

Trends in Modeling Reservoir Fluids

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1. SIMPLIFIED PVT FORMULATIONS

The petroleum industry has historically used simple PVT models to describe phase and volumetric behavior of reservoir fluids. Most engineering calculations, all the way from the reservoir to the wellhead, assume the three fluid phases *gas*, *oil*, and *water* are made up of two hydrocarbon "pseudo" components and a water component. Interestingly, the three pseudocomponents are also called *gas*, *oil*, and *water*! These pseudocomponents are surface products resulting from a simple two- or three-stage separation process.

Some reservoir engineering problems such as gas injection (to increase oil recovery) require more complicated PVT models. These models treat the main components in reservoir fluids as individual compounds (N_2 , CO_2 , H_2S , C_1 , C_2 , C_3 , iC_4 , nC_4 , iC_5 , C_5 , and C_{6s}), and heptanes-plus as a number of fractions. Equilibrium calculations are made using K-values that are known as a function of pressure, temperature, and composition (through the convergence pressure).

Simplified PVT models are still widely used in reservoir and production engineering. These models are used mainly because (1) they are well understood, (2) they are often accurate enough for engineering design, (3) the PVT properties used by these simple models are readily measured or easily estimated, and (4) they are computed fast (particularly important in simulators where reservoirs may be discretized into hundreds of thousands of grid cells).

1.1. Water Treatment (*Salinity and Solubility, that's about it*)

In many petroleum engineering applications we only treat hydrocarbon PVT behavior, neglecting the water component and water phase. When water is considered, the most common assumption is that the water component does not partition in either the gas or the oil phase, and that neither gas or oil pseudocomponents partition in the water phase. We sometimes assume that the gas pseudocomponent partitions in the water phase, with a resulting (minor) effect on water phase volumetric properties. Production engineering calculations may require the estimation of water content in produced gas for hydrate predictions and vertical lift pressure loss calculations.

Reservoir water is almost always saline, consisting mainly of NaCl, in concentrations from a few thousand ppm to more than 300,000 ppm. Water salinity has profound effect on mutual gas & water solubilities. Water chemistry also plays an important role in production operations, where scaling and related production problems are often correlated with reservoir brine and/or injected water composition.

1.2. Traditional Black-Oil Model (*Black Magic*)

The bread-and-butter PVT model used in petroleum engineering is based on the simple assumption that pseudocomponent gas can partition in both oil and gas phases, while pseudocomponent oil partitions only in the oil phase. The amount of pseudocomponent gas that can partition (dissolve) in the oil phase is a monotonically increasing function of pressure.

This model implies that reservoir gas is "lean" or "dry", containing no condensible liquid hydrocarbons. The reservoir gas does not exhibit retrograde condensation or revaporization as pressure drops in the reservoir (at a constant temperature). Neither does produced reservoir gas yield HC liquid (stock-tank oil or "condensate") at surface conditions. The reservoir gas phase consists only of the pseudocomponent gas.

Some basic definitions are needed to set the discussion of black-oil PVT models:

V_o	volume of oil <i>phase</i> at pressure and temperature
V_{oo}	volume of (surface) oil <i>pseudocomponent</i> produced from oil phase
V_{go}	volume of (surface) gas <i>pseudocomponent</i> produced from oil phase
V_g^g	volume of gas <i>phase</i> at pressure and temperature
V_{gg}	volume of (surface) gas <i>pseudocomponent</i> produced from gas phase
V_{og}	volume of (surface) oil <i>pseudocomponent</i> produced from gas phase

Note that $V_{og}=0$ in the traditional black-oil model. Partitioning of gas and oil pseudocomponents in the oil phase is defined by a *solution gas-oil ratio* (GOR) $R_s=V_{go}/V_{oo}$.

The black-oil model assumes pseudocomponents oil and gas have constant physical properties (e.g. specific gravities) that do not vary during depletion of the reservoir. Phase densities are calculated from *formation volume factors* (FVF) B_o and B_g , defined as the ratio of phase volume to product volume, $B_g=V_g/V_{gg}$ and $B_o=V_o/V_{oo}$. FVFs are functions of both pressure and temperature.

It has been found that the traditional black-oil PVT formulation is quite accurate for reservoir oils with initial solution GORs less than about $100 \text{ m}^3/\text{m}^3$, and adequate for GORs up to $150 \text{ m}^3/\text{m}^3$. This model can not be used for gas condensates because of the assumption that reservoir gas contains no condensible liquids ($V_{og}=0$).

1.3. Modified Black-Oil Models (*Better than Black Magic*)

A modification of the traditional black-oil model was proposed in 1973 for gas condensates, {Spivak, 1973 #593} where the oil pseudocomponent was allowed to partition in the reservoir gas phase ($V_{og}>0$). The *solution oil-gas ratio* (OGR), $r_s=V_{og}/V_{gg}$, defines pseudocomponent partitioning in the gas phase. Solution OGR is a function of pressure, with $dr_s/dp>0$ indicating retrograde condensation, and $dr_s/dp<0$ indicating revaporization (at lower pressures). The gas FVF is defined as $B_{gd}=V_g/V_{gg}$ to account for the fact that not all of the reservoir gas remains as a gas after surface separation.

The modified black-oil PVT formulation also proved to be important in describing volatile oil systems ($R_s>150 \text{ m}^3/\text{m}^3$). It was already documented {Cook, 1951 #374} in the 1950s that saturated reservoir gas coming out of solution from high-bubblepoint oils (>300 bar) contained significant amounts of condensible liquids. However, not until the mid-1970s did reservoir simulators include the solution OGR term r_s . For some volatile oil systems, the oil recovery calculated using the modified black-oil PVT formulation is more than twice the oil recovery based on the traditional black-oil PVT formulation.

Historically the modified black-oil model was not used because PVT laboratory studies did not provide r_s and B_{gd} data (particularly for volatile oil systems). Today, however, EOS models that have been tuned to match experimental PVT data are used routinely to simulate depletion PVT experiments, {Whitson, 1983 #504; Coats, 1985 #452} automatically generating the four pressure-dependent modified black-oil PVT properties R_s , B_o , r_s , and B_{gd} .

A further development of the modified black-oil model was proposed by Cook et al., {Cook, 1974 #537} where a new PVT variable G_i was introduced for quantifying the effect of vaporization by lean injection gas (separator gas, nitrogen, etc.). The G_i parameter is basically the amount of injection gas that has entered a given volume of a reservoir (e.g. a grid cell). Saturated PVT properties are modified as a function of G_i , where for increasing values of G_i the oil phase becomes less volatile (lower R_s and B_o) and the gas phase becomes leaner (lower r_s). In a reservoir simulator, the G_i variable is tracked in each grid cell.

Practically, the G_i parameter results in PVT behavior that corresponds to splitting the oil pseudocomponent into many fractions. Oil vaporization (stripping) can be modeled accurately with this approach. The G_i model's drawback is not being able to describe the advantageous near-miscible and miscible phase behavior that develops (at the gas front) in lean-gas vaporizing processes operating at higher pressures (>350 bar).

1.4. Tie-Line Models (*Sophisticated Black Magic*)

A few tie-line PVT models have been proposed, {Tang, 1993 #1580} where three or four pseudocomponents are allowed to partition in the oil and gas phases. These PVT models are not widely used, and it doesn't appear that they will out-compete the simpler two- and three-pseudocomponent black-oil models, or the more-rigorous EOS models which have been developed with as few as four pseudocomponents.

1.5. K-value Models (*OK, but no longer needed*)

The first fully compositional PVT treatment of reservoir fluids used simple K-value models, where K-values ($K_i = y_i/x_i$) were correlated empirically to pressure, temperature, and the composition parameter *convergence pressure*. A simple example of a general K-value equation that exhibits the most important characteristics of K-values for a real system is the modified Wilson equation, {Whitson, 1983 #504}

$$K_i = \left(\frac{p_{ci}}{p_k}\right)^{A-1} \cdot \frac{\exp[5.37 A (1+\omega_i)(1-T_{ri}^{-1})]}{p_{ri}}$$

where A is a function of pressure, with $A=1$ at $p=p_{sc}$ and $A=0$ at $p=p_K$, and an approximate pressure dependence $A=1-(p/p_K)^n$ (with n ranging from 0.5 to 0.8).

In these simple compositional models, VLE calculations are made using K-value correlations, while volumetric properties are computed from an equation of state or empirical correlations. {Standing, 1942 #431; Alani, 1960 #614}

Tabular K-value models are available in some compositional reservoir simulators. The K-value table (only pressure dependent) is generated with an EOS fluid characterization. This approach has certain advantages, and it is easily shown that some reservoir processes are adequately modeled by pressure-dependent K-values. However, generating K-values at pressures greater than the original reservoir fluid saturation pressure may be a problem. One method to extrapolate K-values to higher pressures

(up to the system convergence pressure) is the negative flash. {Whitson, 1989 #330} Another approach would be to inject incipient-phase composition in several stages up to some maximum pressure; unfortunately this method doesn't always result in increasing saturation pressures.

1.6. Needs for the Future *(not much, I think)*

One problem with black-oil PVT models is the calculation of negative total compressibility in some volatile systems. Because these models are not thermodynamically consistent, unphysical behavior can result during reservoir simulation. It would be useful if a rigorous procedure was developed for ensuring physically meaningful results with black-oil PVT models, for all ranges of pressures and gas/oil volume fractions.

Another problem with black-oil PVT models arises when volatile oil and rich gases coexist in a reservoir initially, for example with a saturated gas-oil contact (GOC). The PVT properties generated using reservoir gas are not the same as calculated for the reservoir oil (except at the GOC). One option is to use different PVT tables in the gas cap and in the oil zone. However, the GOC can move (usually downwards) during depletion, in which case the original definition of gas zone and oil zone are no longer valid.

Forecasting compositional production profiles can often be done accurately using black-oil reservoir simulation results. Based only on producing GOR and separator gas & oil compositions, wellstream compositions are readily calculated. Separator compositions are often constant throughout depletion, even for extremely volatile systems. This approach to calculating wellstream production forecasts (for designing process equipment, etc.) could, in many situations, reduce the need for EOS-based compositional reservoir simulation.

2. EQUATION OF STATE MODELS

In the late 1970s and early 1980s cubic equations of state became readily available, providing an important new tool for describing complicated reservoir fluids exhibiting near-critical behavior, strong vaporization, and retrograde condensation.

Cubic equations of state, though relatively simple models, were not readily solved using available numerical techniques. Even when reliable solution algorithms became available in the early 1980s, it took several years before they were implemented efficiently in reservoir simulators.

Another problem using equations of state is the fact that petroleum fluids consist of many hundreds and thousands of heavier components which require quantification using expensive experimental techniques (or mathematical models). It is also necessary to estimate critical properties (used by an EOS) for these heavy fractions.

2.1. Cubic Equations of State *(Simple, Fast, and Accurate)*

Two-Parameter Equations *(Not accurate enough for liquid densities)*

van der Waals started it all in 1873, or thereabouts. $p=RT/(v-b)-a/v^2$. Simple, and relatively accurate. Petroleum engineers have used this equation for 35 years, as proposed by Alani & Kennedy {Alani, 1960 #614} for calculating oil density.

The Redlich-Kwong equation came in 1949. Still simple, and even more accurate. $p=RT/(v-b)-a/v(v+b)$, with constant a being temperature dependent. Petroleum engineers, as with most of the chemical

industry, started using this equation in 1972 when Soave{Soave, 1972 #170} introduced the simple and accurate temperature-correction term for the a constant, $\alpha=[1+m(1-\sqrt{T_r})]^2$, with m being a function of acentric factor. Several oil companies use the Zudkevitch and Joffe{Zudkevitch, 1970 #115} modification of Redlich and Kwong's EOS; the ZJRK equation is significantly better than the SRK equation for liquid density prediction, but at the expense of simplicity.

Peng and Robinson{Peng, 1976 #246} made their enclave in petroleum engineering after a publication by Katz and Firoozabadi{Katz, 1978 #395} in 1978. The PR equation is the most widely used for modeling reservoir fluids. Why? Well, habit (and a bit of prejudice) are probably the only good reasons for choosing the PR over the SRK equation. The SRK equation is probably somewhat better for VLE calculations, and the PR equation better for liquid volumetrics. With volume translation however, the two equations are practically equivalent in all PVT predictions.

Volume Translation (A God-send!)

The novelty of volume translation{Peneloux, 1982 #359} (VT) is (1) its simplicity, $v_{L,corrected}=v_{L,EOS}-\sum x_i c_i$ for the liquid phase and $v_{V,corrected}=v_{V,EOS}-\sum y_i c_i$ for the vapor phase, and (2) the fact that it does not affect VLE results from the original EOS to which VT is being applied. The VT parameters c_i are readily determined by force fitting a key liquid density for each component (e.g. specific gravity or saturated liquid density at $T_r=0.7$), or c_i can be considered as a function of temperature to fit, for example, all saturated liquid densities at $T_r<1$.

If Peneloux and coworkers had only published volume translation ten years earlier (in 1972), at the same time Soave gave us his modification of the Redlich-Kwong EOS, we would never have had to suffer the onslaught of two- and three-constant cubic competitors (Peng-Robinson inclusive!). No one has, and no one probably ever will be able to show that any two- or three-constant cubic EOS consistently outperforms the SRK with VT. On the other hand, the PR equation with VT gives practically identical results to the SRK equation with VT.

Luckily, none of the post-VT three-parameter cubic equations have caught on for modeling reservoir fluids. They don't offer any real advantage. Period. Perhaps the only (somewhat) useful development in cubic equations of state during the past 25 years, other than Soave and Peneloux's improvement of the Redlich-Kwong equation, has been the proposal of "generic" cubic forms.{Martin, 1979 #358; Abbott, 1979 #608} These equations readily reduce to the industry standard two-constant (SRK and PR) equations by specification of numerical constants, thereby saving unnecessary lines of computer code.

Non-Cubic Equations (Only if fast, and measurably better than cubics)

Interestingly, the first EOS used for modeling reservoir fluids was presented by Starling{Starling, 1966 #244} in 1966. The Starling modified BWR equation did not catch on, mainly because it was computationally slower than cubic equations, and partly because this work came too early. EOS-based compositional simulation was not practical until the late 1970s and early 1980s, even using simple cubic equations. More complicated EOS models would have brought these early simulators to their knees.

Today, the speed of inexpensive computers is fast enough to handle a somewhat more complicated EOS model. However, it would only appear that a significant improvement in property predictions could justify a more complicated EOS model. For reservoir fluids, it is still not clear what is actually wagging the dog's tail: inaccuracies in the EOS model, or inability to describe the EOS parameters (and distribution) of heptanes-plus fractions. Even a significant improvement in the EOS model may be rendered useless without methods to accurately define the EOS parameters for undefined plus fractions.

Cubic equations have proven successful in modeling very complex phase and volumetric behavior of reservoir fluids (near-critical phenomena, retrograde condensation, and vaporization). Perhaps the main unresolved problem with cubic equations is accurate prediction of all of these phenomena simultaneously (e.g. during the development of multicontact miscibility).

2.2. EOS Solution Algorithms (*M.L. Michelsen*)

Michelsen{Michelsen, 1980 #1575; Michelsen, 1982 #326; Michelsen, 1982 #327; Michelsen, 1984 #1245; Michelsen, 1985 #328; Michelsen, 1986 #1276; Michelsen, 1988 #1576; Michelsen, 1993 #1573; Michelsen, 1994 #1554} has solved the puzzle of equilibrium calculations that caused great confusion (and suffering) by all of those who first tried to implement cubic equations of state for high-pressure reservoir fluids. Using mathematically rigorous and computationally efficient methods, he has solved even the most difficult phase equilibria problems. Others have smoothed the edges or refined his original procedures, but very few (if any) real improvements on Michelsen's analysis and solution algorithms are found in the literature during the past 15 years. Perhaps our only complaint of his work is its rather terse and not-always-obvious development.

Michelsen's contributions to the modeling of reservoir fluids has been particularly important because his algorithms are computationally efficient and robust, even for difficult near-critical systems.

Two-Phase Flash Calculation (*making it fail-safe, and fast*)

The nuts-and-bolts calculation in reservoir simulation and PVT modeling is the two-phase flash calculation. This calculation should never fail. And it should be fast. Michelsen{Michelsen, 1982 #326; Michelsen, 1982 #327} laid the ground rules for making a fail-safe flash calculation. It relies on good initial estimates of the K-values, which he showed were always available from a stability test. Luckily, accurate K-value estimates are often available from "previous" calculations (which saves the cost of a stability test).

GDEM (General Dominant Eigenvalue Method{Crowe, 1975 #606}) promotion to successive substitution has distinct advantages over many of the other acceleration procedures found in the literature, mainly because it accounts for the fact that two eigenvalues tend to dominate "difficult" flash calculations (near-critical and along phase boundaries). A properly coded implementation of GDEM will almost always converge in less than 30 iterations, even very near a critical point. Numerical roundoff needs to be handled properly in the GDEM method (as in any method).

Newton-Raphson solution of the flash calculation is outlined by Michelsen, in a way that results in the equations being symmetric (due to the use of mole numbers instead of mole fractions). Newton methods are notorious for requiring accurate initial guesses, and reliable back-up schemes must always be available to make sure the solution is valid. Ultimately, the back-up routine may turn into an energy minimization solution. Minimization algorithms have not found use in reservoir simulation because they are expensive, without any real advantages.

An interesting extension of the traditional two-phase flash is the negative flash,{Whitson, 1989 #330} where phase mole fractions are allowed to exceed the range 0 to 1. The resulting equilibrium conditions are continuous through the two-phase region, the saturated state, and into the single-phase region. This continuity allows the method to extend the region where K-value estimates can be used in reservoir simulation. For example, Zick{Zick, 1993 #1579} has shown that the negative flash is much faster than phase stability testing in reservoir simulation.

A fool-proof algorithm for solving the Rachford-Rice{Rachford, 1952 #650; Muskat, 1949 #1229} material balance equation has yet to be published. A severe problem of roundoff errors results when solving the Rachford-Rice equation for phase fraction when one of the components is found in an infinitesimal amount, and the K-value of that component is very small or very large. Such an algorithm has been developed,{Zick, 1985 #1227} but unfortunately Mr. Zick hasn't published it yet.

Phase Stability Test (a great security blanket)

One of the keys to Michelsen's treatment of the two-phase flash problem was a procedure to check if a fluid exists as a single phase, or whether the fluid decreases its energy by splitting into two (or more) phases. The idea behind the phase stability test dates back to Gibbs, and interestingly a graphical review of the Gibbs tangent plane criteria was published by Baker and Luks{Baker, 1982 #616} at the same time Michelsen presented his calculational algorithm for solving the tangent plane stability test.

To reduce the stability test to a level that almost anyone can understand, it basically replaces the equal-fugacity equilibrium condition $f_{Vi}/f_{Li}=1$ (for a two-phase flash) with the condition that $f_{zi}/f_{yi}=S$, where S is a constant (the same for all components), f_{zi} is the fugacity of the feed, and f_{yi} is the fugacity of a test phase. Once a test phase is found that satisfies $f_{zi}/f_{yi}=S$, the constant S determines whether the test phase reduces the energy of the feed. Usually two test phases are searched for in reservoir fluid systems. If either (or both) of the test phases define the feed as "unstable" then a flash calculation is initiated, with initial K-values known from the stability test. If both test phases indicate the feed is "stable" then the fluid can be assumed to exist as a single phase (with 99.99% certainty).

Solving the stability test is relatively time consuming because it can not use initial estimates for test phases without losing reliability. The initial guesses for the test phases should be "poor" guesses, to ensure that a wide range of composition space is searched. The result is a relatively high certainty as to whether the feed is stable or not, but at the expense of solving a relatively tough equilibrium problem (twice!).

As mentioned earlier, the negative flash has been found to provide a reliable and fast alternative to stability testing in reservoir simulation. However, for general EOS modeling of PVT experiments, the stability test still remains the final "litmus" test when a flash calculation converges to a trivial solution ($K_i=1$). Also, the stability test is useful in saturation pressure and multiphase flash calculations.

Saturation Pressure (try and find it, if it exists!)

One of the more important experimental PVT measurements made on reservoir fluids is saturation pressure. Saturation pressures may be measured at several temperatures, from reservoir temperature to as low as 20°C. Saturation pressure may also be measured as a function of injection gas (lean or enriched separator gas, N₂ or CO₂).

Calculation of saturation pressure (or temperature) has been described by Michelsen{Michelsen, 1993 #1573} as one of the most difficult equilibrium calculations, mainly because its existence is not known beforehand. He gives several methods for making the calculation,{Michelsen, 1980 #1575; Michelsen, 1984 #1245; Michelsen, 1985 #328; Michelsen, 1994 #1554} ranging from traces of the entire p-T saturation envelope (safe but slow), to direct methods solving N+1 equations for pressure and incipient phase compositions. The direct calculation methods require a stability test to initiate the calculation, and to keep the pressure estimate within physical bounds.

Phase Envelopes (nice to look at, but not very useful)

The p-T phase envelope tracing algorithms of Michelsen{Michelsen, 1980 #1575; Michelsen, 1984 #1245; Michelsen, 1994 #1554} are relatively fast and safe procedures which can compute through critical

points without problem. A tracing variable (usually the heaviest component $\ln K_i$) is used to eliminate problems associated with tracing saturated states directly in terms of pressure or temperature. The tracing variable is continuous through critical points, and easily correlated with all unknowns (pressure, temperature, and incipient phase compositions).

The phase envelope algorithms can be readily modified to trace other equilibrium lines such as equal-molar fractions, or pressure-composition (p-x) envelopes. The algorithm also has been used for tracing saturated reservoir oil/CO₂ p-x space, including low-temperature three-phase regions. Recently we have looked at using the tracing algorithms for speeding up determination of the gas-oil contact in compositional gradient calculations.

Critical Points (*as fast as a two-phase flash!*)

Who would have believed that we would someday be able to compute critical points of complicated reservoir mixtures as fast or faster than doing a two-phase flash? Michelsen provides such an algorithm, [Michelsen, 1984 #1245; Michelsen, 1988 #1576] based on an idea originally proposed by Heidemann and Khalil. [Heidemann, 1980 #1581] This approach reduces the extremely complicated critical point formulations of earlier authors [Peng, 1980 #105; Baker, 1980 #243] to the simple solution of two equations in two unknowns! Though critical points are not usually needed in reservoir fluid calculations, the ability to compute a critical point efficiently may open up for new applications in the future (e.g. a compositionally consistent treatment of relative permeabilities and capillary pressures in reservoir simulation).

Multiphase Calculations (*stability / flash / stability / flash ...*)

Several applications for multiphase flash calculations of reservoir fluids exist. Low-temperature CO₂/oil systems, low-temperature rich HC gas/oil systems, water/hydrocarbon systems, and solid/fluid systems (wax, asphaltene, and hydrate). The approach for multiphase calculations recommended by Michelsen [Michelsen, 1982 #327; Michelsen, 1993 #1573] involves a sequence of stability tests and subsequent flash calculations.

First the system is tested for stability. More than two test phases may be necessary in some multiphase systems. Once a test phase is found resulting in an unstable condition, a flash calculation is made. The resulting system fugacities for equilibrium phases A and B ($f_{Ai}=f_{Bi}=f_{ABi}$) are then known. A new stability test is conducted on the current system equilibrium (i.e. f_{ABi}). If a new test phase is found that makes this equilibrium condition unstable ($f_{ABi}/f_{yi}=S$) then a multiphase (three-phase) flash is made. A new stability test is made on the resulting equilibrium conditions ($f''_{Ai}=f''_{Bi}=f''_{Ci}=f''_{ABCi}$). This testing procedure is repeated until a test phase can not be found that makes the current multiphase equilibrium condition unstable.

The key to this procedure is locating new test phases that make the current equilibrium system unstable. Some knowledge of the physical system helps, and in the case of low-temperature CO₂/oil or water/hydrocarbon systems, we have an excellent idea of what the test phase(s) look like.

Numerical roundoff errors can pose a serious problem when solving the Rachford-Rice material balance equations for multiphase systems. This problem is caused by near-zero partitioning of some components in some phases; this problem has yet to be solved adequately.

2.3. Heptanes-Plus Characterization

Experimental Methods (*TBP/GC/SIMDIS - costly but necessary*)

The heptanes-plus fraction in a reservoir fluid can make up more than 50% (by mass) of the total mixture. Even small C_{7+} quantities can have a profound effect of gas condensate systems. The amount of C_{7+} in a reservoir fluid usually dictates whether it is an "oil" or "gas" at reservoir conditions. Mixtures with less than about 10 mol-% C_{7+} are usually gases (with retrograde behavior), mixtures with more than 15 mol-% C_{7+} are oils, and mixtures with 10-15 mol-% C_{7+} are typically near-critical.

The C_{7+} molecular weight and specific gravity are always available, but unfortunately these may be the *only* data available for describing what is in fact a mixture of hundreds or thousands of heavy components. Experimental procedures for quantifying single carbon-number (SCN) fractions up to C_{30+} (and heavier) are available and now offered as a routine analysis by most PVT laboratories. Simulated distillation (SIMDIS) by gas chromatography (GC) is less expensive than true boiling point (TBP) distillation. GC analysis provides mass and mole fractions of SCN fractions, and some of the more modern GC methods also determine PNA (paraffin, naphthene, and aromatic) content; PNA data can be used to estimate specific gravity of each SCN fraction, used in property predictions.

It is generally recommended that at least one sample from every isolated reservoir be analyzed by TBP distillation. This is a minimum requirement for process engineering. TBP data can also be useful in developing the EOS characterization for upstream modeling of reservoir fluids. Extended GC analyses of equilibrium samples collected during multicontact gas injection experiments can also be useful when tuning an EOS for miscible{Zick, 1986 #370} (and immiscible{Cook, 1967 #1322}) displacement mechanisms.

Molar Distribution Models (*Exponential & Gamma*)

Mathematical models for describing the distribution of components in the C_{7+} fraction can be useful when measured data are not available. These models can also be fit to measured GC or TBP data.{Whitson, 1983 #503; Whitson, 1990 #508} Molar distribution models allow the heaviest cut (C_{7+} , C_{15+} , C_{21+} , etc.) to be further split into smaller fractions. The three-parameter gamma distribution{Whitson, 1983 #503} has been widely used for describing the heptanes-plus fraction in reservoir fluids. This model simplifies to an exponential distribution, typical of many reservoir fluids, and it has the flexibility to describe very heavy residues that typically have a wider distribution{Brule, 1985 #450} (e.g. log normal).

Properties Estimation (*Bordering on Black Magic*)

An EOS requires molecular weight, critical pressure and temperature, and acentric factor for each component in a mixture. Critical properties and acentric factor of C_{7+} fractions are typically estimated using correlations based on inspection properties (specific gravity and normal boiling point). When inspection properties are not measured, they can be estimated from molecular weight and overall C_{7+} properties (e.g. by assuming similar PNA distribution for each SCN cut).

(Too) many correlations are available for estimating critical properties.{Whitson, 1984 #506} It is unreasonable to expect that any set of correlations will be significantly better than all others for every reservoir fluid. Some correlations are "dangerous" because of unphysical extrapolation for heavier components. The Twu correlations{Twu, 1984 #365} are attractive because of their generality, and supposed ability to predict reasonable properties even for very heavy fractions. The Lee and Kesler correlations{Kesler, 1976 #470} are also widely used.

We have found that the best approach for estimating the properties of C_{7+} fractions is to estimate critical pressure and temperature from a correlation (based on normal boiling point and specific gravity). The EOS is then used, individually for each C_{7+} fraction, to match normal boiling point by adjusting the acentric factor. The volume translation coefficient for each C_{7+} fraction is determined by

fitting the component specific gravity. As mentioned below, using this approach ensures consistency during EOS tuning; normal boiling point is often a primary tuning parameter, due to the uncertainty in its measured value, and because it affects all other properties in a consistent manner (e.g. increasing T_b yields a more paraffinic fraction).

Multiple-Sample Characterization (*For the Sake of Consistency*)

Composition may vary dramatically from the top to the bottom of a reservoir, ranging from a lean gas condensate to a critical mixture to a slightly volatile oil. {Riemens, 1988 #324} Compositional variation is usually due to gravity and/or thermal diffusion (see section 4). Even in the absence of compositional gradients, a reservoir may have a gas cap in equilibrium with an oil (saturated at the GOC). The distribution of C_{7+} fractions in the gas cap will be significantly different than in the oil zone. Average C_{7+} molecular weight, for example, might range from 130 to 250 in the same reservoir.

When developing an EOS fluid characterization in reservoirs with multiple (related) fluids, it is imperative to use a single set of components to describe the fluids throughout the reservoir. The problem is how to determine C_{7+} components, mole fractions and properties that properly describe *all* of the reservoir fluids - consistently. One general method has been proposed for solving this problem, based on application of a modified Gaussian quadrature procedure with the gamma distribution model. {Whitson, 1989 #383} Although this method appears to meet the requirements of characterizing widely varying related fluids, it would seem possible to develop a better and more consistent method for solving the problem (we didn't *really* know what we were doing, mathematically).

2.4. EOS Tuning (*Dangerous, doable, but definitely difficult*)

Modifying EOS Parameters (*A must, but be careful!*)

Even the best (and other good) EOS characterization procedures are *not* good enough for some engineering applications. Predictions of reservoir fluid properties are generally $\pm 2-5\%$ for density and volumetric properties, $\pm 3-10\%$ for saturation pressures, $\pm 5-30\%$ for compositions, and $\pm 10-25\%$ for minimum miscibility pressure and enrichment. To improve the predictions, EOS parameters must be modified. Typically the binary interaction parameters (BIPs) between methane and C_{7+} fractions are modified (unless using the Pedersen et al. {Pedersen, 1989 #1242; Pedersen, 1985 #483} SRK characterization procedures). For the Peng-Robinson EOS, C_1-C_{7+} BIPs are usually positive, and they may be as large as 0.3. Smaller (positive and negative) C_1-C_{7+} BIPs are typical for the SRK EOS.

Other EOS parameters that can be modified include critical properties, acentric factor, and volume translation parameters (for the C_{7+} fractions). We have found it useful to modify the normal boiling point of C_{7+} fractions, which in turn modifies critical properties and acentric factor. Sometimes the EOS constants a & b are modified directly. {Coats, 1986 #362}

Data Quality Control (*Garbage in, garbage out*)

Checking the quality of measured PVT data is an important first-step in EOS tuning. Recommended quality-control methods include graphical plots, material balance calculations, use of empirical property correlations, and comparison with EOS predictions. This last recommendation sounds a bit funny, but the comparison with EOS predictions should give (1) verification of qualitative PVT behavior and (2) identification of "outlier" data.

Material balance calculations can often be made in both directions, starting with a known composition and checking the change in composition during an experiment; else, starting with the final experimental composition(s) and working backwards toward the initial fluid system. Material balance checks in both directions provide useful assessment of compositional data.

Data Selection and Weighting (*Where the shoe hurts*)

Use *all* reliable PVT data from a given reservoir, including as many fluid samples and PVT data as available. The more data, the more difficult to get that "perfect" fit. But, it is very important to cover the largest possible (and practically relevant) range of pressure, temperature, and compositional space where engineering calculations are to be made. This ensures that the EOS model will be interpolating as much as possible, minimizing the need to extrapolate into regions of p-T-x space that may not be adequately modeled.

It has been suggested {Fevang, 1994 #1569} that the samples used in developing an EOS characterization do not necessarily have to be representative of insitu reservoir fluids. It is argued that all fluids produced from a reservoir (unless badly contaminated by oil-based drilling mud) should be as accurately described by the EOS characterization as the insitu reservoir fluids. After all, the produced fluids are equally important (if not more so) than insitu fluids!

A major headache in fitting measured PVT data with an EOS is the specification of weight factors to individual data. I have found the following approach useful. First use unit weight factors for all data. Then look at the contribution of each data to the total sum-of-squares (SSQ) function which is being minimized. Identify individual data that have a particularly large contribution to the total SSQ; reduce the weight factor if the data is not reliable or important (e.g. small concentrations of nitrogen in a low-pressure oil sample). Identify key data that have an unacceptably large deviation, but whose contribution to the SSQ is small; increase the weight factor for such data.

One of the keys to robust EOS tuning is the choice for residuals defining the SSQ function. Sometimes the residual should be a deviation, and sometimes a difference (e.g. data that vary from 0 to 1).

Parameter Selection and Minimization Algorithms (*What do we really need?*)

The philosophy behind choosing regression parameters should be based on the fact that initial parameter estimates are often good, and only minor changes are needed. Seldom, if ever, are initial parameter estimates chosen at random. We should ideally choose parameters that maximize improvement in the SSQ with a minimum change in the parameters. This ensures that parameter changes will have less chance of causing unreasonable predictions in p-T-x space outside the range of data being fit.

Minimizing parameter changes is a major consideration in the minimization algorithm used for EOS tuning. Another important consideration is that the cost of function evaluations is *much much* greater than the cost of operations associated with the non-linear minimization algorithm. These two considerations are quite different than traditionally desired from "optimal" minimization algorithms. This means that the "optimal" minimization algorithm for EOS tuning may look very different from traditional algorithms. We should state clearly our requirements to the experts who develop minimization algorithms, so maybe they'll give us what *we* need (instead of what everybody else needs).

2.5. Pseudoization - Component Reduction (*To reduce reservoir simulation time*)

How Many Components to Use (*Depends of the processes being studied*)

The number of components needed in an EOS characterization may vary from four to thirty-four, depending mostly on the reservoir process being studied. Usually no more than 15 components are needed to describe even the most complicated phase behavior. Sometimes we may want to use more components for a mechanistic study (e.g. studying the effect of test sequence on produced separator samples).

We should begin by developing a "complete" characterization, using as many components as necessary to obtain a desired accuracy. This characterization should then form the basis of comparison (in addition to measured PVT data) for checking the quality of pseudoized characterizations with fewer components.

In general, we should never use more components than necessary. This allows us to use available CPU time to study phenomena other than PVT (e.g. layering and other reservoir heterogeneities using grid refinement). It may be useful to develop several EOS characterizations, each with fewer components. Simulation studies with the different characterizations should reveal differences in reservoir performance, and give guidelines as to how many components are needed to avoid significant deviation from results obtained with the "complete" characterization.

Simple Mixing Rule Approach (*Back-of-the-envelope solution, but why?*)

A first approach to grouping components would be to simply calculate average critical properties. Pedersen, [Pedersen, 1989 #1242] for example, recommends using weight-fraction average properties. The best "direct" pseudoization method was suggested by Coats. [Coats, 1985 #452] He recommends that the overall mixture EOS constants (a & b) should be the same for the original characterization and the pseudoized characterization, thereby ensuring that volumetric predictions of the overall mixture are identical for the original and pseudoized characterizations. Furthermore, the EOS parameters a & b for each pseudocomponent are the same as given by the components (making up the pseudocomponent) in the original characterization. This method is as accurate (or more accurate) than other methods proposed later; for some strange reason, these other methods don't compare their approach with Coats' procedure.

Stepwise Pseudoization Approach (*Tedious but rigorous*)

For complex reservoir systems involving multiple fluids and multicontact processes with large changes in composition and equilibrium conditions (vaporizing-to-critical-to-condensing), simple pseudoization procedures may not be adequate. We have used an approach that is based on reducing the number of components stepwise. For example, from 15 to 12 to 9 to 7 to 5.

First the original (e.g. 15-component) characterization is used to generate PVT data covering a large range of pressure (temperature) and composition space. PVT experiments are simulated with the original characterization, including expansion & depletion tests, multistage separator tests, multicontact gas injection tests, and minimum miscibility pressures. The calculated data (densities, compositions, MMPs, etc.) are automatically stored as "measured" data.

The first pseudoization from 15 to 12 components is made using the Coats procedure to estimate all pseudocomponent properties. A non-linear regression is performed to minimize the SSQ defined by the calculated 12-component results and the 15-component "measured" data. The regression parameters include EOS constants (a & b) for each of the newly-created pseudocomponents, relevant BIPs, and VT parameters.

The second pseudoization from 12 to 9 pseudocomponents is made, again using the Coats procedure to estimate initial pseudocomponent properties. A second non-linear regression is performed to minimize the SSQ defined by the calculated 9-component results and the 15-component "measured" data. The regression parameters include EOS constants (a & b) for each of the newly-created pseudocomponents, relevant BIPs, and VT parameters.

This procedure is continued for fewer and fewer pseudocomponents until the quality of match between the original 15-component characterization and the pseudoized characterization is unacceptable.

3. MISCIBILITY CALCULATIONS

3.1. Miscibility Mechanisms (*Complex thermodynamic/flow processes*)

One of the main reasons we need to model reservoir fluids with an EOS is to describe multicontact miscible processes resulting from the injection of gas in an oil reservoir. The path taken towards developing miscibility in a reservoir oil is complicated due to chromatographic separation of components behind, at, and ahead of the displacement front. Strong vaporization typically dominates behind the front, near-critical behavior is found at the front, and severe condensation may occur just ahead of the front. Other effects include swelling and viscosity changes.

In a one-dimensional displacement, the conditions of pressure or gas enrichment where a miscible displacement first occurs - the *minimum miscibility condition* (MMP/MME) - is completely independent of the porous material through which the flow is occurring. Relative permeability, capillary pressure, and interfacial tension have no effect on MMP/MME. Minimum miscibility conditions are only dependent on the phase behavior of the system. However, the MMP/MME may be (and usually is) dependent on a complex interaction of "flow mixing" and thermodynamics; certainly true for the condensing/vaporizing mechanism. {Zick, 1986 #370} When the interaction of flow mixing and thermodynamics is important, we can not predict MMP/MME conditions with a zero-dimensional PVT calculation.

Other traditional miscibility mechanisms, such as first contact miscibility and the vaporizing mechanism, are independent of flow mixing and can be calculated with a zero-dimensional PVT calculation (e.g. a tie-line approach).

First-Contact Miscibility (*Nobody can afford this process*)

First-contact miscible (FCM) processes are almost never used in practice, because of the high cost of using an injectant that is completely miscible with the reservoir oil. Propane is often mentioned in connection with FCM, usually in a process that consists of injecting slugs of propane followed by lean gas or water. Calculation of FCM is simple. Tracing the saturation pressure versus amount of injection gas (p-x diagram), the maximum is defined as the FCM pressure.

Vaporizing Multicontact Mechanism (*Straight-forward, when it exists*)

Injection of a lean gas (nitrogen or a methane-rich separator gas) may result in miscible displacement of lighter reservoir oils ($\rho_{STO} < 850 \text{ kg/m}^3$ and $R_s > 150 \text{ m}^3/\text{m}^3$) at relatively high pressures (>350 bar). This process results from the gas being enriched by the oil through vaporization. If the gas becomes sufficiently rich in light and intermediate C_{5+} components, miscibility can develop *at the gas displacement front*.

Note that the vaporizing miscibility mechanism can not occur for a reservoir with initial gas saturation; the mechanism will not develop with a free gas saturation ahead of the miscible gas front. Furthermore, the MMP condition determined by a rising bubble apparatus will *always* correspond to the vaporizing MMP.

Condensing Multicontact Mechanism (*A figment of our imagination*)

Historically, the condensing mechanism of developed miscibility was thought to occur when a lean gas enriched in C_2 - C_5 intermediates was injected into an oil reservoir. The mechanism of developing miscibility assumed that the oil at the point of injection would absorb enough of the enriching components from the injection gas to eventually become miscible with the injection gas. Once miscibility was achieved, the injection gas would miscibly displace the enriched oil.

Zick{Zick, 1986 #370} blew a hole in this traditional picture of the condensing mechanism when he reminded us that each time the injection gas contacts the oil at the point of injection: (1) the gas enriches the oil with C_2 - C_5 components, and (2) the oil enriches the gas with components C_{6+} . Oops, we forgot about the vaporization from oil to gas. Zick continues by noting that after only a few contacts, the oil becomes saturated in C_2 - C_5 components, so the first process stops! However, the gas continues vaporizing the C_{6+} material from the oil -- forever (or until the oil disappears); recall that the injection gas doesn't have any C_{6+} components.

The practical consequence of Zick's observations is that the development of miscibility with an enriched gas does not follow the traditional condensing process which accounts only for transfer of C_2 - C_5 components from the gas to the oil. Developed miscibility with enriched gas must, therefore, follow another process (the condensing/vaporizing mechanism).

Condensing/Vaporizing Mixed Mechanism (*Zick technology*)

Zick{Zick, 1986 #370} shows that the minimum miscibility condition developed by the injection of an enriched gas is a combination of condensation (ahead of the front) and vaporization (behind the front). At the front, the condensing and vaporizing behavior is severe, reaching criticality in the limit of zero dispersion. Even with physical dispersion, the condensing/vaporizing front is sufficiently near-critical to result in oil recoveries approaching 100%.

The mixed mechanism also exists for un-enriched separator gases. It also is the mechanism describing most low-temperature CO_2 miscibility processes. The mechanism is easily recognized from one-dimensional displacement simulations at a pressure close to the true MMP/MME condition. If we look at the profile of K-values (or gas and oil densities) along the x-axis, say after 0.6 pore volumes injected, the near-critical front is the middle of an hour-glass shape. Flowing from left to right, the right side of the hour glass is the region of condensation, and the left side of the hour glass is the region of vaporization. If the right side of the hour glass is missing (at the MMP/MME), then the mechanism is dominated by vaporization.

Though, beware! For a highly undersaturated oil, the condensing region may actually be there, but the gas in this region "dissolves" almost immediately into the undersaturated oil. It may require a very fine-grid simulation to see the condensing side of the hour glass. If you misinterpret the mixed mechanism for an undersaturated oil as being a vaporizing mechanism, and use a tie-line method to compute MMP/MME, then the result will be wrong; the vaporizing MMP/MME will always be higher than the mixed mechanism MMP/MME.

3.2. Calculating Minimum Miscibility Conditions (*Be careful!*)

Slimtube Simulations (*Fail-safe if used right*)

The slowest but safest way to compute MMP/MME conditions is to use a 1D "slimtube" compositional simulator. The simulator should be run with an IMPES (implicit pressure, explicit saturation and composition) formulation, with short time steps to avoid instabilities. It is necessary to run displacements for varying numbers of grid cells at each pressure/enrichment, e.g. $N=50, 100, 200,$ and 500 grid cells. At a given pressure/enrichment, oil recovery is plotted versus pore volume injected (PV_{inj}), and the recovery at $1.2 PV_{inj}$ is chosen ($R_{1.2}$). Plotting $R_{1.2}$ versus $1/N$ (or $1/\sqrt{N}$), you extrapolate to $N=\infty$ to obtain a dispersion-free recovery $R_{1.2}^{\infty} \leq 100\%$. Plotting $R_{1.2}^{\infty}$ versus pressure or enrichment, the point where $R_{1.2}^{\infty}$ first reaches 100% is defined as the MMP/MME.

This approach is fail-safe, in that it does not assume a mechanism. The "qualitative" parts of the procedure (e.g. choosing $1.2 PV_{inj}$ instead of $1.4 PV_{inj}$ and the method of extrapolating to $N=\infty$) may

result in an uncertainty in MMP of about 1 bar, but this is certainly acceptable for most applications. The main problem with this method is that it is slow and tedious, and not readily automated.

Vaporizing Multicontact MMP (Tie-line approach OK)

The vaporizing miscibility condition can be modeled using a forward-contact tie-line calculation because the process depends only on what is occurring at the gas front. First the original reservoir oil is contacted with injection gas. The resulting equilibrium gas is taken and contacted with original oil. The procedure is repeated until the equilibrium gas either becomes miscible with the reservoir oil, or gets stuck on an immiscible tie line. Several calculation procedures have been proposed for MMP calculation of the vaporizing mechanism, {Jensen, 1990 #1266; Luks, 1987 #573} the most efficient being the method proposed by Jensen and Michelsen. {Jensen, 1990 #1266}

If the true (slimtube) MMP/MME reflects the mixed C/V mechanism, then the MMP from a vaporizing mechanism will *always* be greater than the true MMP. If the MMP/MME truly reflects a vaporizing process, then the C/V mechanism won't exist; this usually doesn't occur unless the injection gas is very lean.

Condensing Multicontact MMP/MME (It's not what you think it is!)

The traditional condensing mechanism doesn't exist. Let me know when you find a real reservoir fluid and a realistic injection gas that develops condensing miscibility -- without the *actual* mechanism being first-contact miscible or vaporizing. If you find such a system, send me the fluids and EOS characterization. If you're right, I'll send you a box of delicious Norwegian candies!

If you insist on computing a miscibility condition for the traditional condensing mechanism, this can be done with a backward-contact tie-line approach. First the injection gas contacts the original oil. An equilibrium oil and gas result. Thereafter, fresh injection gas is contacted with the equilibrium oil resulting from the previous contact. This process is continued until either no changes occur (you're stuck on an immiscible tie line) or miscibility is reached.

If you increase the pressure or enrichment to the first point where this process leads to a miscible condition (the injection gas is on the extension of a critical tie line through the equilibrium oil), you probably will find one of two things has happened: (1) the pressure equals the first-contact miscibility pressure, or (2) the process has turned into a vaporizing mechanism! The second result is easily confirmed by simulating a one-dimensional displacement (at the tie-line-determined MMP) and observing that gas miscibility develops at the displacement front (with a strongly vaporized region behind the front); no gas is ahead of the front as would be expected for a true condensing mechanism.

Condensing/Vaporizing Multicontact MMP/MME (It can be done, but how?)

The MMP/MME of a mixed C/V mechanism can be calculated using slimtube simulations, as outlined earlier. It can not be calculated with a simple forward-contact or backward-contact tie-line method. Zick has developed a procedure based on the interpretation of results from a multicell calculation procedure (similar to the one proposed by Metcalfe {Metcalfe, 1973 #27}). Data are interpreted in a way that eliminates numerical dispersion, providing mixed mechanism MMP/MME results that are precise (± 0.1 bar) and very close to dispersion-free slimtube simulation results.

4. COMPOSITIONAL GRADIENTS

More and more reservoirs are being discovered today with large structural relief or thick sections that cover hundreds of meters from top to bottom, and sometimes more than 1000 meters. The occurrence of reservoirs with significant compositional gradients has increased, and the industry is currently using

compositional gradient models on a regular basis to determine initial fluids in place, and estimation of the gas-oil contact (sometimes used in choosing where to drill delineation wells).

A problem we have is not knowing whether the thermodynamically rigorous isothermal gravity/chemical equilibrium model is truly valid for non-isothermal systems (*all* reservoirs have temperature gradients, usually ranging from 0.01 to 0.03°C/m). If the isothermal model is not valid, what should we use?

4.1. Isothermal Gravity/Chemical Equilibrium (*Gibbs said it's OK, so it's OK*)

The equations governing isothermal gravity/chemical equilibrium were outlined by Gibbs. The equations are solved by first specifying a reference depth, pressure, and composition. The equilibrium calculation at any depth (above or below the reference depth) results in pressure and composition at the specified depth.

Already in the 1930s the isothermal gravity/chemical equilibrium problem was applied to petroleum reservoirs using simple thermodynamic models (Muskat, {Muskat, 1930 #379} and Sage and Lacey {Sage, 1939 #587}). About 15 years ago the model was first applied using cubic equations of state. {Schulte, 1980 #381} A thorough review of the literature and application of this model to petroleum reservoirs is given by Whitson and Belery. {Whitson, 1994 #660}

The main advantages of the isothermal model are that it has a rigorous thermodynamic basis, the gradient calculation is fast and exact (as exact as any other equilibrium calculation), and it can be solved from one depth to another depth without knowing the solution in between (the solution is known, implicitly, at all depths).

4.2. Gas-Oil Contact Determination (*We need it efficiently and precisely*)

Determination of the gas-oil contact (GOC) is a tricky problem. The GOC is defined (here) as the depth where the fluid changes from having a dewpoint to having a bubblepoint (at constant reservoir temperature). Two situations can occur. First, the GOC can represent a saturated condition where the reservoir pressure equals the saturation pressure. All physical properties have a discontinuity at a saturated GOC.

A second situation is when composition has a transition from a dewpoint to a bubblepoint at undersaturated conditions (with reservoir pressure greater than the saturation condition). The only way this can occur is that the saturation pressure of the fluid *at* the point of transition is a critical point. This defines an undersaturated GOC.

Computing the GOC, independent of whether it is saturated or not, requires a condition that takes into account both types of GOCs. One approach is to minimize the function $F = \Delta p \Delta c$, where Δp is the difference between reservoir and saturation pressure ($\Delta p = p_R - p_s$), and $\Delta c = \sum \ln K_i$, with $K_i = K$ -values at the saturation pressure. Numerical derivatives are used to solve the depth derivative dF/dh in the Newton-Raphson routine. We are also looking at faster methods based on Michelsen's approximate phase envelope algorithm. {Michelsen, 1994 #1554}

4.3. Thermal Diffusion/Gravity Zero-Mass-Flux Model (*A mass of confusion*)

Including a temperature gradient with depth precludes solving a thermodynamic equilibrium problem. Because a thermal gradient exists, thermodynamic equilibrium can not be achieved. What *may* develop is a system with zero net-mass flux of components resulting from all existing driving potentials (chemical, gravity, and thermal). If we assume zero convection.

On the other hand, convection may result from the thermal gradient, in which case the compositional variation is no longer a 1D problem, but must be solved in three dimensions. The convection problem must also consider rock and rock/fluid property variations throughout the reservoir. Lateral temperature variations may play a role, as well as geologic regional compositional gradients. From a practical point of view, the problem can't be solved. Even if we try, the problem is to first agree on the fundamental physics (something that doesn't seem easy to do).

What *would* be nice is to have a one-dimensional zero net-mass transfer model that could be used to compare with the isothermal gravity/chemical equilibrium model. Several non-isothermal models have been proposed for petroleum reservoirs, {Belery, 1990 #372; Faissat, 1994 #1555} based on non-equilibrium thermodynamics. Only the Belery and da Silva model has been solved for a multicomponent reservoir system. We plan to compare the models formulated by Faissat et al. with the Belery-da Silva model to identify any significant differences.

An unfortunate problem with all of the non-isothermal models is the need to solve (integrate) the equations discretely from the reference depth to some other depth. Discretization makes the result susceptible to numerical inaccuracies, and it is more difficult to include calculated results in a fluid characterization scheme based on non-linear regression.

4.4. Including Gradient Data in EOS Tuning (*We need better field data*)

One area we are looking at is the use of measured compositional gradient information (compositions, PVT properties, and gas-oil contact) as part of the EOS tuning procedure. An inherent problem is the quality of gradient data. Saturated gas-oil contact may be the only data we can rely on (from RFT pressure measurements), unless new depth-specific methods for sampling (RFT/MDT) prove successful. Another problem is which gradient model should be used (isothermal or non-isothermal).

When using gradient data in EOS tuning, the regression parameters should no longer be limited to EOS parameters. The reference depth, reference pressure, and depths of samples all have a degree of uncertainty. It is too early to report results from our studies, but we are hopeful that this research will improve our understanding of observed compositional gradients, and methods for calculating gradients.

REFERENCES

