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A new simplified compositional simulator

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Rice University, 1994

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RICE UNIVERSITY
A NEW SIMPLIFIED COMPOSITIONAL SIMULATOR

by

JAMES L BUCHWALTER

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IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE

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May, 1994

ABSTRACT

A New Simplified Compositional Simulator

by

James L. Buchwalter

A new simplified fully implicit compositional simulator has been developed. This simulator is different from existing models because it combines the conventional black oil equations with a compositional injection component equation. Sets of two dimensional pvt and injection component K value tables at constant pressure and variable mole fraction injection component are generated using a cubic equation of state used in the compositional simulator. The data are generated from a series of cells loaded with the initial composition of the reservoir. Pore volume increments of injection gas are cycled through the cells in sequence, with oil and gas volumes passing downstream in proportions calculated by the relative permeability curves. This pvt test replicates a one dimensional compositional cycling process at fixed pressure. The resulting data describes a unique compositional path through the phase diagram for constant pressure and variable mole fraction injection gas, and this path is independent of cell position in the simulator. The simulator runs at speeds that far exceed the speeds in current compositional simulators, primarily because the speed is independent of the number of components. Small problems with several hundred cells typically run about 10 times faster, and larger speed increases are realized for bigger problems. The simulator has been tested successfully for gas cycling projects including the Third SPE Comparative Solution Project and CO₂ flooding projects. Results for constant and variable pressure cycling, with and without vertical crossflow were in good agreement with a compositional model.

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Chapter 1 - INTRODUCTION

Compositional simulation is one of the most important tools for hydrocarbon recovery prediction. In the United States, the majority of the original reserve base has been produced with depletion and water drive energy, and a significant fraction of the remaining oil can be recovered with carbon dioxide flooding or lean gas cycling. Compositional simulation is the only tool in the oil industry that can provide a detailed prediction of optimal well locations and injection rates for these reservoirs.

Practical applications exist - the economics of scale make carbon dioxide flooding an attractive economic project, even at current oil prices. Texaco and other majors have large scale CO₂ projects in the western United States. In addition, lean produced gas cycling is critical to efficient oil recovery in high yield gas condensate and volatile oil reservoirs.

The fully compositional simulator with molar flow equations coupled to a cubic equation of state (EOS) package is the only popular approach for simulating compositional behavior in oil reservoirs. A minimum of 4-5 molar flow equations must be included, resulting in models that may run 100 times slower than simpler black oil models that are written in stock tank volume units and group the hydrocarbon components into only oil

and gas phases. The compositional approach is normally limited to explicit representation of the interblock relative permeabilities. Fully implicit interblock relative permeabilities require a larger matrix structure that is practical only for smaller problems even on a supercomputer. Unfortunately, many compositional problems have an unfavorable mobility ratio between injection and reservoir fluids, which leads to instability problems. The unfavorable mobility ratio accentuates grid orientation effects that must be solved with grid refinement and/or nine point flow equations. Both solutions can drastically increase CPU time to the point that a pattern study may be the only alternative for a large reservoir.

In the past 20 years a search for a simple accurate equivalent to the fully compositional simulator has been pursued. A straightforward simplified compositional formulation for the general problem has not been achieved to date, and modified black oil simulators have not accurately represented the compositional behavior in the reservoirs. A step towards this solution is the focus of the work presented here.

Chapter 2 - LITERATURE REVIEW

2.1 Structure of Black Oil Simulators - Impes and Fully Implicit

Black oil simulators are used to represent fluid flow in oil reservoirs. This is accomplished by first dividing the reservoir into a number of compartments called grid blocks. The grid blocks are usually rectangular, with a common face connecting adjacent grid blocks. Fluid flow equations are written within each grid block to represent flow to adjacent grid blocks, and the pressure change due to changes in fluid content and compressibility effects within the block. These equations are written in stock tank volume units for oil, water, and gas ¹⁻³. The development of the pressure equations requires first writing the equation of continuity that describes conservation of mass.

$$\text{Accumulation of Mass} [=] \text{Flow into block} - \text{Flow out of block}$$

The phase behavior is characterized by black oil pvt properties, specifically oil/water/gas compressibilities and viscosities, gas solubility in the oil phase, and oil solubility in the gas phase, that are dependent only on pressure.

Laminar fluid flow within a sand body can be represented by Darcy's law, which states that fluid flow volume is proportional to pressure drop ΔP and inversely proportional to the distance of flow Δx .

$$\text{Volumetric flow rate} = \text{Constant} * K_{rel} * \frac{\Delta P}{\Delta x}$$

K_{rel} [=] *Relative permeability*

The relative permeability term K_{rel} is necessary when multiple phases are flowing simultaneously, and is a function of saturation and independent of pressure. All variables are defined on page 83.

The equation of continuity is combined with Darcy's law for flow in porous media to write stock tank volume equations for the oil, water, and gas phases in each grid block. The oil, water, and gas equations are listed below. These equations assume grid block (i,j,k) communicates only with grid block (i+1,j,k) for brevity. Extension to the case of communication with all adjacent grid blocks is straightforward.

Oil Equation:

$$\begin{aligned}
 & V_{pn_{ijk}}/D_t \left((1+C_{rock}[P_{ijk}-P_{n_{ijk}}]) \frac{S_{o_{ijk}}}{B_{o_{ijk}}} - \frac{S_{on_{ijk}}}{B_{on_{ijk}}} \right) = \\
 & \frac{T_X K_{ro_{up}}}{\mu_o B_o} (P_{ijk}-P_{i+1,j,k}+\rho_o[E_{L_{ijk}}-E_{L_{i+1,j,k}}]) \\
 & -Q_o
 \end{aligned} \tag{3}$$

The first term is the accumulation term and includes the rock compressibility C_{rock} to adjust the pore volume with pressure, the formation volume factor B_o to correct the oil volume from reservoir conditions to stock tank conditions, the time increment Dt , and the pore volume V_p . The second term represents fluid flow in/out of the grid block using Darcy's law. T_X is the transmissibility term that groups all constants, K_{ro} is the oil relative permeability, E_L the elevation of the block, and μ_o the oil viscosity. The pressure drop is added to the gravity correction due to elevation. The last term is the well production term for the oil phase. Also note that the relative permeability term is weighted on the upstream or high pressure side to minimize stability problems.

The oil equation includes two sets of variables that can be organized into dependent and independent sets. The dependent variables have an n subscript and are known at the beginning of a timestep. The other variables, specifically pressure and saturations at the end of the timestep are not known and must be calculated.

Water Equation:

$$\begin{aligned}
 & V_{pn_{ijk}}/D_t \left((1+C_{rock}[P_{ijk}-P_{n_{ijk}}]) \frac{S_{w_{ijk}}}{B_{w_{ijk}}} - \frac{S_{wn_{ijk}}}{B_{wn_{ijk}}} \right) = \\
 & \frac{T_x K_{rwup}}{\mu_w B_w} (P_{ijk} - P_{i+1,jk} + [P_{cow_{ijk}} - P_{cow_{i+1,jk}}] + \rho_w [E_{L_{ijk}} - E_{L_{i+1,jk}}]) - Q_w
 \end{aligned} \tag{4}$$

The water equation includes a oil/water capillary pressure term $[P_{cow_{ijk}} - P_{cow_{i+1jk}}]$ to account for the pressure difference produced by the curvature of the oil-water interface within the reservoir rock. The capillary pressure accounts for the difference in oil and water phase pressures created by different interfacial tensions for the 2 phases with the reservoir rock.

Gas Equation:

$$\begin{aligned}
 & V_{p_{ijk}} / D_t \left((1 + C_{rock} [P_{ijk} - P_{n_{ijk}}]) \left[\frac{S_{o_{ijk}}}{B_o} R_{so} + \frac{S_{g_{ijk}}}{B_{g_{ijk}}} \right] - \left[\frac{S_{on_{ijk}}}{B_{on_{ijk}}} R_{son_{ijk}} + \frac{S_{gn_{ijk}}}{B_{gn_{ijk}}} \right] \right) = \\
 & \frac{T_x K_{ro_{wp}}}{\mu_o B_o} (P_{ijk} - P_{i+1jk} + \rho_o [E_{L_{ijk}} - E_{L_{i+1jk}}]) R_{so} \\
 & + \frac{T_x K_{rg_{wp}}}{\mu_g B_g} (P_{ijk} - P_{i+1jk} + PC_{og_{ijk}} - PC_{og_{i+1jk}} + \rho_g [E_{L_{ijk}} - E_{L_{i+1jk}}]) \\
 & - Q_o RSO - Q_g
 \end{aligned} \tag{5}$$

The gas equation includes a oil/gas capillary pressure term $[P_{cog_{ijk}} - P_{cog_{i+1jk}}]$ to account for the pressure difference between the oil and gas phases. R_{so} is the solution gas in the oil phase, and B_g is the gas formation volume factor representing the ratio of reservoir gas volume to stock tank gas volume.

For the general case each grid block communicates with 6 other blocks in a 5 point solution for a 3 dimensional rectangular system.

If shift derivatives are used the independent variables can be equivalently stated in terms of a shift for the timestep as illustrated below :

$$S_{oijk} = S_{oijk_n} + D_{S_o} \quad (6)$$

Using shift derivatives for the independent variables one can use a straightforward accounting procedure to organize the equations for each grid block into a matrix with 3 lines and 3*3 matrix sub blocks as shown below for a 1-D system with 3 grid blocks. The left hand side has partial derivatives with respect to the independent variables, and the right hand side has all constants grouped into one term.

$$\begin{bmatrix} O_{11} & 0 & O_{11} & O_{11,imp} & 0 & O_{11} & 0 & 0 & 0 & D_{so_1}+1 \\ 0 & W_{at} & W_{at} & 0 & W_{at,imp} & W_{at} & 0 & 0 & 0 & D_{sw_1}+1 \\ G_{as} & G_{as} & G_{as} & G_{as,imp} & G_{as,imp} & G_{as} & 0 & 0 & 0 & D_{p_1}+1 \\ O_{11,imp} & 0 & O_{11} & O_{11} & 0 & O_{11} & O_{11,imp} & 0 & O_{11} & D_{so_1} \\ 0 & W_{at,imp} & W_{at} & 0 & W_{at} & W_{at} & 0 & W_{at,imp} & W_{at} & D_{sw_1} \\ G_{as,imp} & G_{as,imp} & G_{as} & G_{as} & G_{as} & G_{as} & G_{as,imp} & G_{as,imp} & G_{as} & D_{p_1} \\ 0 & 0 & 0 & O_{11,imp} & 0 & O_{11} & O_{11} & 0 & O_{11} & D_{so_{1-1}} \\ 0 & 0 & 0 & 0 & W_{at,imp} & W_{at} & 0 & W_{at} & W_{at} & D_{sw_{1-1}} \\ 0 & 0 & 0 & G_{as,imp} & G_{as,imp} & G_{as} & G_{as} & G_{as} & G_{as} & D_{p_{1-1}} \end{bmatrix} = \begin{bmatrix} Rhs_{oil_{1+1}} \\ Rhs_{wat_{1+1}} \\ Rhs_{gas_{1+1}} \\ Rhs_{oil_1} \\ Rhs_{wat_1} \\ Rhs_{gas_1} \\ Rhs_{oil_{1-1}} \\ Rhs_{wat_{1-1}} \\ Rhs_{gas_{1-1}} \end{bmatrix} \quad (7)$$

Oil,Wat,Gas [=] Oil, water, gas equation derivative terms

Oil,Wat,Gas imp [=] Oil, water, gas equation fully implicit upstream
relative permeability derivatives

Dso,Dsw,Dp [=] Oil, water, and pressure changes over the timestep

Rhs [=] Constants grouped into right hand side

The terms denoted by imp denote implicit derivative terms, specifically the saturation derivatives for the inter block relative permeability terms. An example of an implicit term is given below for the oil relative permeability term :

$$K_{ro_{N+1}} [=] K_{ro_N} + \left[\frac{DK_{ro}}{D_{so}} \right]_N * D_{so_{N+1}} \quad (8)$$

The implicit relative permeabilities limit flow into the downstream grid block to the volume corresponding to the relative permeability at the end of the timestep for the upstream cell. Negative saturations in upstream cells due to unrealistic exiting flow rates based on explicit relative permeabilities at the beginning of the timestep in the upstream cell can usually be averted. This is particularly important for vertical gas movement, and water/gas coning problems with very small grid blocks.

Solving the three equations in each grid block without further reduction of the unknowns is called fully implicit, with the two saturations and pressure retained as independent variables. If the imp terms are not considered the oil/water/gas equations for each block can be collapsed into one independent equation with pressure, and two dependent saturation/pressure expressions. To accomplish this the left inverses of the 3*3 diagonal submatrices are calculated, and this matrix is multiplied by the diagonal and off diagonal matrices as well as the right hand side. The matrix above becomes as follows with mod

denoting the modified terms.

$$\begin{bmatrix}
 1 & 0 & 0 & 0 & 0 & O_{il_{mod}} & 0 & 0 & 0 & D_{so_l}+1 \\
 0 & 1 & 0 & 0 & 0 & W_{at_{mod}} & 0 & 0 & 0 & D_{sw_l}+1 \\
 0 & 0 & 1 & 0 & 0 & G_{as_{mod}} & 0 & 0 & 0 & D_{p_l}+1 \\
 \\
 0 & 0 & O_{il_{mod}} & 1 & 0 & 0 & 0 & 0 & O_{il_{mod}} & D_{so_l} \\
 0 & 0 & W_{at_{mod}} & 0 & 1 & 0 & 0 & 0 & W_{at_{mod}} & D_{sw_l} \\
 0 & 0 & G_{as_{mod}} & 0 & 0 & 1 & 0 & 0 & G_{as_{mod}} & D_{p_l} \\
 \\
 0 & 0 & 0 & 0 & 0 & O_{il_{mod}} & 1 & 0 & 0 & D_{so_{l-1}} \\
 0 & 0 & 0 & 0 & 0 & W_{at_{mod}} & 0 & 1 & 0 & D_{sw_{l-1}} \\
 0 & 0 & 0 & 0 & 0 & G_{as_{mod}} & 0 & 0 & 1 & D_{p_{l-1}}
 \end{bmatrix} = \begin{bmatrix}
 Rhs_{oil_{mod_{l+1}}} \\
 Rhs_{wat_{mod_{l+1}}} \\
 Rhs_{gas_{mod_{l+1}}} \\
 \\
 Rhs_{oil_{mod_l}} \\
 Rhs_{wat_{mod_l}} \\
 Rhs_{gas_{mod_l}} \\
 \\
 Rhs_{oil_{mod_{l-1}}} \\
 Rhs_{wat_{mod_{l-1}}} \\
 Rhs_{gas_{mod_{l-1}}}
 \end{bmatrix} \quad (9)$$

The first two equations for each grid block have saturations and pressure as variables, but the third equation for each grid block has only one variable, pressure (all off diagonal implicit terms are ignored for IMPES). These pressure equations can be organized into a new system of equations, with pressure solved independently, and the dependent saturations calculated by back substitution into the modified oil and water equations symbolically illustrated above. It is interesting to note that this elimination also rescales the system of equations for each grid block to maintain diagonal dominance. As a consequence, this step is also helpful as a first step for a fully implicit matrix.

2.2 Structure of a Compositional Simulator

Compositional simulators link component flow equations with thermodynamics described with a cubic equation of state and fugacity equalities between phases. These simulators are necessary for cycling projects where an injected phase can mix and strip the original hydrocarbon components in the reservoir. Within the individual grid cells of the model thermodynamic equilibrium is assumed at each time step. The assumption of constant stock tank oil and gas compositions used in the black oil model is no longer valid.

The construction of a compositional simulator requires careful ordering of the defining equations to minimize the independent variables to be solved in the resulting matrix. Young ⁴, Coats ⁵, Thele ⁶, and Todd ⁷ all provide excellent descriptions for the creation/solution of the matrix for this system. The set of independent equations considered are listed below :

Equation Set A $\Rightarrow$ Equality of the fugacities for each component in the gas and liquid phases. Unknowns include pressure, and component phase mole fractions. If NC is the number of components then NC equations are written per grid block.

$$Fug_{liq_i} [X_i, P] = Fug_{gas_i} [Y_i, P]$$

$$X_i \text{ can be replaced by noting } Z_i = V Y_i + (1-V) X_i \quad (10)$$

When this is done the fugacity equality is :

$$Fug_{liq_i} [Z_i, Y_i, V, P] = Fug_{gas_i} [Y_i, P]$$

V represents the fraction of the total hydrocarbon which is in the vapor phase, and X_i , Y_i , Z_i are the respective mole fractions of component i in the liquid, vapor, and total mixture. The elimination step changes the unknowns to Z_i , Y_i , V, and P in equation 10. Normally water is assumed to be immiscible with the hydrocarbon phases.

Equation Set B => Saturation constraint.

$$1 - F \left[\frac{(1-V)}{\rho_o} + \frac{V}{\rho_g} \right] - \frac{W}{\rho_w} = 0$$

where :

$$S_o = F \frac{(1-V)}{\rho_o} \quad (11)$$

$$S_w = \frac{W}{\rho_w}$$

$$S_g = F \frac{V}{\rho_g}$$

The molar densities in equation 11 are dependent on pressure and the respective liquid and gas mole fractions of the components in the system. F represents the moles hydrocarbon per unit volume, and W is the moles water per unit pore volume.

Equation Set C => Material balance flow expressions for the individual components. Individual component mole fractions and pressure are the variables. NC-1 component equations are written per grid block. Each equation consists of an accumulation term to account for mole changes over the timestep, and flow terms to account for Darcy flow and any injection or production.

$$V_{ijk} (F_{ijk}^{n+1} Z_{ijk}^{n+1}) + \sum_{s=1}^m T_s P_s^{n+1} - T_{ijk} P_{ijk}^{n+1} = RHS$$

where:

(12)

ijk [=] *grid block*
 s [=] *blocks surrounding block (i,j,k)*
 F [=] $\frac{\text{moles hydrocarbon}}{\text{unit volume}}$
 V_{ijk} [=] *Volume of block (i,j,k)*

The first two terms are the implicit part of the accumulation and darcy flow terms. The right hand side of equation 12 includes all constant explicit terms - an explicit production term is included here for simplicity in the derivation.

Equation Set D => Overall hydrocarbon mole balance. One equation per grid block.

$$V_{p_{ijk}}(F_j^{n+1}-F_j^n)+\sum_{k=1}^m T_j P_k^{n+1} - T_{ijk} P_{ijk}^n = RHS \quad (13)$$

The overall hydrocarbon balance equation could alternatively be replaced by a constraint that the summation of the Zi terms equals 1.

Equation Set E => Water mole balance. One equation per grid block.

$$V_{p_{ijk}}(W_{ijk}^{n+1}-W_{ijk}^n)+\sum_{s=1}^m T_s P_s^{n+1} - T_{ijk} P_{ijk}^n = RHS \quad (14)$$

The equations are organized 1 to 6 in the matrix below. First order shift derivatives are calculated for each independent variable, and the equations are written with a left hand side grouping the derivatives in a matrix and a right hand side grouping the constants in a residual term. The equations in the matrix are listed below.

Equation No. in matrix	Description	No. of equations	Unknowns
1	eqn. 10	NC-1	Y_i, V, Z_i, P
2	eqn. 10	1	Y_i, V, Z_i, P
3	eqn. 11	1	F, V, Z_i, P, W
4	eqn. 13	1	F, P
5	eqn. 14	1	W, P
6	eqn. 12	NC-1	F, V, Z_i, P

The saturation constraint, equation 11 makes one of the hydrocarbon component balances in equation 12 dependent. Equation 10 is listed twice, with the second listing corresponding to the equation for component NC. The equations count to $2NC+2$. The unknowns for Z_i and Y_i are counted from $i=1$ to $NC-1$. The total unknown count becomes F, V, W, P , and $2NC-2$ Y_i/Z_i values, for a total of $2NC+2$ unknowns.

The structure of the matrix is listed below for one grid block.

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 1 \\ 2 & 2 & 2 & 0 & 0 & 2 \\ 0 & 3 & 3 & 3 & 0 & 3 \\ 0 & 0 & 0 & 4 & 0 & 4 \\ 0 & 0 & 0 & 0 & 5 & 5 \\ 0 & 6 & 6 & 6 & 0 & 6 \end{bmatrix} \begin{bmatrix} \Delta Y_i \\ \Delta V_t \\ \Delta Z_i \\ \Delta F_t \\ \Delta W_t \\ \Delta P_t \end{bmatrix} \quad (15)$$

The numbers 1-6 in the matrix above correspond to the equation numbers stated in the table on the last page, and are included for the nonzero entries of the matrix.

An independent variable minimizing procedure called Newton Rhapson ⁴ is now used to simplify the matrix structure. If the first equation is used to eliminate the first term of the second equation, and then the modified second equation is used to eliminate the first term of the third equation a diagonal matrix structure results for equations 1-5. These equations can then be used to eliminate the first three terms of equation 6. The resulting matrix structure is shown below where M denotes modified terms.

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 1 \\ 0 & M & M & 0 & 0 & M \\ 0 & 0 & M & M & 0 & M \\ 0 & 0 & 0 & 4 & 0 & 4 \\ 0 & 0 & 0 & 0 & 5 & 5 \\ 0 & 0 & 0 & 0 & 0 & M \end{bmatrix} \begin{bmatrix} \Delta Y_t \\ \Delta V_t \\ \Delta Z_t \\ \Delta F_t \\ \Delta W_t \\ \Delta P_t \end{bmatrix} \quad (16)$$

The modified saturation constraint equation 16 can now be solved directly for pressure, and the $2*NC+1$ remaining variables per grid block are found directly by back substituting into the modified matrix.

Inner iterations for a fully compositional simulator (defined as successive updates of the independent variables for a timestep) are further complicated by the necessity to calculate

the bubble or dew point for all single phase cells at each inner iteration to confirm that a second phase does not form.

2.3 Pseudo Compositional Simulators

For the reasons outlined previously, considerable incentive exists for creating an accurate simplified compositional model. Large problems could be run on supercomputers, stability problems minimized, and modest problems could be solved on personal computers. The search for a simpler formulation has focused on two areas, an improved black oil approach, and a simpler compositional formulation.

Unfortunately, the search for a better compositional simulator has been discouraged by several factors. Probably most important is the complexity of the task. Every compositional simulator in industry use is selected from a small consortium of companies that have spent the last 20 twenty years developing robust code. It is difficult for these companies to allocate the resources necessary to tackle this difficult problem, especially when it is doubtful that current simulators will ever be completely replaced.

Unlike the simpler black oil simulator with 3 unknowns per reservoir grid block (2 saturations and pressure), the compositional simulator was shown above to have $2N_C + 2$ unknowns per grid block. Accurate representation of pvt behavior usually requires a minimum of 6-7 components resulting in 14-16 unknowns per grid block. The Newton

Rhapson minimizing process produces a matrix with the same structure as the normal black oil matrix, but the minimizing and back substitution procedure is very costly in terms of CPU time. As a result the compositional simulator may require as much as 100 times the CPU time of a black oil simulator for a modest problem, and large fine grid simulations may not be practical even with supercomputers. Typically, very coarse grids or pattern models are constructed to limit CPU problems. In addition, a fully implicit formulation, with interblock upstream relative permeabilities treated implicitly can minimize stability problems but prevent collapsing the original set of equations to only pressure as an independent variable. One commercial simulator today (SSI's COMP3 model) has a fully implicit compositional option, but it is practical only for small problems.

One of the earliest attempts to simplify the compositional problem was published by R.Cook et al of Gulf Oil in 1973 ⁸. This model starts with the normal black oil set of equations written for oil, water and gas in stock tank volumes. A fourth equation is added to this set representing the stock tank cumulative pore volume of injected tracer that passes through each grid cell. The variables in the four equations are saturations, pore volumes tracer, pressure, and pvt properties (viscosities, formation volume factors, gas oil ratio, and condensate yield). The pvt properties are assumed to be functions of pressure and cumulative pore volumes injected, and become dependent variables. The original variable list collapses to 3 saturations, pressure, and cumulative pore volumes injected. Recognizing that the saturations sum to one eliminates one saturation, and

allows a unique solution of the four remaining independent variables.

The construction of the equations described by R.Cook is a straightforward exercise. The important new concept that they introduced was the ability to correlate the pvt properties to both pressure and a compositional parameter - cumulative pore volumes injected. The cumulative pore volume correlation if accurate, would allow simplified compositional simulation. The results would be in standard volume units, in place of molar units for the compositional simulator.

The idea for correlating the pvt to a compositional parameter was actually introduced in an earlier paper by a second author also named Cook in 1969⁹. The object of this paper was to try to create general K value correlations for the individual components using a new pvt test and cubic equation of state package flash calculations. Their calculations loaded a series of identical cells in sequence with the reservoir oil composition, and injected a series of fixed pore volumes of lean gas into the first cell. An equilibrium flash at reservoir temperature and cycled pressure was made, and gas with the equilibrium composition was removed off the top of the first cell to restore the original cell volume. The gas was then added to the second cell, and the steps repeated for the remaining cells in sequence. At the completion of the sequence a new incremental pore volume of dry gas was reinjected into the first cell. The pvt properties were measured in various cells as a function of cumulative pore volumes injected (CGI). The loop was repeated until all of the cells contained liquid phases with heavy ends and very low

volatility. A. Cook⁹ found that his results were relatively insensitive to the incremental pore volume of dry gas injected in the first cell, and to cell number after the tenth cell. These observations were the major conclusions in the paper.

For the system A.Cook chose the pvt behavior was relatively insensitive to cell number. The resulting pseudo compositional data was later used by R.Cook in his pseudo compositional model to match a fully compositional simulation.

Caution should be used when viewing his results - overall production rates and gas oil ratios matched well, but detailed compositional mole fractions could not be compared (because the pseudo compositional model was based on stock tank volumes). In addition, a wide variety of real life problems were not tested. A.Cook chose a lean natural gas to cycle, and the compositional dependency on system properties in this injection gas is not as important as for CO₂, thus minimizing difficulties. Practically speaking, these authors showed that their procedure worked for methane cycling in a moderate yield gas condensate reservoir with single phase flow. This was an excellent piece of work that has provided the building blocks and inspiration for my work.

R.Cook's model constructed with the A.Cook method of correlating pvt properties was a first step, but unfortunately the correlation to CGI proved to have significant limitations when other situations were considered. Henry¹⁰ was the first to uncover the problem. He discovered a poor correlation to CGI for a volatile oil problem with lean gas

cycling. R. Cook's response was that the correlation wasn't bad for a simple approach. Some of my test cases with CO₂ cycling show that the approach by these authors has serious errors, larger than those presented by Henry. The dispute effectively eliminated any further research in this direction for a decade. Work on multicomponent flow to be presented in the theory section will explain why the Cook correlation is not general.

Mott¹¹ improved the Cook work by correlating to mole fraction injection gas. A fourth equation written in terms of stock tank molar densities was added to the three black oil equations to track the tracer, and two cells were chosen to generate the pvt properties using a scheme that replicated Cook's work. Differences in the pvt behavior between the two cells were corrected by adding an additional correlating parameter. Mott chose lean gas cycling in a retrograde gas condensate reservoir (SPE Third Comparative Solution Project) and applied the correction parameter to the oil in solution variable, R_{vo} . The K value of the injection gas was assumed constant.

Mott's work was a fundamental improvement on the Cook work. The correlation to the current mole fraction of tracer in the cell is better than correlating to cumulative pore volumes that have passed through a cell. Mott chose a problem where R_{vo} is the only important pvt parameter that changes. For the general problem, for example CO₂ cycling, all of the pvt properties change significantly. His correlation for cells 1 and 2 are different, and he uses a correction parameter to split the difference in the R_{vo} values. For the general problem the pvt correlations must hold for 15-30 cells, and a correction

parameter is not practical.

Mott assumes that the K value for the recycled lean gas component is constant, and this is not true in the general case. Cases illustrating this will be presented in the results section.

Keith Coats of SSI ¹² and later Fanchi at Marathon ¹³ discuss a simple approach to the lean gas cycling problem. The black oil system of equations includes solution gas in the oil phase (called R_{so}), but normally ignores oil in solution in the free gas phase (condensate yield, R_{vo}). This assumption is inconsequential for a normal black oil reservoir, but critical in a gas condensate or volatile oil reservoir, where most of the free oil is immobile, and the majority of oil will be produced as a dissolved component of the gas phase. The R_{vo} data are correlated versus pressure in an identical fashion to the other black oil pvt properties.

Coats' modifications do an excellent job of replicating compositional model results for gas condensate and volatile oil reservoirs under depletion or secondary water drive. Interestingly, SSI has chosen not to release this enhanced black oil code to the public, but they use the code for internal reservoir studies. The code runs at the speed of a black oil model because the number of unknowns is unchanged, and the one additional dependent pvt parameter, R_{vo} is correlated versus pressure.

Coats ¹² notes that for lean gas cycling cases the Rvo correction alone will not yield good results. The pvt behavior for this case is dependent on pressure and composition, and the modified black oil model will not match the fully compositional results.

Another approach that simplifies the compositional problem and does not require modifying the compositional code has been developed by the French consulting company Franlab ¹⁴. The Franlab approach is to group the dead oil components into a single component with properties representing an average of the individual components. Likewise, the injected gas and reservoir gas can be grouped into 2 additional components. The 3 component system can then be used in a fully implicit simulator. This technique is very similar to pseudoization (which will be discussed in the pvt section), and in many problems will give acceptable results. Care must be taken because lumping a complex group of components into an average component will not always yield an accurate pvt envelope.

In summary, aside from the Rvo approach which is valid only in the absence of lean gas cycling, no fundamental basis is given for the general compositional problem. Certain of the approaches discussed seemed promising, but all had shortcomings.

2.4 Laboratory Measurement of PVT Properties

The differential expansion test expands the original reservoir mixture in a series of cell volume changes at constant temperature. The pressure is reduced at each increment by increasing the cell volume. The liberated gas is then removed at constant pressure while at the same time reducing the cell volume to restore a single phase oil in the cell. The test continues until stock tank conditions are reached. If the original reservoir mixture is undersaturated the original cell volume is expanded but no fluid is removed, and cell volumes at each pressure are measured.

The differential expansion test is used to approximate the behavior of a normal gravity oil reservoir, where the more mobile gas phase is often preferentially produced as reservoir pressure declines. Of course, this may not always be the case. For example, consider a reservoir that is originally undersaturated with well completions only in the downdip part of the reservoir. A large secondary gas cap that is not produced may form, and this behavior would be better characterized by removing oil off the bottom of the cell in the pvt test. Nevertheless, from a practical standpoint the pvt results from both tests would normally be in very close agreement because in practice the properties are strongly dependent on pressure, and only very weakly dependent on overall cell composition.

The constant volume expansion test is used to measure the pvt behavior for gas condensate reservoirs. This test requires loading the original reservoir fluid at reservoir

conditions, and then removing gas off the top of the cell in a series of pressure decreases at constant cell volume. Gas and liquid volumes in the cell at each step are measured, and the test is continued until stock tank conditions are reached. The test replicates the production in most gas condensate reservoirs, where oil dissolved in the gas phase is produced and most of the free oil that drops out of the condensate remains in the reservoir.

All of the laboratory tests measure liquid and gas volumes, and corresponding gas deviation or compressibility factors (Z factors) at different pressures. In the oil industry the composition and Z factor dependency is often expressed in terms of pvt parameters measured directly in the laboratory tests, specifically as formation volume factors (reservoir phase vol./stock tank phase volume), gas oil ratios (solution gas in oil), and viscosities. These parameters are input directly into the black oil model.

2.5 Cubic Equation of State Pvt Package - fundamental relationships

The pseudo compositional model that will be presented uses pvt data generated from a general cubic equation of state package, and consequently a review of the accepted methods for creating these packages is necessary ¹⁵⁻²¹.

A robust pvt package must accomplish several goals. The package should have both

successive substitution iteration routines (SSI) for quick convergence away from the critical point, and the more stable Newton-Raphson first order derivative based technique (MVNR) for more stable convergence close to the critical point. Phase changes must be recognized, and bubble/dew point pressure calculations are necessary as a consequence of these changes. Good initial guesses for K values of the individual components is critical for convergence.

The fundamental relationships used in the equation of state (eos) package will now be developed. For simplicity most of the equations will be shown for the liquid phase, although identical expressions hold for the gas phase.

A generalized form capable of representing all cubic equations of state was developed by Martin ¹⁵ and was used in the equation of state developed for this work. For simplicity, the Redlich-Kwong EOS will be assumed for now. The cubic expression is :

$$\begin{aligned}
 FUG_{i_{vap}} [Y_i Z_V] &= FUG_{i_{liq}} [X_i Z_L] \\
 \text{where :} \\
 Z_L^3 - Z_L^2 + Z_L [A_L - B_L (B_L + 1)] - A_L B_L &= 0 \\
 Z_V^3 - Z_V^2 + Z_V [A_V - B_V (B_V + 1)] - A_V B_V &= 0
 \end{aligned}
 \tag{17}$$

The A and B terms are calculated using mixing rules :

$$\begin{aligned}
 A_L &= \sum_i \sum_j X_i X_j a_{ij} \\
 \text{where: } a_{ij} &= (1 - \delta_{ij}) \sqrt{a_i} \sqrt{a_j} \\
 a_i &= \Omega_i \frac{P_{ri}}{T_{ri}^{2.5}} \\
 B_L &= \sum_{i=1}^n X_i \beta_i \\
 \text{where: } \beta_i &= \Omega_i \frac{P_{ri}}{T_{ri}}
 \end{aligned} \tag{18}$$

This equation shows the mixing rules for the liquid phase, and all X_i values are replaced by Y_i for the gas phase. The δ_{ij} coefficients are binary interaction coefficients between components i and j . The X_i values represent mole fraction of component i in the liquid phase, and P_{ri}/T_{ri} are the reduced pressure and temperature.

If L and V represents the overall hydrocarbon mole fractions in the liquid and vapor phases then :

$$L + V = 1 \tag{19}$$

The overall mole fraction of component i can now be expressed as the sum of the contributions of the mole fractions in the liquid and vapor phases :

$$L X_i + V Y_i = Z_i \quad (20)$$

The sum of the mole fractions in the liquid and gas phases are also equal.

$$\sum X_i = \sum Y_i = 1 \quad (21)$$

Equations 17 to 21 completely describe the system of independent unknowns, with $2NC+4$ unknowns (L, V, Z_L, Z_V , and X_i, Y_i for $i [=] 1 \Rightarrow NC$) and an equal number of equations. Unfortunately the equations are coupled in such a way that no direct solution exists.

Equations (19),(20), and (21) can be conveniently combined to form the Rachford-Rice equation. To show this first rewrite equation (21) as :

$$\sum [X_i - Y_i] = 0 \quad (22)$$

Now equations (19) and (20) can be combined to yield material balance expressions for X_i and Y_i , and then combined with equation (22) to yield the desired Rachford-Rice flash equation :

$$\begin{aligned}
 [1-V] X_i + [V] Y_i &= Z_i \\
 \text{rewriting : } [1-V] [X_i - Y_i] &= Z_i - Y_i \\
 \text{rewriting : } X_i &= \frac{Z_i}{[1+V(K_i-1)]} \quad Y_i = K_i \frac{Z_i}{[1+V(K_i-1)]} \\
 \text{with } K_i &= \frac{Y_i}{X_i} \quad (23) \\
 \text{rewriting (22): } \sum [Y_i - X_i] &= 0 \\
 \text{substituting } X_i, Y_i : \sum_{i=1}^{N_c} Z_i \frac{(K_i-1)}{1+V(K_i-1)} &= 0
 \end{aligned}$$

The Rachford Rice equation can be solved for V given an approximate set of K values, pressure, and temperature. First order Newton Rhapsion derivatives and an initial V estimate of 0.5 is typically assumed. If the calculated V is less than 0 the system is in the single phase vapor region, and if V is greater than 1 a single phase liquid region exists.

2.6 Construction of EOS Package

Many researchers have published papers for creating stable cubic equation of state pvt packages using the Minimum Variable Newton Raphson (MVNR) procedure¹⁶⁻²¹. One of the simplest to understand is a comprehensive review presented by Fussell and Yanosik¹⁶.

The MVNR second order solution can take the form of one of three different sets of equations- a L-X set of equations (total and component liquid mole fractions) solves two phase systems that are principally vapor, and V-Y (total and component vapor mole fractions) solves two phase systems that are principally liquid. A third set of equations called P-X (saturation pressure and component mole fractions) calculates the bubble/dew point pressure for undersaturated mixtures.

The minimum Newton-Raphson procedure is used to minimize the number of unknowns to NC for the two phase region (L and NC-1 Xi's for the L-X iteration) and NC+1 for bubble/dew point calculations (Psat and NC Yi's for bubble point). To see how this is accomplished first take partial derivatives of equations (19) and (20), noting that all Xi/Yi are constant in the first expression, and L and V are held constant in the second expression.

$$\begin{aligned}
 \frac{\partial L_{[x_i, i=1, nc]}}{\partial X_i} + V \frac{\partial Y_i}{\partial Y_j} - \frac{\partial Z_i}{\partial Y_j} &= 0 \\
 \text{rewriting : } \frac{\partial X_i}{\partial Y_j} &= -\frac{V}{L} \text{ for } i=j, 0 \text{ if } i \neq j
 \end{aligned} \tag{24}$$

The partial derivatives in equation (24) are first order derivatives of equations (19) and (20), and these partial derivatives allow the elimination of either Xi or Yi and L or V as independent variables. The independent equations in the system become the fugacity equality between the 2 phases, and the Rachford Rice Flash equation. Either the Xi/L or Yi/V variable set can be chosen as independent unknowns depending on whether the system is predominately liquid or vapor.

The partial derivatives with respect the dependent component mole fraction set in the fugacity equality expressions are eliminated as follows :

for X_i as a independent variable :

$$\frac{\partial Term_1}{\partial Y_i} = \frac{\partial Term_1}{\partial X_i} \frac{\partial X_i}{\partial Y_i} \quad (25)$$

Note that the final partial derivative is simply one of the partial derivative expressions derived in equation (24). Summarizing, this procedure when applied to the L-X or V-Y procedure, results in the Rachford Rice flash equation and NC-1 fugacity equality expressions between phases to completely describe the independent variables in the system. A jacobian is created, and first order partial derivatives are taken using the chain rule (or shift derivatives as explained in the theory section). When good initial guesses are made, the matrix will usually converge in 2 or 3 iterations.

For the P-X iteration at the bubble/dew point the flash equation is replaced by the following expression relating fugacities to the saturation pressure.

$$P_s = \sum_{i=1}^n \frac{F_{iL}}{F_{iV}} P Y_i \quad (26)$$

P_s replaces V in the set of independent unknowns.

2.7 Convergence Problems with MVNR

The MVNR procedure converges quickly, but has stability problems if the initial guesses are not accurate. A number of researchers have studied this problem, and contributed many practical techniques for minimizing convergence problems and maximizing convergence speed. The first problem is good initial guesses for the K values of the individual components. Most commercial equation of state packages use a correlation created by Wilson ¹⁶. This correlation is only approximate, and generally holds at pressures less than 500 psia. A second correlation by Varotsis at Schlumberger ¹⁸ is stated to be more accurate than the Wilson correlation. Unfortunately his paper contains errors in some of the constants used in the correlation, and to date no corrections have been published.

The K values calculated directly by Wilson will usually diverge when they are entered directly into the MVNR process if the system pressure exceeds 500 psia. Because this is almost always the case a hybrid method has been developed by Abhvani ²¹ combining a successive substitution iteration (SSI) with the MVNR technique. This procedure is as follows.

First, K values are estimated at either the system pressure, or at 500 psia if the system pressure exceeds 500 psia.

Second, the Rachford-Rice flash equation is next solved for V using first order derivatives. If V is calculated to be less than 0 or greater than 1 during the iteration process a single phase is present and a reformulation procedure described below is used to reformulate the problem.

Third, the X_i and Y_i values are updated using the new vapor mole fraction V and the expressions developed in equation (23).

Fourth, the equation of state is solved for the component fugacities in both phases.

Fifth, the K values are updated based on the ratios of the fugacity coefficients or :

$$K_i = \frac{\frac{F_{iL}}{X_i P}}{\frac{F_{iv}}{Y_i P}} \quad (27)$$

The updated K values are now used to reloop to step 2 and recalculate the vapor mole fraction V . The looping is continued until converge is achieved, and then the pressure is incremented by 500 psia and steps 2 to 4 repeated until the system pressure is reached. At the final pressure one SSI iteration is performed, and if convergence is not reached the MVNR procedure is used for further iterations.

The possibility exists for crossover into the single phase region during the pressure stepping process. Risnes ¹⁵ has developed a simple approach for the phase change. If $V < 0$, then the single phase is liquid so set V to 0, and $X_i = Z_i$. If $V > 1$, then the single phase is vapor so set V to 1 and $Y_i = Z_i$.

Combining the first order SSI and second order MVNR results in a hybrid method that is both quick and reliable, and this method was chosen in the pvt package created for this work. Other hybrid methods exist, but a comparison of the convergence rates for different methods by Abhvani ²¹ found the method described above superior.

2.8 Pseudoization and Regression

Cubic equations of state (EOS) are the popular choice for representing the pvt behavior in modern compositional simulators. Although higher order equations of state may be more accurate a process called regression is used to minimize cubic EOS errors.

In this method, pvt behavior for the actual reservoir mixture is first measured in one of the laboratory tests that have been described. A jacobian process is then used to write a minimizing function F in terms of the errors between the equation of state and measured pvt data, and the jacobian iterates for user specified parameters (eg. binary interaction coefficients) until a minimizing fit is obtained. Coats ⁵ shows an expression

that can be used for minimization.

$$F = \sum_{j=1}^J W_j \left[\frac{(d_j - d_j^c)}{d_j} \right]$$

(28)

F = objective function

d_j^c = calculated eos value

d_j = observed value

W_j = weight factor

Weighting factors can be attached to the different errors; typically bubble/dew point is weighted higher than perhaps oil formation volume factors. The resulting regressed fit is usually excellent, and if the lab pvt data were generated over a pressure range comparable to the operating pressure range in the field, the resulting compositional model can represent the pvt behavior closely.

An approximation called pseudoization is attempted to minimize the number of components used in the regression. The original mixture of 10-15 primary components including a plus fraction lumping heavy components is divided into 3 to 7 pseudo components and new equation of state parameters are assigned to these imaginary components using the regression. In many real applications grouping the components leads to errors. For example grouping C5 thru C30 components and regressing will lead to a pseudo component that has cubic parameters that looks like something between a C5

and a C6 because these two components influence most of the vaporization curve used in the regression. Likewise the pvt for this imaginary component acts like a C5 or C6, and although it may represent the first 80% of the vaporization process accurately, the last 20% of the vaporization curve cannot be matched because the real oil mixture is mostly heavier components. The end result is unrealistically high oil vaporization rates in the model at lower oil saturation values.

For the work presented here a commercial compositional model, the SSI COMP3 PVT model, was used to regress the pvt data. The regressed parameters were then passed to the cubic equation of state package developed to calculate the new compositional data. The pseudoization step is eliminated in the new model, because as will be seen in equation development for the new model, only the injection component compositional equation is included.

Chapter 3 - Theory

3.1 Preview

The focus of this work was the development of a simplified compositional simulator. The early work used a compositional simulator to verify correlations for the new simulator. K values were the convenient choice for testing correlations. The first section will prove that for a given pressure, temperature, and set of K values the X/Y mole fractions and corresponding black oil properties are unique.

The second section will investigate the simplest modification that yields a pseudo compositional formulation- including the dissolved oil component in the gas phase in a black oil model. This model was introduced in the literature search section - but the applicability and limitations of this method were not covered.

The third section will discuss the success of the Cook pseudo compositional model introduced in the literature review section - and show both its successes and failures.

The fourth section will discuss the steps required to construct a pvt test capable of representing the compositional behavior, and introduce a new correlation for depletion/secondary drive and the more difficult gas cycling problem. The validity of the correlation using theory for multicomponent multiphase flow will be discussed.

The fifth section will discuss a new system of flow equations that can be combined to represent a compositional reservoir, and the corresponding finite difference approximations. These equations are independent of the number of components in the hydrocarbon mixture, and in fact solution of this system will be shown to have speeds almost identical to a black oil system.

The sixth section will describe the mathematical reduction of the independent unknowns for the system of equations to construct a matrix, matrix operations required to maintain stability, and the back substitution calculations to calculate the dependent variables.

3.2 Proof that a set of K values corresponds to unique black oil properties

A popular misconception in the oil industry is that a black oil simulation approach cannot model volatile oil or gas condensate reservoirs under a depletion or water injection process. These people have traditionally used a compositional simulator with K values correlated to pressure to model these reservoirs, and created a computational headache for themselves in the process. Because the new model we will construct assumes that a black oil approach is valid for these reservoirs, it may be instructive to prove that a unique set of K values does assure unique black oil pvt properties.

The simplest proof comes from looking at the Gibbs phase rule that states for NC components and P phases the degrees of freedom are $NC - P + 2$. With two phases present

the degrees of freedom equal NC, and if pressure and temperature are given the unknowns are reduced to NC-2. These remaining variables can be represented by NC-2 K value expressions.

Consequently, for a given pressure, temperature, and set of K values the X/Y mole fractions and black oil pvt properties are unique. For example R_{so} and R_{vo}, the terms for gas in solution in the oil phase and oil in solution in the gas phase are a function of Z_L, Z_v, and the X_i/Y_i mole fractions.

3.3 Black Oil Model With Dissolved Oil Term

The simplest approach that allows many compositional problems to be modeled is accomplished by adding R_{vo}- the dissolved oil in the gas phase ^{13,14}. Traditionally, this term has been ignored in black oil models for two reasons. First, this term is negligible for the majority of oil reservoirs. Second, for higher gravity oil and gas reservoirs where R_{vo} is not negligible the compositional model is the industry choice. This is primarily because these reservoirs often cycle lean gas to maintain R_{vo} yields high, and for most of these reservoirs the pvt behavior is dependent on both pressure and composition. When this is the case the R_{vo} modification alone cannot model these reservoirs, because the pvt behavior for this simpler formulation is still dependent only on pressure. Coats ¹³ shows this to be the case for gas condensate reservoirs.

The application of the Rvo/black oil formulation in gas condensate reservoirs under depletion or water injection recovery is well documented ¹³, and the Rvo data are commonly reported in lab pvt reports. Conversely, the applicability of this method to volatile oil reservoirs is not widely understood in the oil industry. In fact, I am not aware of any papers that show case studies for this application. The major difficulty that reservoir engineers face in modeling volatile oil reservoirs with the Rvo modification is calculating the Rvo parameters. A conventional differential expansion test does not measure Rvo for volatile oil reservoirs (although it is possible that it could be measured), and correlations have not been published to date.

For the purpose of testing the volatile oil problem laboratory differential expansion test data were matched using a regression procedure in Scientific Software's pvt package. The regressed data were entered into the pvt package created in this work, and the cubic equation of state replicated the differential expansion test while at the same time predicting Rvo. The data from the pvt package were entered into the modified black oil model, and the regressed pvt data were entered into SSI's compositional model COMP3 for comparison purposes.

The results from the two models are for all practical purposes identical, confirming that the modified black oil model gives accurate results when the reservoir fluid properties are dependent only on pressure. The results section will show detailed comparisons between the two models.

The validity of this simple pseudo compositional formulation provided the first important building block necessary to represent the more complex goal- cycling lean gas in an oil or gas reservoir.

3.4 Pseudo-compositional model based on cumulative pore volumes injected

One of the most promising attempts for creating a pseudo compositional model adopted a modified black oil approach but did not include compositional equations. Black oil equations are based on stock tank volumes, and as a consequence a volume correlation was attempted- cumulative pore volumes injected gas (CGI). The details of this model created by R. Cook ⁸ were discussed in the literature review section. Recall that all cells must have the same black oil properties at a given CGI. Unfortunately, this is not always true, and in serious error for some hydrocarbon mixtures that cycle lean gas. The results section will discuss in detail the limitations of this correlation.

3.5 Construction of a pvt test to represent lean gas cycling - background

The first step in creating an accurate modified compositional formulation required a simple and accurate correlation for the compositional dependency of black oil pvt data. The logical choice for investigating the validity of any new correlations is the fully

compositional model.

Many researchers have adopted the opposite approach- constructing a new model and then trying to show that somehow it would match the compositional model. This approach is time consuming- a great deal of work is required to prove/disprove any new formulation. Some researchers become favorably biased towards a formulation that holds promise for some problems, but does not offer replicability for other problems. These problems are sometimes solved with correcting parameters that have little or no basis in theory and may be impossible to calculate for an arbitrary problem (unless you know the solution). Many of these ideas could be disproved in a few hours using a fully compositional simulator.

The compositional behavior of an oil reservoir with lean gas is almost overwhelming at first glance. The oil and gas compositions change continually, both as a function of pressure and lean gas stripping or swelling. Previous correlations were based on some type of volume parameter, for example cumulative pore volumes dry gas injected. The logical intuitive choice would be to correlate to some type of mole based parameter, since the K values for the individual components are based on mole fractions entered into the cubic equation of state. As discussed previously, the CGI volume correlation is not always accurate.

3.6 PVT Generation Procedure for Simplified Model

The first step in creating an accurate modified compositional formulation is to develop a simple and accurate correlation for the compositional dependency of black oil pvt properties. The procedure used here is basically that of Cook et al ⁸ but with a different correlating parameter, as discussed below. A linear sequence of between one and thirty cells of equal volumes is chosen for the calculation. All are taken to be initially at specified values of temperature and pressure. The composition is that of the initial reservoir for undersaturated cycling, and is found by expanding the cells in a series of pressure drops for the two phase region. For example, the cell volume in the first cell is restored at each step by moving fluids to the second cell in proportion to the relative permeability curves. The process is repeated in the remaining cells. The cells have almost identical liquid and gas component mole fractions when cycling begins.

A fixed volume of lean cycled gas is injected into the first cell to start the cycling test. The same equation of state used in the compositional simulator carries out a constant composition expansion to determine liquid and gas properties at the specified pressure. Then a volume of fluid equal to the injected volume is transferred from the first to the second cell. Different methods were investigated for this step including transferring only gas and using relative permeability tables from the simulator to determine the relative amounts of liquid and gas transferred. A considerable improvement in the correlation was seen in the latter case. The process of expansion and fluid transfer is repeated in

sequence for all of the cells. Then another increment of gas is injected into the first cell and the entire process repeated. Additional increments are injected until all of the cells are filled with gas and a liquid phase containing only heavy components with low volatility.

This multicell, multicontacting scheme is a simple model of a one dimensional linear cycling process at constant pressure with lean gas injected into the first cell and a reservoir fluid/lean gas mixture produced from the last cell. A one dimensional calculation employing the compositional simulator without dispersion could be used instead, as could the generalized chromatographic scheme of Helfferich ²³. All these methods basically determine a path through the multidimensional phase diagram along which system composition falls. That is, a compositional wave develops which passes through the formation. Fluid compositions and properties found for a given point on this wave are the same for all cells. In practice deviations are sometimes seen, particularly in the first few cells, as a result of the finite cell size and injected gas increments.

Each point on the composition path obtained in this way can be identified by the mole fraction Y_{inj} in the gas phase of the primary component of the injected gas or, if no gas is present, by the liquid mole fraction X_{inj} of this component. Formation volume factors B_o and B_g , the dissolved gas R_{so} in the oil, and the condensate yield R_{vo} of the gas can be found by determining with the equation of state package the behavior of the individual liquid and/or gas phases upon expansion to separator pressure. K_{inj} or (Y_{inj}/X_{inj}) for

the primary injection component can be found whenever two phases are present.

The procedure used by R.Cook et al ⁸ is inferior to ours because values of their correlating parameter CGI, the cumulative pore volumes of injected gas that have passed through a cell, are not uniquely related to points on the compositional path. If the compositional wave is spreading, for example, where each composition travels through the formation at different speed, it is easily shown that the value of CGI for which a particular composition is reached in a cell varies with cell position in the sequence. In contrast, Y_{inj} is obviously the same for the same composition in all cells. While Mott¹¹ was the first to propose Y_{inj} as the correlating parameter, he required K_{inj} to have the same value for all compositions in the two phase region at a given pressure. As shown below, K_{inj} can vary significantly in some gas injection processes.

It is useful to view behavior in terms of a ternary diagram. The diagram on the next page shows a ternary representation of phase behavior at one pressure for a CO₂-crude oil system whose behavior is considered in more detail below. The two-phase region and tie-lines are shown, as are compositions of the initial reservoir fluid and injection gas, which are connected by line A. When the first increment of gas is injected into the first cell, mixing yields an overall composition such as R, which is a mixture of liquid and gas having compositions P and Q. As indicated above, some of the liquid and gas are transferred to the second cell. With subsequent increments of injected gas, overall composition of the first cell varies along the path S with corresponding liquid and gas

compositions moving along their respective coexistence curves. Ultimately, the composition of this cell should approach the injected gas composition D. When more components are included for this system, however, the heavy components of the liquid have such low volatility that they are not fully vaporized for practical amounts of injected gas. Accordingly, the path does not reach D. As the multicontacting process proceeds, compositions in each cell follow the same path, provided that cell volumes and injected increments are sufficiently small, in accordance with the general theory of one-dimensional multiphase, multicomponent transport described by Helfferich²³.

It is noteworthy that specifying Y_{inj} for a true ternary system in the two-phase region, e.g., Y_{CO_2} in the figure, determines the equilibrium tie-line and fluid properties independently of the above procedure. With more components, however, the system has additional degrees of freedom, and a value of Y_{inj} is not, in general, sufficient to determine a unique tie-line. If the reservoir fluid is initially in the single-phase region, Y_{inj} (or X_{inj}) is sufficient to specify the compositions and properties, whatever the number of components present, because the injected gas simply mixes with the fluid until the dew point (or bubble point) is reached. However, if a single-phase region arises during the multicontacting process, Y_{inj} (or X_{inj}) is not sufficient to specify its composition even for a ternary diagram, as may be seen from the diagram on the last page, and again a procedure such as that described above is required to supply the additional information.

The linear sequence of cells and the above method can be used to obtain black oil PVT properties and K_{inj} as a function of Y_{inj} for a series of pressures bounding the operating pressure range. Properties at intermediate pressures which might be required during a simulation are obtained by interpolation. This method of handling pressure variations in the reservoir has so far proved to be successful, as discussed below.

3.7 Description of the Flow Equations

Excellent Y_{inj} correlations were established for both CO₂ and lean methane gas cycling. These correlations established that all black oil pvt properties could be represented as a function of two variables, pressure and Y_{inj} . A three dimensional simulator will now be developed with pvt properties correlated to pressure and Y_{inj} using the procedure described in the previous section.

The normal set of black oil equations are written in units of stock tank volumes, and by themselves are incapable of tracking the Y_{inj} dependency. The logical choice is to add a compositionial tracer equation to the set of black oil equations to track Y_{inj} . This new set of equations is neither a black oil or compositionial formulation - a modified compositionial system results.

The compositional molar equation that represents the tracer, Y_{inj} can be stated as follows :

$$\begin{aligned}
 & V_{p_n} \Delta T [S_g Y_i \rho_g + S_o X_i \rho_o]_n - V_{p_{n+1}} \Delta T [S_g Y_i \rho_g + S_o X_i \rho_o]_{n+1} + \\
 & [T_{o_{up}} X_i \rho_o + T_{g_{up}} Y_i \rho_g] [\Delta P + \Delta P_c + \rho_{avg} \Delta D_{eph}] + \\
 & P_{id} X_i \rho_o \frac{K_{ro}}{\mu_o} [P_{well} - P_n] + \\
 & P_{id} Y_i \rho_g \frac{K_{rg}}{\mu_g} [P_{well} - P_n] = 0
 \end{aligned} \tag{29}$$

The first two terms correspond to accumulation for component i in the grid block, the third term is the Darcy flow term, and the last two terms are for oil/gas production. The avg subscript denotes an average of the variable in the upstream and downstream cells. This equation would normally be included as one of a set of NC component equations in the fully compositional model. Fortunately, the ability to correlate all of the K values to Y_{inj} and pressure allows the original set of NC equations to be reduced to one independent equation for the injection component, and NC-1 dependent equations. Complex mixtures of injection components are treated by correlating the primary component in the injection gas for the tracer equation.

The resulting system has 4 independent expressions- specifically the oil, water, gas, and tracer equations. The new Y_{inj} variable is added to the normal black oil unknowns, two saturations and pressure. The condensate dissolved in the gas phase, R_{vo} is included in

the oil expression. The new oil equation becomes :

$$\begin{aligned}
 & V_{p_n} \Delta T \left[S_g \frac{R_{vo_l}}{B_g} + \frac{S_o}{B_o} \right]_n - V_{p_{n+1}} \Delta T \left[S_g \frac{R_{vo_l}}{B_g} + \frac{S_o}{B_o} \right]_{n+1} + \\
 & \left[\frac{T_{o_{up}}}{B_o \mu_o} \right] [\Delta P + \rho_{o_{avg}} \Delta D_{eph}] + \left[T_{g_{up}} \frac{R_{vo_{avg}}}{B_g \mu_g} \right] [\Delta P + \Delta P_{c_{go}} + \rho_{g_{avg}} \Delta D_{eph}] + \quad (30) \\
 & P_{id} \frac{K_{ro}}{B_o \mu_o} [P_{well} - P_{cell}] + \\
 & P_{id} \frac{K_{rg} R_{vo}}{B_g \mu_g} [P_{well} - P_{cell}] = 0
 \end{aligned}$$

The first two terms are accumulation terms and include free oil as well as dissolved oil in the gas phase. The next two terms correspond to free oil and dissolved oil moving from Darcy flow, and the last two terms are the production terms. The gas equation becomes :

$$\begin{aligned}
 & V_{p_n} \Delta T \left[S_o \frac{R_{so_l}}{B_o} + \frac{S_g}{B_g} \right]_n - V_{p_{n+1}} \Delta T \left[S_o \frac{R_{so_l}}{B_o} + \frac{S_g}{B_g} \right]_{n+1} + \\
 & \left[\frac{T_{g_{wp}}}{B_g} \right] [\Delta P + \Delta P_{c_{og}} + \rho_{g_{avg}} \Delta D_{epth}] + \left[T_{o_{wp}} \frac{R_{so_{avg}}}{B_o} \right] [\Delta P + \rho_{o_{avg}} \Delta D_{epth}] + \\
 & P_{id} \frac{K_{rg}}{B_g \mu_g} [P_{well} - P_{cell}] + \\
 & P_{id} \frac{K_{ro} R_{so}}{B_o \mu_o} [P_{well} - P_{cell}] = 0
 \end{aligned} \tag{31}$$

The tracer equation becomes the component equation developed above with the i subscript replaced with inj - the primary injection component mole fraction. The correlation variable can be either X_{inj} or Y_{inj} , with the X_{inj} correlation used if an undersaturated liquid is present, and the Y_{inj} correlation used for other regions in the phase envelope:

$$\begin{aligned}
 & V_{p_n} \Delta T [S_g Y_{inj} \rho_g + S_o X_{inj} \rho_o]_n - V_{p_{n+1}} \Delta T [S_g Y_{inj} \rho_g + S_o X_{inj} \rho_o]_{n+1} + \\
 & [T_{o_{wp}} X_{inj} \rho_o] [\Delta P + \rho_{o_{avg}} \Delta D_{epth}] + [T_{g_{wp}} R_{v_{avg}} Y_{inj} \rho_g] [\Delta P + \Delta P_{c_{go}} + \rho_{g_{avg}} \Delta D_{epth}] + \\
 & P_{id} X_{inj} \rho_o \frac{K_{ro}}{\mu_o} [P_{well} - P_{cell}] + \\
 & P_{id} Y_{inj} \rho_g \frac{K_{rg}}{\mu_g} [P_{well} - P_{cell}] = 0
 \end{aligned}
 \tag{32}$$

The pvt properties, specifically the formation volume factors (B_o, B_w, B_g), dissolved gas (R_{so}), condensate yield (R_{vo}), viscosities, and oil and gas densities can be characterized as dependent variables. These pvt variables are functions of both pressure and Y_{inj} , in comparison to the normal black oil approach where the data is dependent on pressure but independent of Y_{inj} .

3.8 Shift Derivatives in the Simplified Model

The finite difference representations of the descriptive flow equations are organized into a matrix, with partial derivatives taken with respect to each independent variable. These partial derivatives are calculated using shift derivatives as illustrated below for the accumulation term for the oil equation.

$$\begin{aligned}
 Accum(S_o, P, Y_{inj}) [=] & \theta V_{P_{n+1}} \frac{S_o}{B_o} \\
 Shift \text{ for } S_o \rightarrow \frac{\delta Accum}{\delta S_o} [=] & \frac{\theta V_{P_{n+1}} \frac{S_o + \delta S_o}{B_o} - \theta V_{P_{n+1}} \frac{S_o}{B_o}}{\delta S_o} \\
 Shift \text{ for } Y_{inj} \rightarrow \frac{\delta Accum}{\delta Y_{inj}} [=] & \frac{\theta V_{P_{n+1}} \left[\frac{S_o}{B_o + \frac{\delta B_o}{\delta Y_{inj}} \delta Y_{inj}} - \frac{S_o}{B_o} \right]}{\delta Y_{inj}}
 \end{aligned} \tag{33}$$

$$Shift \text{ for Pressure} \rightarrow \frac{\delta Accum}{\delta P} [=] \frac{\theta \left[\frac{S_o \left[V_p + \frac{\delta V_p}{\delta P} \delta P \right]}{[B_o + \frac{\delta B_o}{\delta P} \delta P]} - V_p \frac{S_o}{B_o} \right]}{\delta P} \tag{34}$$

The partial derivatives with respect to Y_{inj} and pressure requires 3-D interpolation from the set of 2-D pvt tables generated for variable Y_{inj} at different cycling pressures. Shift derivatives are used, and shifts are kept small to maintain accurate approximations of the partial derivatives. Shift derivatives avoid mistakes made when deriving partial derivative expressions. This advantage for the expressions above is minimal- real advantages are only realized for complicated expressions. For example, consider the complex mole fraction derivatives in the cubic equation of state- an hour or more can be spent deriving/checking this one partial derivative. Shift derivatives can be coded in a few minutes.

3.9 Organization and solution of the system of flow equations

Shift or partial derivatives are found with respect to each independent variable for each term in the system of flow equations, and the equations are then organized into the following symbolic structure with the changes in the independent variables over the time step as unknowns :

$$\begin{aligned}
 & \begin{bmatrix}
 O_{ii} & O_{ii} & 0 & O_{ii} & O_{ii} & O_{ii,imp} & 0 & 0 & 0 & 0 & 0 & 0 & D_{p_{i-1}} \\
 Wat & 0 & W_{\alpha i} & 0 & Wat & 0 & W_{\alpha i,imp} & 0 & 0 & 0 & 0 & 0 & D_{so_{i-1}} \\
 G_{as} & G_{as} & G_{as} & G_{as} & G_{as} & G_{as,imp} & G_{as,imp} & 0 & 0 & 0 & 0 & 0 & D_{sw_{i-1}} \\
 I_{nj} & I_{nj} & I_{nj} & I_{nj} & I_{nj} & I_{nj,imp} & I_{nj,imp} & I_{nj,imp} & 0 & 0 & 0 & 0 & D_{y_{nj,i-1}} \\
 \\
 O_{ii} & O_{ii,imp} & 0 & 0 & O_{ii} & O_{ii} & 0 & O_{ii} & O_{ii} & O_{ii,imp} & 0 & 0 & D_{p_i} \\
 Wat & 0 & W_{\alpha i,imp} & 0 & Wat & 0 & W_{\alpha i} & 0 & Wat & 0 & W_{\alpha i,imp} & 0 & D_{so_i} \\
 G_{as} & G_{as,imp} & G_{as,imp} & 0 & G_{as} & G_{as} & G_{as} & G_{as} & G_{as} & G_{as,imp} & G_{as,imp} & 0 & D_{sw_i} \\
 I_{nj} & I_{nj,imp} & I_{nj,imp} & 0 & I_{nj} & I_{nj} & I_{nj} & I_{nj} & I_{nj} & I_{nj,imp} & I_{nj,imp} & 0 & D_{y_{nj,i}} \\
 \\
 0 & 0 & 0 & 0 & O_{ii} & O_{ii,imp} & 0 & 0 & O_{ii} & O_{ii} & 0 & O_{ii} & D_{p_{i+1}} \\
 0 & 0 & 0 & 0 & W_{\alpha i} & 0 & W_{\alpha i,imp} & 0 & W_{\alpha i} & 0 & W_{\alpha i} & 0 & D_{so_{i+1}} \\
 0 & 0 & 0 & 0 & G_{as} & G_{as,imp} & G_{as,imp} & 0 & G_{as} & G_{as} & G_{as} & G_{as} & D_{sw_{i+1}} \\
 0 & 0 & 0 & 0 & Y_{lnj} & Y_{lnj,imp} & Y_{lnj,imp} & 0 & Y_{lnj} & Y_{lnj} & Y_{lnj} & Y_{lnj} & D_{y_{lnj,i+1}}
 \end{bmatrix}
 =
 \begin{bmatrix}
 R_{hs_{oil,i-1}} \\
 R_{hs_{wat,i-1}} \\
 R_{hs_{gas,i-1}} \\
 R_{hs_{ynj,i-1}} \\
 \\
 R_{hs_{oil,i}} \\
 R_{hs_{wat,i}} \\
 R_{hs_{gas,i}} \\
 R_{hs_{ynj,i}} \\
 \\
 R_{hs_{oil,i+1}} \\
 R_{hs_{wat,i+1}} \\
 R_{hs_{gas,i+1}} \\
 R_{hs_{ynj,i+1}}
 \end{bmatrix}
 \end{aligned}
 \tag{35}$$

Three grid blocks organized into a one dimensional flow problem are illustrated above, but the organization is completely general for the 3-D problem as well. The equations

are ordered oil/water/gas/ tracer, and the independent variables are ordered P/So/Sw/Yinj.

The order of the equations is unimportant, and the equation structure above can be collapsed into one independent equation for the IMPES structure. Back substitution can solve for the dependent variables. This will be illustrated in the discussion below.

The system of equations is rescaled by calculating the left inverse of the 4 by 4 diagonal matrix for each grid block. The inverse matrix, when multiplied through the original diagonal, off diagonal blocks, and right hand side yields :

$$\begin{bmatrix}
 1 & 0 & 0 & 0 & O_{ll_{mod}} & O_{ll_{imp}} & 0 & 0 & 0 & 0 & 0 & 0 & D_{p_{l-1}} \\
 0 & 1 & 0 & 0 & W_{at_{mod}} & 0 & W_{at_{imp}} & 0 & 0 & 0 & 0 & 0 & D_{so_{l-1}} \\
 0 & 0 & 1 & 0 & G_{as_{mod}} & G_{as_{imp}} & G_{as_{imp}} & 0 & 0 & 0 & 0 & 0 & D_{sw_{l-1}} \\
 0 & 0 & 0 & 1 & I_{nj_{mod}} & I_{nj_{imp}} & I_{nj_{imp}} & I_{nj_{imp}} & 0 & 0 & 0 & 0 & D_{yn_{l-1}} \\
 \\
 O_{ll_{mod}} & O_{ll_{imp}} & 0 & 0 & 1 & 0 & 0 & 0 & O_{ll_{mod}} & O_{ll_{imp}} & 0 & 0 & D_{p_l} \\
 W_{at_{mod}} & 0 & W_{at_{imp}} & 0 & 0 & 1 & 0 & 0 & W_{at_{mod}} & 0 & W_{at_{imp}} & 0 & D_{so_l} \\
 G_{as_{mod}} & G_{as_{imp}} & G_{as_{imp}} & 0 & 0 & 0 & 1 & 0 & G_{as_{mod}} & G_{as_{imp}} & G_{as_{imp}} & 0 & D_{sw_l} \\
 I_{nj_{mod}} & I_{nj_{imp}} & I_{nj_{imp}} & 0 & 0 & 0 & 0 & 1 & I_{nj_{mod}} & I_{nj_{imp}} & I_{nj_{imp}} & 0 & D_{yn_l} \\
 \\
 0 & 0 & 0 & 0 & O_{ll_{mod}} & O_{ll_{imp}} & 0 & 0 & 1 & 0 & 0 & 0 & D_{p_{l+1}} \\
 0 & 0 & 0 & 0 & W_{at_{mod}} & 0 & W_{at_{imp}} & 0 & 0 & 1 & 0 & 0 & D_{so_{l+1}} \\
 0 & 0 & 0 & 0 & G_{as_{mod}} & G_{as_{imp}} & G_{as_{imp}} & 0 & 0 & 0 & 1 & 0 & D_{sw_{l+1}} \\
 0 & 0 & 0 & 0 & Y_{ln_{mod}} & Y_{ln_{imp}} & Y_{ln_{imp}} & 0 & 0 & 0 & 0 & 1 & D_{yn_{l+1}}
 \end{bmatrix} = \begin{bmatrix} R_{hs_{od_{l-1}}} \\ R_{hs_{wat_{l-1}}} \\ R_{hs_{gas_{l-1}}} \\ R_{hs_{tn_{l-1}}} \\ \\ R_{hs_{od_l}} \\ R_{hs_{wat_l}} \\ R_{hs_{gas_l}} \\ R_{hs_{tn_l}} \\ \\ R_{hs_{od_{l+1}}} \\ R_{hs_{wat_{l+1}}} \\ R_{hs_{gas_{l+1}}} \\ R_{hs_{tn_{l+1}}} \end{bmatrix} \quad (36)$$

If an IMPES formulation can yield a stable solution the off diagonal implicit (imp) saturation and Y_{inj} terms are not present. The first equation in the matrix blocks is only a function of pressure, and these pressure equations for the grid blocks can be organized into a structure that can be solved directly for pressure. Back substitution into the last three equations solves for the remaining dependent variables, 2 saturations and Y_{inj} .

The reduction of the original set of 4 independent unknowns into one unknown is the general problem - but care must be taken to consider other subsets of these variables. For example, initially most of the cells in the model do not contain tracer, and Y_{inj} must be not be included as an unknown or else a 0 will result along one of the diagonal bands. A rigorous solution to this problem was found for the general problem by including all 4 equations, and checking for zeros in the diagonal elements. If zeros are found the equations are reordered, and all matrix operations on this block recognize that one or more variables are not present in this grid block.

For undersaturated cells the water saturation change can be calculated using the relationship $DSW = -DSO$, and bubble/dew point change can be used to replace DSW as an independent variable in the four original equations for each grid block.

Variables such as Y_{inj} must sometimes be included even though they are not present in a cell at the beginning of a time step. For example, suppose lean gas has entered an upstream grid block during a time step. The next time step requires the Y_{inj} variable be

included in the downstream cell (even though Y_{inj} was 0 here)- otherwise the injection gas could not move into the downstream cell.

3.10 Comparing Simplified Model to Classical Approaches

The system of equations that are used in this work is unique - traditionally researchers have either modified the original set of black oil equations or simplified the compositional formulation using pseudo-components. Neither approach offers a complete solution- the compositional dependency has not been shown to be represented by any simple volume type of correlation (for example CGI). Compositional model speeds are slow because four to seven pseudo components are still needed to represent the pvt properly.

The new system of equations described creates a reasonable marriage of the black oil and compositional formulations. The fundamental pvt behavior used in the compositional model is still generated. The difference lies in the fact that these data are generated in the preprocessor, and table lookup is used in the simulator. The compositional simulator requires calculating pvt properties using the cubic equation of state for each cell in the model at every time step. The speed of the compositional simulator is directly tied to these calculations. In addition, combining the three black oil equations with the compositional injection equation completely describes the system, and eliminates all

dependency on the number of components in the system without pseudoization.

One important difference from the classical approach was also made in the finite difference approximations. Note that the R_{vo} term in the oil equation is based on the upstream cell, as compared to the R_{so} term that is calculated from the arithmetic average of the upstream and downstream cells. Classical development of the finite difference approximations for the flow equations always uses an arithmetic average for the R_{so} term, but when this approximation was tried for the R_{vo} term stability problems were encountered.

This problem was caused when large volumes of injected dry gas created two cells in contact where the upstream cell had a very low oil saturation composed primarily of heavy ends, and the downstream cell had a higher oil saturation with primarily light ends. If the arithmetic average R_{vo} was used, the predicted dissolved condensate movement from the upstream to the downstream cell exceeded the original oil in place in the upstream cell (both as condensate and free oil). As a result negative oil saturations were calculated for the upstream cell.

The solution required using the R_{vo} term based on the upstream cell. For example, in the SPE Gas Cycling Comparative Solution problem stable time steps increased from 0.3 days to 25 days after the change was made.

RESULTS

4.1 Compositional Runs on COMP3 Simulator

The earliest work used the Scientific Software simulator COMP3 to investigate possible correlations that could be used as the building blocks for a simplified compositional formulation. These correlations were made by viewing the K value fits for different cells in 1-D and 3-D problems. These plots are identical to viewing correlations for the various black oil properties, and this proof was given in the theory section.

The first set of plots in Figures 1 to 3 verify that K values for two different volatile oil reservoirs correlate to pressure independent of cell number for a depletion drive mechanism. The compositions of the Henry fluid is given in Appendix 1. PVT data were calculated from an original mixture with C1 to C10 components and a C11 plus fraction. C1 to C5 components plus a C6+ fraction were used to approximate the original mixture. The first reservoir was a sample COMP3 data set, and the second reservoir was the volatile oil reservoir chosen by Henry¹⁰. Compositional simulation tests were run with 15 cells in a radial pattern with a producing well in the last cell. The arrangement of the cells is shown in Figure 4. Cell permeabilities were set at 5 darcys

Figure 1 -Volatile oil reservoir, 2688 GOR at Pb=4088

4*4*1 pattern with cell (1,1,1) producing

Figure 2 - Volatile oil reservoir, Henry paper, depletion drive

C1 correlation

Figure 3 - Volatile oil reservoir, Henry paper, depletion drive

C6+ pseudo component correlation

Figure 4

RADIAL PATTERN FOR COMPOSITIONAL PVT CORRELATIONS

to minimize pressure differences between the cells. The figures show the correlation for both C1 and a heavy end component. These figures illustrate that a black oil formulation with the Rvo condensate yield modification can replicate compositional model results for primary production in volatile oil and gas condensate reservoirs. Some scatter in the data is evident- primarily because it is difficult to hold the pressure constant in all of the cells. Overall the fit is excellent confirming Coats'¹² previous conclusion.

The next logical step was to extend the correlation to gas cycling problems. These problems are sensitive to pressure and the current oil composition- as cycling proceeds at constant pressure the light ends vaporize and the remaining oil takes on the properties of a lower gravity oil. A number of correlations were attempted, and as discussed in the theory section the mole fraction injection component (Y_{inj}) correlated best because at constant pressure a compositional wave sweeps across the reservoir. Once again the compositional simulator was used to study correlations.

Figures 5 and 6 illustrate the Y_{inj} correlation for the Henry data set. Recall that the Henry data were shown to have a poor correlation to cumulative pore volumes injected, the fit parameter in the Cook study. The test was run with 10 cells in a radial pattern- a C1 injector was placed in the first cell (the center of the radial pattern) and a producing well in the tenth cell (the outer limit of the radial pattern) as illustrated in Figure 4. Both the injection and producing wells were pressure specified - that is the wells produced whatever rates were possible with a specified flowing bottomhole pressure. The injection

Figure 6 - Henry data, volatile oil reservoir, C1 cycling

Cycle C1 at 4000-4150 psia, radial geometry

Figure 6 Henry data, volatile oil reservoir, C1 cycling

Cycle C1 at 4000-4150 psia, radial geometry

pressure was set 150 psi higher than the producing cell pressure to maintain the average reservoir pressure. Cell permeabilities were set at 5 darcies to minimize pressure differences between the cells. Some scatter in the data is evident- primarily because it is difficult to hold the pressure constant in all of the cells. In general the correlation is excellent.

Many projects cycle gas in three dimensional problems under conditions where pressure is highly nonuniform. Consequently, it was necessary to show in the compositional simulator that the one dimensional correlation to Y_{inj} at constant pressure could yield accurate interpolations in a two and three dimensional reservoir problems with variable pressure. The radial geometry shown above was chosen, the cell permeabilities were reduced to one millidarcy, and the injection/producing cell pressures were set to 3500 and 2000 psi respectively.

The results of this test are shown in Figure 7. The solid lines in Figure 7 represent K value fits versus Y_{inj} at various constant pressures. These lines were obtained in a manner similar to that described above for Figures 5 and 6. The radial geometry described above was modified by placing an injector in the first cell. Next a variable pressure process was created - C1 was injected at a rate lower than the producing rate. The K values in the various cells changed with time as pressure decreased and Y_{inj} increased. The point by point data in Figure 7 shows the K value/ Y_{inj} combination in cells 4,10 and 12 at pressures corresponding to the line pressures. These points were

Figure 7 - K values versus Y_{inj} for variable pressure paths in compositional simulator

obtained by using a fully compositional simulator for the variable pressure data. The points fall close to the lines, confirming that 3-D pvt table lookup for a set of 2-D K values generated at variable Y_{inj} and constant pressure is accurate. Recall that the PVT behavior is independent of cell position because the compositional path remains unchanged. Figure 7 illustrates that interpolation between the known compositional paths at various pressure in two dimensional space can be extended to three dimensional space with pressure as the added variable.

4.2 Third SPE Comparative Solution Project - comparing the simplified model to COMP3 for gas cycling in a retrograde condensate reservoir

The preliminary studies in the previous section suggested that the modified compositional simulator method described in Chapter 3 looked very promising. The next step required building a pvt package to calculate the Y_{inj} correlation. The Third SPE Comparative Solution project ²³ was chosen as the first test case. The problem description is given in Appendix 2. This problem cycles a lean gas in a retrograde gas condensate reservoir. A 9 by 9 grid with 4 layers is used. Gas is injected in corner block (1,1) in the top two layers, and oil is produced from block (7,7) in the bottom two layers. The producing well makes gas at a constant rate of 1500 MCF per day, and the injection well pressure is fixed at 4000 psi. The original gas mixture has a dew point of 3443 psi and an original condensate yield equal to 160 BBL oil per MMCF gas. The PVT behavior is

described by C1 to C5 fractions and a C6 plus fraction to approximate the remaining components. Reservoir horizontal permeability was 130, 40, 20, and 150 millidarcies in the four respective layers, and vertical permeability was set to ten percent of these values.

Figures 8 to 12 show the Y_{inj} correlations for the various black oil properties and oil/gas molar densities at 2000 psia. Cells 10, 22, and 30 were chosen for comparison purposes. These figures generated from the pvt package show that at 2000 psia the pvt properties are relatively insensitive to Y_{inj} , except at Y_{inj} values greater than approximately 98 percent. For cycling at this pressure the Rvo modification with a black oil formulation would closely approximate the results from a fully compositional simulator. The K values versus Y_{inj} at 2000 psia are presented in Figures 13 and 14. The K values for all of the components are nearly constant and independent of Y_{inj} - reconfirming that the Y_{inj} dependency is minimal.

Figures 15 to 20 show the Y_{inj} correlation at 3000 psia for sample black oil properties and gas molar densities. Figures 8 and 15 show the difference between cycling lean gas at 2000 and 3000 psia on volume fraction liquid versus Y_{inj} plots. The lean gas does not pick up appreciable liquid at 2000 psia, where the volume fraction liquid stays close to 21 percent except at high Y_{inj} values. In contrast Figure 15 shows the lean gas picks up the free oil phase readily at 3000 psia, with less than 2 percent free oil remaining at Y_{inj} equal to 0.80.

FIGURE 8 - CYCLING VOLUME FRACTION LIQUID PLOT
THIRD SPE COMPARATIVE SOLUTION-2000 PSI CYCLING

FIG 9 -CYCLING GAS FORMATION VOLUME FACTOR PLOT
THIRD SPE COMPARATIVE SOLUTION-2000 PSI CYCLING

FIGURE 10 - CYCLING GAS VISCOSITY PLOT
THIRD SPE COMPARATIVE SOLUTION-2000 PSI CYCLING
Gas cycling in retrograde condensate reservoir

FIGURE 11 - CYCLING RV PLOT
 THIRD SPE COMPARATIVE SOLUTION-2000 PSI CYCLING
 Gas cycling in retrograde condensate reservoir

FIGURE 12 - CYCLING GAS DENS
THIRD SPE COMPARATIVE SOLUTION-2000 PSI CYCLING
Gas cycling in retrograde condensate reservoir

FIGURE 13 - CYCLING K VALUE PLOTS
 THIRD SPE COMPARATIVE SOLUTION-2000 PSI CYCLING
 Gas cycling in retrograde condensate reservoir

FIGURE 14 - CYCLING K VALUE PLOTS
THIRD SPE COMPARATIVE SOLUTION-2000 PSI CYCLING
Gas cycling in retrograde condensate reservoir

FIGURE 15 - CYCLING VOLUME FRACTION LIQUID PLOT
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING

Gas cycling in retrograde condensate reservoir

FIG 16 -CYCLING OIL FORMATION VOLUME FACTOR PLOT
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING

FIG 17 -CYCLING GAS FORMATION VOLUME FACTOR PLOT
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING

Gas cycling in retrograde condensate reservoir

FIGURE 18 - CYCLING GAS VISCOSITY PLOT
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING

Gas cycling in retrograde condensate reservoir

FIGURE 19 - CYCLING RV PLOT
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING
Gas cycling in retrograde condensate reservoir

FIGURE 20 - CYCLING GAS DENSITY
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING
Gas cycling in retrograde condensate reservoir

The pvt properties at 3000 psia are strongly dependent on Y_{inj} . To see this compare the Rvo correlation at 2000 psia in Figure 11 to the Rvo correlation at 3000 psia in Figure 19. The Rvo correlation at 2000 psia is insensitive to Y_{inj} , while the Rvo correlation at 3000 psia is strongly dependent on Y_{inj} for mole fractions greater than 40 percent. All of the correlations at 3000 psia in Figures 15 to 20 are close regardless of cell number.

The corresponding K value correlations for several components at 3000 psia are shown in Figures 21 and 22. In contrast to the K value plots at 2000 psia in Figures 13 and 14 the K value plots at 3000 psia show a strong dependency on Y_{inj} .

The pvt test was run at a range of pressures covering the operating pressure range for the reservoir - 1500 to 3500 psi - and the Y_{inj} dependency was correlated at each pressure versus Y_{inj} . The resulting pvt properties are shown in Figures 23 to 32. The pressures cover a range from the original reservoir pressure in the undersaturated region to economic limit of the reservoir in the two phase region.

These pvt properties were entered into the simplified compositional model and compared to the results in the COMP3 compositional simulator. Figure 33 shows the oil saturation distribution at 3650 days in the top layer for the fully compositional simulator with a 6 pseudo component approximation. Figure 34 shows the oil saturation distribution at 3650 days in the top layer for the fully compositional simulator with 12 components and the distribution for the simplified compositional simulator. Six pseudo components were

FIGURE 21 - CYCLING K VALUE PLOTS
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING

Gas cycling in retrograde condensate reservoir

FIGURE 22 - CYCLING K VALUE PLOTS
THIRD SPE COMPARATIVE SOLUTION-3000 PSI CYCLING
Gas cycling in retrograde condensate reservoir

FIG 23 -CYCLING OIL FORMATION VOLUME FACTOR PLOT
THIRD SPE COMPARATIVE SOLUTION

FIG 24 -CYCLING OIL FORMATION VOLUME FACTOR PLOT
THIRD SPE COMPARATIVE SOLUTION

FIG 25 -CYCLING GAS FORMATION VOLUME FACTOR PLOT
THIRD SPE COMPARATIVE SOLUTION

FIGURE 26 - CYCLING GAS VISCOSITY PLOT
THIRD SPE COMPARATIVE SOLUTION

FIGURE 27 - CYCLING RV PLOT
THIRD SPE COMPARATIVE SOLUTION

FIGURE 28 - CYCLING OIL DENS
THIRD SPE COMPARATIVE SOLUTION

FIGURE 29 - CYCLING GAS DENSITY
THIRD SPE COMPARATIVE SOLUTION

FIG 30 -CYCLING OIL FORMATION VOLUME FACTOR PLOT
THIRD SPE COMPARATIVE SOLUTION

FIGURE 31 - CYCLING GAS VISCOSITY PLOT
THIRD SPE COMPARATIVE SOLUTION

FIGURE 32 - CYCLING RV PLOT
THIRD SPE COMPARATIVE SOLUTION

Figure 33: compositional model oil saturation distribution at 3650 days

Figure 34 - COMP3 model oil saturation distribution at 3650 days

12 pseudo components

Third SPE Comparative Solution Project - top layer

Simplified compositional model oil saturation distribution at 3650 days

6 pseudo components

Third SPE Comparative Solution Project - top layer

used in the simplified model pvt package to generate the model pvt data as indicated in the figure. The simplified compositional simulator gives a reasonable saturation profile.

Figures 35 to 38 show the oil saturation profile comparisons for the second, third and fourth layers at 3650 days. Agreement is reasonable, although some differences are evident. These differences are in part created by vertical movement of fluids. Recall that the unique compositional path is only guaranteed in one dimensional problems.

Part of the error seen in comparing the compositional and simplified compositional runs is no doubt due to the treatment of some of the variables. For example the simplified compositional model linearizes the relative permeabilities over a timestep, that is to say that if inner iteration are made the slope of the relative permeability curve remains fixed. This approximation minimizes material balance errors by guaranteeing that the relative permeabilities are linear. Most of the compositional formulations update the relative permeability slopes for multiple inner iterations (multiple iterations with the same time step size to minimize the residual term), and as a result the two models will never exactly match. This problem becomes worse if large volumes of gas move vertically, because small relative permeability errors are multiplied by the large gas volumes.

A six pseudo component mixture was created and regressed using the known dew point and constant composition expansion data. The fully compositional model was rerun, and Figure 37 compares the oil saturation profile in the second layer at 3650 days for the six

and twelve component fully compositional cases. The results are shown in Figure 37 show larger differences than the differences in Figure 36 between the 6 component compositional model and the simplified model. Infact comparing both the simplified model and the 6 pseudo component compositional model to the 12 component compositional model shows a closer fit for the simplified model. We cannot infer that the simplified model will in general be better than a pseudoized fully compositional model, but for many problems the errors introduced by these two simplifications of the the original compositional model may be comparable. Most compositional simulations require a 3-5 pseudo component simplification of the original mixture components to minimize cpu times.

Figure 39 shows a comparison of oil rates versus time for the three runs. The oil rates for new simplified model fall between the 6 pseudo component and 12 component fully compositional runs. Errors caused by the simplified model are evident, but the resulting pseudoized run is no more accurate than the simplified pseudoized compositional model. These errors are caused because fluids move vertically, and the compositional path independent of cell position is only guaranteed in a one dimensional problem. It can be argued than more pseudo components are necessary, but as the pseudo component count increases towards the original component count the cpu time advantage for pseudoization is also minimized. Simulation time per timestep is proportional to the number of components squared. For example, the solver for a nine component system will have approximately nine times the CPU time of a three component system because $9^2/3^2 = 9$.

Figure 39- gas cycling of retrograde condensate reservoirs

Third SPE Comparative Solution Project - case 1

Recall that our simplified model has 4 variables and would be approximately $9^2/4^2$ or 5 times faster. This time is only for the solver in the simulator, and in addition equation of state phase change calculations and costlier jacobian building in the preprocessor are required for the compositional simulator.

4.3 CO₂ Cycling in a Single Layer Case for a Normal Black Oil Reservoir - simplified compositional model versus fully compositional model

The success of the simplified model in representing lean gas cycling for a retrograde condensate reservoir encouraged me to try to extend the theory to a CO₂ cycling process in a normal oil reservoir. It was decided to test the simplified compositional model on data for an actual large scale CO₂ flood that Texaco started in the early 1980's in Paradis Louisiana. Fully compositional runs were already in place for comparison purposes, and a full suite of reservoir data was available.

The Paradis reservoir is a clean sand with 26 degrees API oil gravity, a reservoir temperature equal to 193 F, and 1090 scf/stb GOR at an original bubble point pressure equal to 3950 psia. Primary recovery was estimated to be 20% from a partial water drive. CO₂ was injected at the top of the reservoir, and simulation showed that a gravity stable CO₂/oil bank formed and gradually swept downdip towards the producing wells. Laboratory slim tube experiments established that at a flooding pressure of 3500 psia

CO₂ and oil were partially miscible as illustrated on the ternary diagram in the theory section. The CO₂ rich oil bank that forms was predicted to sweep the remaining oil in the reservoir to less than 10 percent oil saturation.

A one dimensional pvt cell arrangement as described in the theory section was used to generate the pvt data. Sixteen equal volume cells were placed in the pvt model, and 0.3 cell volumes CO₂ (30 % of the volume in one cell) were injected at each step of the test. The injection gas composition was 91 mole percent CO₂ and 9 mole percent nitrogen.

Figures 40 to 47 show the black oil properties and gas/oil molar density correlations at 4500 psia. Figure 40 shows the volume fraction liquid versus gas fraction CO₂ in the injection gas at 4500 psia. A CO₂/oil bank forms and sweeps through the reservoir to approximately 20 percent oil saturation at the 0.55 Y_{inj} value. After this point a CO₂ rich gas phase continues to sweep the remaining oil to approximately the 9 percent oil saturation, after which heavy ends remain and vaporization is negligible.

Figures 41, 43 and 45 give a clear picture of the CO₂ partitioning during the flood. The CO₂ first contacts the cells and swells the oil phase. The oil formation volume factor and gas oil ratio in Figures 41 and 43 both increase. The condensate yield R_{vo} in Figure 45 remains nearly constant until the CO₂/oil bank passes through the cells, and then the condensate yield drops and the oil density increases.

FIGURE 40 - CYCLING VOLUME FRACTION LIQUID PLOT
CO₂ CYCLING IN OIL RESERVOIR

FIG 41 - CYCLING OIL FORMATION VOLUME FACTOR PLOT
CO₂ CYCLING IN OIL RESERVOIR

FIGURE 42 - CYCLING GAS DENSITY
THIRD SPE COMPARATIVE SOLUTION

FIGURE 43 - CYCLING GAS OIL RATIO PLOT
CO₂ CYCLING IN OIL RESERVOIR

FIG 44--CYCLING GAS FORMATION VOLUME FACTOR PLOT
CO2 CYCLING IN OIL RESERVOIR

FIGURE 45 - CYCLING RV PLOT
CO₂ CYCLING IN OIL RESERVOIR

FIGURE 46 - CYCLING OIL DENSITY
CO2 CYCLING IN OIL RESERVOIR

FIGURE 47 - CYCLING GAS DENSITY
CO₂ CYCLING IN OIL RESERVOIR

The K values for the individual components are shown in Figures 48 to 50. The K values for the lighter components- specifically CO₂ in Figure 48, and C₁ in Figure 49 remain nearly constant and then increase at Y_{inj} values greater than 0.5 reflecting that these components are less soluble in the oil phase at higher oil densities. Recall that Mott¹¹ assumed that K_{inj} is constant, and this is not the case in Figure 48. Figures 49 and 50 show the K value trends for the intermediate and heavy end components. These components vaporize easily at low Y_{inj} values, but the vaporization rates drop as the oil density increases.

The theory section discusses an alternative approach to the fully compositional model using a modified black oil model proposed by R.Cook et al ⁸ with cumulative pore volumes injected gas (CGI) as the correlating parameter. Figures 51, 52, and 53 show the oil formation volume factor, gas oil ratio, and condensate yield correlations to Y_{inj} for the Paradis CO₂ flood data at 4500 psia. Comparisons can be made to the Y_{inj} correlated data for these parameters in Figures 41, 43, and 45. For example the spread in the data between cells 4 and 10 at Y_{inj} equal to 0.5 is 50 stb/mmcf for the CGI correlation, and 5 stb/mmcf for the Y_{inj} correlation. The Cook correlation is in serious error, and has little hope of accurately representing the CO₂/oil vaporization process.

An additional check of the correlation at 4500 psia was accomplished by plotting pvt for cells 12 and 16 as shown in Figures 54 to 56. The pvt converges as the cell count increases. In comparison the Cook correlation to CGI for cells 12 and 16 shown in

FIGURE 48 - CYCLING K VALUE PLOTS
CO2 CYCLING IN OIL RESERVOIR

FIGURE 49 - CYCLING K VALUE PLOTS
CO₂ CYCLING IN OIL RESERVOIR

FIGURE 50 - CYCLING K VALUE PLOTS
C02 CYCLING IN OIL RESERVOIR

FIG 51 --CYCLING OIL FORMATION VOLUME FACTOR PLOT
CO2 CYCLING IN OIL RESERVOIR

FIGURE 52 - CYCLING GAS OIL RATIO PLOT
CO₂ CYCLING IN OIL RESERVOIR
4500 PSI CYCLING - COOK CORRELATION

FIGURE 53 - CYCLING RV PLOT
CO2 CYCLING IN OIL RESERVOIR

FIG 54--CYCLING OIL FORMATION VOLUME FACTOR PLOT
CO2 CYCLING IN OIL RESERVOIR

FIGURE 55 - CYCLING GAS OIL RATIO PLOT
C02 CYCLING IN OIL RESERVOIR

FIGURE 56 - CYCLING RV PLOT
CO2 CYCLING IN OIL RESERVOIRS

Figures 57 and 58 have a poor fit.

The Yinj correlation for sample black oil pvt properties at 3500 psia is shown in Figures 60 to 63. This pressure is slightly below the original bubble point of the reservoir at 3950 psia. Nevertheless, a partially miscible oil bank still forms in Figure 64 and vaporization eventually reduces the residual oil saturation to 10 percent.

The Cook CGI correlation for CO₂ cycling at 3500 psia is shown in Figures 65 and 66. The correlation to CGI has very noticeable errors at 3500 psia.

The CO₂ cycling tests described above were repeated for a range of pressures covering the operating pressure range for the CO₂ flood. Data were generated for pressures from 2000 to 4500 psia in 500 psia increments and then used in 3-D table lookup in the simplified model. The property correlations for each of these pressures is presented in Figures 67 to 74.

Figures 67 to 74 show pvt trends that match our intuitive thoughts - at higher pressures CO₂ is more miscible in the oil phase and vaporizes the oil components more easily.

Several interesting observations can be made in Figure 72- the R_{vo} correlation. At higher pressures the Yinj dependency is critical, but at lower pressures the Yinj dependency is less important. This is not true for some of the other pvt properties, for example the RSO

FIG 57-CYCLING OIL FORMATION VOLUME FACTOR PLOT
CO₂ CYCLING IN OIL RESERVOIR
4500 PSI CYCLING , COOK CORRELATION

FIGURE 58 - CYCLING RV PLOT
CO₂ CYCLING IN OIL RESERVOIR
4500 PSI CYCLING . COOK CORRELATION

FIGURE 59 - CYCLING VOLUME FRACTION LIQUID PLOT
C02 CYCLING IN OIL RESERVOIR

FIG 60-CYCLING OIL FORMATION VOLUME FACTOR PLOT
CO2 CYCLING IN OIL RESERVOIR

FIGURE 61 - CYCLING GAS OIL RATIO PLOT
CO₂ CYCLING IN OIL RESERVOIR

FIGURE 62 - CYCLING RV PLOT
CO2 CYCLING IN OIL RESERVOIR

FIG 63 -CYCLING OIL FORMATION VOL. FACTOR PLOT
CO2 CYCLING IN OIL RESERVOIR
3500 PSI CYCLING . COOK CORRELATION

FIGURE 64 -CYCLING OIL FORM. VOLUME FACTOR PLOT
CONSTANT PRESSURE CURVES , CO2 CYCLING

FIGURE 65 - CYCLING GAS OIL RATIO PLOT
CO₂ CYCLING IN OIL RESERVOIR

FIGURE 66 - CYCLING RV PLOT
CO2 CYCLING IN OIL RESERVOIR

FIGURE 68 - CYCLING OIL VISCOSITY PLOT
CONSTANT PRESSURE CURVES , CO2 CYCLING

FIGURE 69 - CYCLING GAS OIL RATIO PLOT
CONSTANT PRESSURE CURVES - CO₂ CYCLING

FIGURE 70 -CYCLING GAS FORM. VOLUME FACTOR PLOT
CONSTANT PRESSURE CURVES - CO2 CYCLING

FIGURE 71 - CYCLING GAS VISCOSITY PLOT
CONSTANT PRESSURE CURVES - CO2 CYCLING

FIGURE 72 - CYCLING RV PLOT
CONSTANT PRESSURE CURVES - CO2 CYCLING

FIGURE 73 - CYCLING OIL DENSITY
CONSTANT PRESSURE CURVES -CO2 CYCLING

FIGURE 74 - CYCLING GAS DENSITY
CONSTANT PRESSURE CURVES - CO2 CYCLING

correlation in Figure 69. Nevertheless, at lower pressures the CO₂ becomes less miscible and Yinj dependency smaller. At sufficiently low pressures the Yinj dependency would be negligible- unfortunately these pressures are too low to be practical if appreciable oil recovery is expected.

The 3-D pvt tables were next included in the simplified compositional model, and comparisons were made to the fully compositional COMP3 simulator.

A simple 2 dimensional grid was chosen for comparison purposes with a 25 cells arranged in a 5 by 5 pattern. The original reservoir pressure of 4400 psi was decreased to 3500 psia by producing oil from a cell at location (5,5,1). When the average reservoir pressure hit the 3500 psia mark CO₂ was injected in cell (1,1,1) to maintain the reservoir pressure at 3500 psia. The production well continued to produce with 3300 psia flowing bottomhole pressure. A flood at this pressure is a multiple contact partially miscible process.

PVT properties for the model were entered from cell 10 in the pvt model. Cell 16 was also tested for sensitivity, and results were very close to the cell 10 data.

The simplified model predicted vaporization of the oil phase in the model cells to saturations below the residual oil saturation realized in the pvt cells. This was due to the rapid CO₂/oil bank movement through the system of cells. The oil solubility in the CO₂

gas phase decreases quickly, and the IMPES formulation can overpredict the oil vaporization during the timestep when the oil bank passes through the cell. An artificial constraint was imposed on the simplified model to fix this problem - all oil phase vaporization at saturations below the residual oil saturation predicted by the pvt tests is prevented. This problem is not unique to the new simplified compositional model; saturations below the residual oil saturation also occurred in the compositional simulator.

Results comparing the simplified compositional model to COMP3 are presented in Figures 75 to 86. Figure 75 shows the gas oil ratio (GOR) versus time match. The new model with pvt based on cell 10 is very close to the compositional results. When the residual oil saturation (SOR) constraint is imposed on the model results are almost identical to the case without the SOR constraint.

Figure 76 shows the mole fraction CO₂ (YCO₂) in the produced cell history comparisons. The simplified model with cell 10 pvt gives an excellent match in comparison to the YCO₂ trend in the compositional model. Adding the SOR constraint did not improve the match. The match for pvt based on cell 16 is also shown, and this fit is very close to the match for pvt based on cell 10.

Figure 77 compares the average reservoir pressure for the various cases. The original reservoir pressure is dropped to 3500 psia, and then CO₂ cycles in the reservoir. The gas oil ratios in the producing well increase rapidly with time, and because CO₂ injection

Figure 15 - Comparing COMP3 to simplified comp. model

CO2 cycling in oil reservoir above minimum miscibility pressure at 3500 psia

Figure 76 - Comparing COMP3 to simplified comp. model

CO2 cycling in oil reservoir above minimum miscibility pressure at 3500 psia

Figure 78 - Comparing COMP3 to simplified comp. model

Figure 79 - Comparing COMP3 to simplified comp. model

Figure 80 - Comparing COMP3 to simplified comp. model

Figure 81 - COMP3 oil saturation profile at 1460 days, 3500 psi cycling

Figure 82 - New model - oil saturation using cell 10 pvt, 1460 days, 3500 psi cycling

COMP3- total mole frac. CO₂ , 1460 days , cell 10 pvt, 3500 psi cycling

Figure 83

New model- total mole frac. CO₂ , 1460 days , cell 10 pvt, 3500 psi cycling

Figure 84

Figure 85 - COMP3 total mole fraction CO₂ at 1460 days, 3500 psi cycling

Figure 86 - New model- total mole fraction CO₂ at 1460 days using cell 10 pvt with sor, 3500 psi cycling

cannot maintain this pace the reservoir pressure decreases to approximately 3200 psia at 2400 days. The match for all cases is very close.

Figure 78 shows the fits for the oil saturations in the corner cell at (5,1,1) as a function of time. The results are remarkably close - reflecting the accuracy of the oil vaporization prediction in the simplified model between the original oil saturation equal to 80 percent and the final oil saturation equal to 33 percent.

Figure 79 shows the oil saturation fit for the producing cell at (5,5,1). Notice that the fit is excellent to approximately 40 percent oil saturation, but the simplified model deviates from the compositional model at lower oil saturations. The residual oil limitation in the model improves the fit, but the oil saturation at 2200 days still deviates from the compositional model by approximately 10 percent.

This error can also be viewed in the pvt plots in Figures 60 to 62. Small deviations in the pvt correlations between cells 4 and 10 are evident for Y_{inj} values greater than 0.70. These errors do not have a fatal result on the model because most of the vaporization curve in these figures is still accurately represented. Interestingly, the pvt plots at 4500 psia in Figures 41 to 47 have a much better fit at high Y_{inj} values. Simulations confirmed that cycling at 4500 psia gave even better agreement than the 3500 psia case.

A more rigorous evaluation of the simplified compositional model was accomplished by

plotting the oil saturation and total mole fraction CO₂ profiles at various times. These results are presented in Figures 81-86 at 1460 days.

The simplified compositional model predicts the profiles to be almost identical to the profiles in the compositional model. The results confirm that the simplified compositional model can accurately reproduce all of the compositional effects in a fully compositional simulator in this case.

4.4 CO₂ Cycling in a Multiple Layer Case for a Normal Black Oil Reservoir - simplified compositional model versus fully compositional model

Multicomponent multiphase flow theory does not guarantee that the CO₂ correlation to mole fraction CO₂ will hold for cases with strong lateral gas flow. The problem discussed above was modified to include 3 layers with the same well conditions. The producer and injector were both placed in the third layer. The alignment of the wells allowed maximum lateral gas flow. Placing the injector in the third layer forced gas to move vertically to the first layer, and placing the producer in the third layer forces gas to eventually cone down to the producing well. Five millidarcy vertical permeability was used to slow the vertical flow of the gas and prevent CO₂ from shooting to the top layer.

The results for this case are presented in Figures 87-90 at 3650 days, and Figure 91 and

Figure 87 - COMP3 total CO₂ mole fract, in top layer, 3 layer case, crossflow

Figure 88. Simplified total CO₂ mole fraction in top layer, 3 layer case with crossf

Figure 89 - COMP3 oil sat. in top layer, 3 layer case, crossflow

3650 days

COMP3 oil saturation in middle layer

COMP3 oil saturation in bottom layer

Figure 90 Simpl. model oil sat. in top layer, 3 layer case, crossflow

3650 days

Oil sat. in middle layer

Oil sat. in bottom layer

92 at 4745 days. Figures 87-88 compare the corresponding total mole fraction CO₂ for the two cases, and Figures 89-90 and 91-92 compare the oil saturation profiles. Agreement is reasonable in all of the figures. Comparing figures 89-90 and 91-92 illustrate as expected that the errors in the simplified model grow as time increases.

Vertical crossflow was maximized for the test case. Simplistically viewing the problem, we may think that a significant fraction of the gas moves vertically within the first few grid blocks, and after this the gas stays into the top layer until it coned down to the production well. In other words, the majority of the gas spends its time in the top layer, and the 3-D problem really became a 2-D problem. This is not the case - the vertical permeability used in this problem was chosen to be a value that limited vertical gas movement and maximized crossflow in all of the grid blocks as seen in the saturation profiles in Figure 89.

Consequently, the correlation is still good for a vertical crossflow case. Further testing in other reservoirs is required to verify the claim for the general problem.

The CPU advantage of the simplified model is proportional to the square of the number of variables. In this case the simplified model has 4 components, oil/gas/water/tracer, and a fully compositional model has 7 components plus water, so the compositional model is approximately $8^2/4^2$ or 4 times slower on the same platform.

Figure 92 · Simpl. model oil sat. in top layer, 3 layer case, crossflow, 4745 days

4.5 CO₂ Cycling in a Two Dimensional Problem with Variable Pressure

The two dimensional CO₂ cycling problem described in section 4.3 was modified to allow cycling in a variable pressure process. The changes included reducing the reservoir permeability from 500 millidarcys to 5 millidarcys to create pressure profiles, setting the injection well pressure to 3400 psi, and setting production at 50 BBLs oil per day. The results are presented in Figures 93-100. Pressure profiles between 2400 and 3400 psi were generated in various cells in the model.

Figures 93 and 94 shows the gas production rate and gas injection rate comparisons between COMP3 and the simplified compositional model. Differences between the two models are evident at times greater than 1095 days. The production wells in both models hit the maximum GOR before 2300 days. Results here have larger errors than Figures 76-80 where the pressure gradients were negligible. This is expected because linear interpolations between the two dimensional compositional pvt tables is only approximate.

Figures 95-100 summarize the pressure, oil saturation, and total mole fraction CO₂ profiles at 1460 and 1825 days respectively. Figure 95 shows the pressure profiles at 1460 days. Cell pressures vary between 2500 and 3400 psia. It is interesting to view the pvt behavior between these pressures. For example in Figure 72 the condensate yield varies from 10 to 60 BBLs oil per MMCF, and the corresponding drive from a partially

Figure 95

Simplified model pressure distribution @ 1460 days, 5x5x1 grid, variable pressure

Comp3 gross pressure distribution @ 1460 days, 5x5x1 grid, variable pressure

Figure 96

Simplified model oil sat @ 1460 days, variable pressure, 5x5x1 grid

COMP3 oil sat @ 1460 days, variable pressure, 5x5x1 grid

Figure 97

COMP3 total frac.CO2@1480 days, variable pressure case, 5x51 grid

Simplified model total frac.CO2@1480 days, variable pressure, 5x51 grid

Figure 98

COMP3 pressure distribution @ 1825 days, variable pressure, 5x5x1 grid

Simplified model pressure distribution @ 1825 days, variable pressure, 5x5x1 grid

Figure 99

COMP3 oil sat @ 1825 days, variable pressure, 5x5x1 grid

Simplified model oil sat @ 1825 days, variable pressure, 5x5x1 grid

Figure 100

COMP3 total frac.CO2@1825 days, variable pressure, 5x5x1 grid

Simplified model total frac.CO2@1825 days, variable pressure, 5x5x1 grid

miscible to a nearly immiscible process.

Figure 96 shows the comparison for the total mole fraction CO₂ at 1460 days, and Figure 97 shows the oil saturation comparison at 1460 days. Both figures show reasonable agreement.

Figures 98-100 show the corresponding pressure, total mole fraction CO₂, and mole fraction oil at 1825 days. Agreement between the fully compositional model and the simplified compositional model is reasonable.

Chapter 5 - Conclusions

A simplified compositional model has been constructed. The model runs at speeds that approach a black oil simulator, but still retains the compositional information necessary to accurately model gas cycling projects. As a result the simplified compositional simulator can use features that are normally only applied in only black oil studies-including an fully implicit formulation, and a nine point option.

The simplified model achieves speed increases by moving the equation of state calculations from the simulator to the preprocessor. In addition the number of unknowns in the simplified model is independent of the number of components in the reservoir fluid. The fully compositional simulator requires linking the equation of state and including a independent equation for each component.

The fully compositional model will still have an important role in compositional simulation. To understand this we should recall the assumptions made in the simplified model. First the pvt data and black oil properties were generated assuming constant separator conditions. Second the injection gas composition must be nearly constant.

The most important assumption is that the dependence of black oil PVT properties and K_{inj} on Y_{inj} and pressure is the same for a two-dimensional or three-dimensional cycling process with variable pressure as for the linear array of cells at various constant

pressures used to develop the PVT correlations. In other words, compositions at each pressure are assumed to lie on the compositional wave generated at that pressure. The results presented above suggest that this assumption may be reasonable under many circumstances. Its validity may be questionable for some reservoirs with strong lateral crossflow, although a lateral crossflow case was tested and found to match reasonably well.

The first two assumptions generally apply. Recycled lean gas composition is often approximately constant over the life of the flood, and separator conditions usually cause only small changes in the pvt properties. Both of these problems can be investigated in the PVT package for the simplified model - different lean gas compositions can be cycled to test the composition effect. The test can be run at different separator conditions to test the second effect.

Summarizing, the new simplified compositional model can provide an important tool for studying cycling processes because it has computing speeds that are a small fraction of the times required for current compositional simulation. The pvt package linked to the compositional model has the ability to generate accurate sets of two dimensional PVT tables dependent on both pressure and composition, allowing interpolation with respect to pressure and composition.

NOMENCLATURE

B_o, B_w, B_g = oil/water/gas formation vol.factors

C_{rock} = rock compressibility

D_t = time step

E_L = elevation

F = fugacity

F_M = moles per unit volume

G/g = gas subscript

K = relative permeability

K_l = mole fraction ratio, gas/oil

L = liquid mole fraction

NC = number of components

O/o = oil subscript

P = pressure

PC = capillary pressure

R_{so} = gas oil ratio, scf gas/stb oil

R_{vo} = dissolved oil gas ratio, bbls oil/mmcf gas

S = saturation

T = transmissibility

t = time

V = vapor mole fraction

V_p = pore volume

W = moles water per unit volume

X = mole fraction liquid phase

Y = mole fraction gas phase

Z = overall mole fraction

Z_L, Z_g = liquid, gas deviation factors

RHS = constant term

ρ = density

δ = derivative

δ_{ij} = binary interaction coefficient i, j components

μ = viscosity

θ = porosity

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Appendix 1 - Henry data¹⁰

Comp.	Mol Weight	Critical Temp	Specific Gravity	Acentric Factor	Mole Fraction	Inj. Gas Mol Fraction	Critical Pressure
Methane					.5645	0.94327	
CO2					.01025	0.00721	
Ethane					0.06396	0.04500	
Propane					0.04195	0.00369	
Butane					0.01774	0.00031	
Pentane					0.02947	0.00052	
Hexane	88	900	0.66714	0.290	0.01444	0.0	450
Heptanes	97	958	0.70630	0.325	0.01542	0.0	445
Residue	252	1340	0.83468	0.710	0.24227	0.0	225

Reservoir Grid data

NX=NY = 9, NZ=4
 DX=DY = 293 ft.
 Porosity = 0.13
 Datum = 7500 ft.
 Pg = Po = 3550 psi @ 7500 ft

Layer	Horiz. Perm. md	Vert. Perm. md	Thickness ft.	Depth to center , ft.
1	130	14	30	7330
2	40	4	30	7360
3	20	2	50	7400
4	150	15	50	7450

Saturation Data :

Phase Sat.	Krg	Kro	Krw	Pcgw
0.04	0.005	0	0	50
0.08	0.013	0	0	50
0.16	0.04	0	0	50
0.20	0.058	0	0.002	32
0.28	0.10	0.005	0.020	15.5
0.40	0.187	0.04	0.066	7.0
0.60	0.40	0.196	0.227	2.1
0.72	0.562	0.40	0.390	1.0
0.84	0.740	0.800	0.62	0.5

Production Well Data :

Location , I=J=7
 Perforation, K=3,4
 Rate, 1500Mcf/d
 Min Fbhp = 500 psi

Injection Well Data :

Location , I=J=1
 Perforations, K=1,2
 Rate, 4000 psi injection pressure

Hydrocarbon make up in injection gas :

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Component	Mole Percent
Methane	65.99
Ethane	8.69
Propane	5.91
Butane	5.01
Pentane	2.69
Hexane	1.44
Heptane	1.50
Octane	1.05
Nonanes +	7.72