Fig. 10 - Typical K-value curves for a component at two convergence pressures.