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Phase behavior in reservoir simulation

The pressure-volume-temperature（PVT）handling of fluids in reservoir simulation (/Reservoir_simulation) describes the phase behavior (/Thermodynamics_and_phase_behavior) of gas, oil, and water at reservoir and surface conditions. PVT considerations are important in setting up the proper parameters when undergoing reservoir simulation.

Phase behavior of a mixture with known composition consists of defining the number of phases, phase amounts, phase compositions, phase properties (molecular weight, density, and viscosity), and the interfacial tension (IFT) between phases. In addition to defining the phase behavior of mixtures at a specific reservoir pressure, knowing the derivatives of all phase properties with respect to pressure and composition is important in reservoir simulation.

Contents

Representing phase behavior

The calculation of phase behavior in a reservoir model can be made in one of the two following ways:

- Using a "black-oil" approach[1][2][3][4][5] based on simple interpolation of PVT properties as a function of pressure
- Using a "compositional" approach based on a thermodynamically-consistent model such as a cubic equation of state (/Equations_of_state) (EOS).[6][7]>

With either approach, the PVT quantities required by a reservoir simulator are essentially the same. Modern reservoir simulators[6][1] are usually written with a general compositional formulation, whereas black-oil PVT properties are converted internally to a two-component "compositional" model; the two components are surface gas and surface oil.

A reservoir simulator keeps track of overall composition in each computational grid cell (/Gridding_in_reservoir_simulation) as a function of time. A grid cell's overall composition changes because of cell-to-cell fluxes and because of production or injection in wells. The phase fluxes and component movement within the reservoir are greatly affected by phase behavior (e.g., the mobility of each phase and which components are carried in each phase). The surface products from wells are dependent on the phase behavior of produced wellstreams, but at conditions far removed from reservoir pressure and temperature.

In most reservoir simulators, the water phase and water component are treated in a simplified manner—namely, that the water component does not partition into the hydrocarbon phases, and the hydrocarbon components do not partition into the water phase; the term "hydrocarbon" also includes N_2, CO_2, and H_2S. Because of relatively high CO_2 solubility in water, and the potential importance of CO_2 "accounting" in CO_2 floods, some compositional models allow CO_2 partitioning in the water phase.[8]

Conceptually and computationally, it is feasible to allow complete partitioning of all components in all phases in reservoir simulation. The partitioning related to the water phase and the water component could be treated with simple pressure-dependent tables, or even with an EOS model. The water-related *K*-values have simple composition dependence that would make EOS-based fugacity (/Glossary:Fugacity) updates almost trivial. The main problem would be treating the impact of changing salinity on water-related *K*-values. From a practical point of view, however, modeling water-related component partitioning will have a marginal impact on reservoir performance. Hereafter, only phase behavior of nonaqueous phases will be discussed.

Number of phases and phase type

The starting point for PVT calculations in a model grid cell is to determine if the overall composition is single-phase or two-phase at the current pressure estimate. If a cell is single-phase, the phase "type" (gas or oil) may also be needed to select the proper relative permeability and capillary pressure (/Relative_permeability_and_capillary_pressure) curves. For a black-oil PVT model (i.e., any model with simple pressure-dependent *K* -values), determining the number of phases and phase identification is trivial.

For EOS models, two methods can be used for establishing how many phases exist: the Michelsen[9] phase stability test or a saturation pressure calculation.[9] The stability test is relatively "slow" because good *K*-value estimates are not used to initiate the calculation, whereas a saturation pressure can be quite fast because good *K*-value estimates are often available. A stability test is more reliable in the sense of giving a conclusive result, whereas a near-critical saturation pressure test may not be found[10] or converge correctly to a nontrivial solution. Another advantage of using saturation pressure is that it gives a consistent method to define phase type for single-phase cells, something that is not provided by the stability test. The choice of which method to use depends on the tradeoff between speed and reliability. Both methods, if detecting two phases, give excellent starting *K*-values to initiate the two-phase flash calculation.

Two-phase flash

Having established that two phases exist in a cell, one must perform a flash calculation. The flash calculation uses the overall moles n and molar composition z_i to determine the molar amounts of each phase (n_g and n_o), and the phase compositions (y_i and x_i). For simple pressure-dependent *K*-value models, the Rachford-Rice[11][12] (RR) procedure is used to find molar amounts and compositions,

$$\sum_{i=1}^{N}(y_i - x_i) = \sum_{i=1}^{N}\frac{z_i(K_i - 1)}{1 + \alpha_g(K_i - 1)} = 0,$$ (/File:Vol5_page_1450_eq_001.png)....................(1)

solving for $\alpha_g = n_g / (n_g + n_o)$, with $x_i = z_i / [1 + \alpha_g (K_i - 1)]$ and $y_i = K_i x_i$.[13]

For an EOS model, using the RR solution can be used, but an additional constraint must be satisfied; the fugacity of each component must be the same in each phase,[14] $f_{gi} = f_{oi}$. Using an initial set of K_i estimates, the RR equation is solved. Resulting compositions y and x are then used to calculate fugacities f_{gi} and f_{oi}. If the constraint $f_{gi} = f_{oi}$ is not satisfied for all components, a new set of *K*-values is estimated using some form of a successive substitution (SS) update K_i new = $K_{i\text{old}}\ (f_{oi} / f_{gi})$.

For reservoir simulation, a Newton solution of the flash equation should be much faster than SS methods. Including the equal-fugacity constraint within the set of nonlinear equations used to solve for model pressures "automatically" provides the first Newton update of the flash equation.[14] Usually only one additional Newton iteration of the flash equation is needed to converge the fugacity constraints to required tolerance.

In summary, *K*-values alone determine the phase amounts and phase compositions (from the Rachford-Rice equation). The EOS model guarantees rigorous thermodynamic consistency through the equal-fugacity constraint, ensuring that *K*-values properly account for pressure and composition dependence of the phase split and component partitioning.

Having completed the flash calculation in a cell, the following information is known: phase moles, phase masses, phase densities, phase volumes (saturations), and phase compositions. The viscosity and gas/oil interfacial tension (IFT) can be calculated using compositional correlations,[13] or interpolated from pressure-dependent tables for a black-oil model. The impact of PVT properties on reservoir performance will consider individual PVT properties and their impact on individual terms in the flow equations.

Density

Phase molar amounts, n_g and n_o, are converted to phase volumes using phase molecular weights and densities: $V_g = n_g M_g / \varrho_g$ and $V_o = n_o M_o / \varrho_o$, where $S_g = V_g / V_{\text{block}}$ and $S_o = V_o / V_{\text{block}}$. Saturations determine relative permeabilities, which can have a dramatic impact on phase fluxes. Typically, $k_r \sim S^n$, where $n \sim 2$ to 4. For $n = 3$, a 5% error in density results in a 15% error in k_r.

For reservoirs with sufficiently high vertical permeability, gravity will often play an important role in recovery. Gravity segregation is caused by vertical fluxes driven by the potential terms $\nabla\varrho_g = d(p_g + \varrho_g gz + P_{cgo}) / dz$, $\nabla\varrho_o = d(p_o + \varrho_o gz) / dz$, and $\nabla\varrho_w = d(p_w + \varrho_w gz + P_{cwo}) / dz$. Errors in densities have a direct impact on gravity segregation. It is actually the density difference between flowing phases that determines the magnitude of gravity segregation (i.e., $\Delta\varrho_{wo} = \varrho_w - \varrho_o$, $\Delta\varrho_{go} = \varrho_o - \varrho_g$, and $\Delta\varrho_{wg} = \varrho_w - \varrho_g$). Likewise, the condition for equilibrium initialization $\nabla\varrho_g = \nabla\varrho_o = \nabla\varrho_w = 0$ results in saturation-depth distributions, which must honor input $\Delta\varrho_{go}g = P_{cgo}(S_g)$ and $\Delta\varrho_{wo}g = P_{cwo}(S_w)$ relationships.

A +5% error in oil density (e.g., 630 instead of 600 kg/m^3) and a –5% in gas density (e.g., 380 instead of 400 kg/m^3) results in gravity segregation potential ($\Delta\varrho_{go} = \varrho_o - \varrho_g$) in error by 25% (250 instead of 200 kg/m^3). Similarly, in the initialization of a water/oil system, the inadvertent use of $\varrho_w = 62.5$ lbm/ft^3 instead of the correct value of 70.0 lbm/ft^3 for a high-salinity brine could easily cause a 25% error in initial oil in place for a low-permeability (large capillary transition zone), low-API oil.

In black-oil models, it is particularly easy to model densities incorrectly because of the inadvertent use of "arbitrary" surface densities. The reservoir phase densities are not input directly in a black-oil model. Instead, they are calculated using the formation volume factors (FVF) B_o, B_g, and B_w, solution gas/oil and oil/gas ratios R_s and r_s, and surface densities ϱ_{gs}, ϱ_{os}, and ϱ_{ws}, based on the relations $\varrho_g = (\varrho_{gs} + p_{os}\, r_s) / B_g$, $\varrho_o = (\varrho_{os} + R_s\, \varrho_{gs}) / B_o$, and $\varrho_w = \varrho_{ws} / B_w$. Because reservoir densities are not usually tabulated as output by reservoir simulators, the user may not know how "wrong" the densities might be.

A well-tuned EOS using volume shift factors[15] should always predict reservoir and surface densities within 2 to 4%, and often within 1 to 2%. The author’s experience has found it generally unnecessary to use different volume shift factors for reservoir and surface calculations unless all densities are needed with accuracies of 1 to 2%. The use of either Peng-Robinson[16] or Soave-Redlich-Kwong[17] EOS with volume-shift factors provides densities as good or better than the more-complicated ZJRK[18] EOS model; in this author’s opinion, the ZJRK no longer has a role in reservoir simulation, as supported by decreasing industrial use (almost to nonexistent) during the past 5 years.

Component partitioning

The partitioning of components in gas and oil phases, as dictated by *K*-values, is important for properly describing vaporization and condensation.

- Vaporization is the process of "stock-tank oil" (STO) components (C_{6+}) moving from the oil phase to the gas phase.
- Condensation is the process of intermediate (C_3_C_{10+}) components moving from the gas phase to the oil phase.

Retrograde condensation is particularly important in the depletion of gas condensate reservoirs, where in-situ retrograde condensation results in decreasing surface liquid yields.[1][13][19]

For most gas-injection projects, vaporization will play an important role. Proper modeling of vaporization usually requires a compositional model that uses a detailed description of the heavier (C_{7+}) components, typically three to five fractions.[1][20][21] The lightest fractions (C_7 to C_{12}) will typically vaporize 80 to 100%, while intermediate heavies (C_{13} to C_{20}) may vaporize in varying amounts from 30 to 90%, and the heaviest components C_{20+} may vaporize from 0 to 50%. The degree of vaporization depends primarily on the local pressure and composition of displacing gas. Cook *et al*.[3] suggested a modification of the black-oil model that allows saturated properties to change as a function of how much injection gas has contacted a given cell, thereby allowing reasonable description of a vaporization-dominated process. Tang and Zick[22] propose a limited three-component compositional model that allows accurate description of developed miscibility for use in models in which grid-related dispersion may result in underpredicted conditions of miscibility using an EOS-based simulator.

In some gas-injection processes, the injection gas may be enriched (1) during injection by adding natural gas liquids (NGLs) (C_3 to C_5 components) and/or (2) within the reservoir by multiple contacts with reservoir oil, which gradually enriches the injection gas with intermediate components C_3 through C_{10}. For either type of enrichment, the vaporization process can become extremely efficient and result in a near-miscible or miscible displacement with near-100% recovery of the oil. When such a displacement results, it is often associated with the development of a complex process whereby the near-miscible front consists of upstream vaporization and downstream condensation—the "condensing/vaporizing" gas drive mechanism first described by Zick.[23]

For an EOS model to properly describe complex phase behavior related to vaporization, condensation, and near-miscible mechanisms, special PVT experimental data should be measured and used to tune the EOS. For immiscible processes with significant vaporization, a single-cell multicontact PVT test is useful, quantifying the degree of vaporization in terms of oil volumetric stripping and gas compositional changes. For near-miscible or miscible processes, a swelling-type test which has the following features is strongly recommended:

1. Five to seven mixtures of reservoir oil and injection gas are used, with two to three mixtures being bubblepoints and two to three mixtures being dewpoints
2. Constant composition expansion is conducted on each mixture, where saturation pressure and the oil relative volumes are measured and reported
3. Single equilibrium "flash" somewhat near the critical point is used for obtaining a set of equilibrium gas and oil compositions (*K*-values).

Proper EOS tuning of the complex phase behavior measured in such an experiment is difficult, and requires the ability to match near-critical volumetric and compositional changes. Such predictions are almost never available *a priori* with an EOS model that has been tuned only to simple depletion data. Small but important modifications of the heavy-end properties and binary interaction parameters are usually required to obtain a satisfactory match of near-critical PVT data provided by this special "swelling" test. A tuned EOS model that is able to match all PVT data, including near-critical phase behavior, has a good chance of properly predicting true multicontact near-miscible/miscible behavior.[13][23]

Viscosity

Gas viscosities (/Gas_viscosity) are typically estimated by correlation[13] within 5 to 10%, and they are almost never measured experimentally. Such accuracy is adequate for most applications, and gas viscosities seldom vary beyond the range of 0.02 to 0.03 cp. For gas-injection processes at high pressure or near-miscible displacements, gas viscosities can range from 0.03 to 0.1 cp. Gas-viscosity correlations are not usually accurate for this higher range of viscosity, and errors up to 20 to 30% may be expected; compositional viscosity correlations also have the same level of accuracy.

Oil viscosities (/Oil_viscosity) are notoriously inaccurate based on correlations,[13] at best being within 10 to 30%, but often in error by 50% or more. Oil viscosities should always be measured and used to tune a viscosity model. A minimum requirement would be measurement of stock-tank oil viscosities, and normally live-oil viscosities are available from a differential liberation test.

For gas condensates, oil viscosities are almost never measured. This may be a serious problem if condensate blockage has a significant impact on well deliverability.[24] Condensate viscosities are difficult to measure because retrograde condensate volumes can be very small. The use of a separator condensate sample is recommended. Bring it to reservoir conditions (T and P) for density and viscosity measurements, then tune the viscosity model to these data. This approach is feasible for any gas condensate; it is not expensive, and it is better than relying on untuned compositional viscosity correlations.

Our experience has been that the compositional viscosity correlation by Lorenz, Bray, and Clark[25] (LBC) is not predictive, and it is highly dependent on accurate density predictions. Tuning the heavy-component critical volumes and, sometimes, careful modification of the higher-order constants in the LBC equation, provide the required accuracy for gas and oil viscosities in most reservoir processes. Unfortunately, modification of the LBC correlation to match a limited number of viscosities (in a narrow range of pressure and composition typical of depletion experiments) can lead to unphysical viscosity predictions at conditions developed during a gas injection process.

The Pedersen *et al*.[26] compositional viscosity correlation, though more complicated and CPU-intensive than the LBC correlation, has quite good predictive capabilities. The correlation is based on a corresponding states formulation in which methane viscosity is the reference compound.

Gas/oil interfacial tension (IFT)

Gas/oil IFTs may be used in a reservoir simulator[27] to modify input capillary pressures P_{cgo} , relative permeabilities k_{rog} and k_{rg} , and residual oil saturation S_{org} . As IFT decreases, P_{cgo} decreases proportionately. Relative permeabilities and residual oil saturation change only marginally until IFT reaches a fairly low value (e.g., 1 mN/m), whereas at lower IFTs, the relative permeability-related properties change approximately as log(IFT).

Practically, IFT impact on capillary pressure is limited to fractured reservoirs[28] in which displacement efficiencies may be strongly linked to the balance of gravity and capillary forces on a relatively small distance scale (e.g., block heights of 1 to 10 m).

IFT impact on relative permeabilities and residual saturations may have an impact on some gas-injection processes, though near-miscible and miscible processes have minimal IFT dependence because they are usually dominated by the strong compositional effects (vaporization and condensation) that result in near-100% recoveries. In fact, displacements that are miscible should, by definition, be independent of the relative permeabilities and residual oil saturation.

IFT impact on near-well relative permeabilities in gas condensate reservoirs can, together with high velocities, result in large capillary numbers, which have the tendency to "straighten" relative permeabilities and improve flow performance. It has been shown[29][30] in a number of recent publications that this effect can have an important impact on gas-condensate well deliverabilities. Neglecting IFT and velocity dependencies of relative permeability can lead to overly conservative prediction of well deliverability (i.e., overprediction of condensate blockage).

Black-oil PVT models

Black-oil PVT properties are generated in one of two ways. For low- to medium-gas-oil-ratio (GOR) oils (< 150 Sm^3 /Sm^3), a traditional differential liberation experiment (DLE) is used, with corrections for separator flash to calculate oil formation volume factor (FVF) B_o and solution GOR R_s, as well as the gas FVF B_g.[13] This approach assumes the reservoir gas contains unsubstantial amounts of condensate in solution, with solution oil/gas ratio $r_s \sim 0$.

The more common and general approach to generating black-oil PVT properties uses an EOS model to simulate a depletion-type PVT experiment (differential liberation, constant volume depletion, or constant composition expansion), with the equilibrium gas and equilibrium oil at each stage in the depletion being individually processed to surface conditions to provide the four black-oil properties[1][17]:

- B_o
- R_s
- B_g
- r_s

For highly volatile oils, the EOS method gives substantially different and improved black-oil properties compared with the traditional laboratory DLE/separator-corrected approach.

The conversion of black-oil PVT data (R_s, B_o, r_s, and B_g) to a compositional model[3] uses K-values of surface gas and oil pseudo "components" $K_{gs} = (R_s + C_{os}) / (1 + r_s C_{os}) / R_s$ and $K_{os} = r_s(R_s + C_{os}) / (1 + r_s C_{os})$, with $C_{os} = (RT_{sc} / p_{sc})(\varrho_{os} / M_{os})$. The reservoir-phase densities are calculated from $\varrho_g = (\varrho_{gs} + \varrho_{os} r_s) / B_g$ and $\varrho_o = (\varrho_{os} + R_s \varrho_{gs}) / B_o$, while phase molecular weights are given by $M_g = (M_{gs} + r_s M_{os} C_{os})/(1 + r_s C_{os})$ and $M_o = (R_s M_{gs} + M_{os} C_{os}) / (R_s + C_{os})$. Viscosities and gas/oil IFTs are interpolated directly from input tables.

Coats *et al*., [1] Coats *et al*.,[2] and Fevang *et al*.[4] have shown that black-oil models can be used for practically any type of reservoir produced by depletion or waterflooding, including reservoirs with large compositional gradients. Some issues require special treatment for complex fluids systems, including fluid initialization and the method for generating black-oil tables. In a nutshell, the recommended procedures[4] are to generate the black-oil tables with an EOS model using the fluids with the highest saturation pressure (e.g., at the gas/oil contact) and to initialize with solution GOR ($R_s$and r_s) vs. depth—not saturation pressure vs. depth.

A common problem with black-oil models is the calculation of "negative compressibility," [31] meaning that a small pressure drop results in a reduction in total (gas + oil) volume. Another problem is physical extrapolation of saturated PVT properties to saturation pressures higher than given in the input table (e.g., caused by gas injection, gravity segregation in undersaturated reservoirs, or near-well behavior during rate reductions).

When can the black-oil PVT treatment not be used? Basically, for any gas-injection process with significant component partitioning that changes during the displacement.[4][20] This would include processes with high-pressure vaporization using lean gas, condensation from enriched injection gas, and developed-miscibility processes such as the condensing/vaporizing mechanism. Surprisingly, a black-oil treatment is sometimes adequate even for complex gas injection problems, though it is not usually known *a priori*. To check the validity of a black-oil model in a gas injection project, the reservoir process should first be simulated with a compositional model, and preferably a relevant 3D model that captures all important flow characteristics.

Equation-of-state models

The most common EOS used in reservoir simulation are the PR and the SRK models. Both models have two constants, a and b. Each constant must be calculated for each component based on component critical properties (T_c and p_c) and acentric factor (ω).

The PR EOS has two versions—the original 1976 version[17] and the modified 1979 version[32]; the latter uses a third-degree polynomial expression for the correction term to constant a. For some systems, the difference in equilibrium calculations for the two PR EOS models is significant.

The Peneloux[15] volume shift factors should always be used with two-constant EOS models to ensure accurate oil and gas densities. The volume shift factors have no impact on calculated K-values or compositions, only densities. As mentioned earlier, the ZJRK[18] EOS is outdated and was used before the volume-shift method was introduced in 1980, with complex correction functions to constants a and b to improve liquid density predictions.

Binary interaction parameters (BIPs) k_{ij} are important for adjusting predictions of equilibrium properties (K-values and compositions).[33] These parameters represent a correction of the form $(1 - k_{ij})$ to the $a_i a_j$ term in the quadratic mixing rule for EOS constant a. BIPs can be positive or negative; they are symmetric ($k_{ij} = k_{ji}$); they are usually ~0 for most hydrocarbon-hydrocarbon pairs, except C_1 to C_{7+} pairs which may reach values as high as 0.25; and they are generally close to 0.1 for nonhydrocarbon (N_2, CO_2, H_2S)-hydrocarbon pairs.

Three-phase PVT behavior

Three-phase (L1-L2-V) behavior is an occasional but serious problem for EOS-based compositional models. The third phase (L2) is usually a light liquid and typically appears at low temperatures (< 140°F) in gas-injection processes (/Miscible_flooding) using CO_2 or NGL-enriched gas.[34] Physically, three phases may actually exist, and the EOS model is correctly predicting the behavior. Sometimes a three-phase system is predicted without one physically existing; this may result for lower temperatures when the heaviest component properties are improperly modified to fit two-phase gas/oil PVT data.

For reservoir simulators, the three-phase problem is caused by the EOS formulation "allowing" only two phases. If three phases actually exist, the two-phase flash may find any of the three possible two-phase combinations: L1-V, L2-V, or L1-L2. These false two-phase solutions may indicate a single-phase condition, or they may actually appear as a valid solution (meeting the equal fugacity constraints). Unfortunately, the reservoir model, in a given cell during a given timestep, may flip-flop between two of the possible solutions, resulting in unstable behavior because the pressure solution is not continuous from one two-phase solution to the other. Models may have to simply give up because of repeated timestep reductions, which result from the inadequacy of the EOS two-phase model handling a three-phase condition.[35]

Surface phase behavior

In compositional simulation, the surface calculations are usually made using multistage separation with an EOS model, with fixed K-values for each separator, or using so-called "gas plant" factors, which define the fraction of a wellstream component that is processed into the stock-tank oil.

For black-oil models, the surface separation is "built in" to the PVT tables. Consequently, if the surface process changes during a model run, all black-oil PVT tables must be reentered at the appropriate time. This also requires that vertical flow performance (VFP) tables be reentered because surface rate and volume ratio nodes change with the process change.

It is difficult to use traditional black-oil models for fields with various well groups that have significantly different processing facilities.[2]

Thermal model PVT requirements

Additional PVT requirements for thermal processes such as steamflooding (/Steamflooding) include quantifying the temperature dependence of K-values, densities, and viscosities. Water-phase behavior of liquid and steam must also be defined in terms of pressure and temperature. Water-hydrocarbon phase behavior is still assumed to be simple, without water/hydrocarbon component partitioning.

An EOS model can be tuned to distillation data for improving the predictive capabilities of K-value dependence; otherwise, a simple correlation of the form $K_i = a_i \exp(- b_i T) / p$ may be used for distillable components.[36] Using distillation data is an indirect approach to defining K-value behavior, and it is used in lieu of high-temperature gas/oil/water phase-behavior experiments, which are not usually available. Oil viscosities in thermal processes may be difficult to correlate with a compositional correlation, so empirical correlations may be used instead.

Fluid initialization

As with rock and other petrophysical properties such as permeability and porosity, a reservoir simulator model must also initialize the spatial distribution of initial fluids. For an EOS-based model, the initial molar compositions are defined, $z_i(x,y,z)$. For a black-oil model, the initial solution gas-oil ratio R s and solution oil-gas ratio r s ratio are defined, $R_s(x,y,z)$ and $r_s(x,y,z)$; sometimes saturation pressures are used instead, $p_b(x,y,z)$ and $p_d(x,y,z)$, but this is not recommended.[37] Specifying a saturated gas-oil contact (GOC) is also a means to initialize fluids vertically in a reservoir simulator, where solution GOR R_s (and bubblepoint) are assumed constant below the GOC, while solution OGR r_s decreases upwards from the GOC to honor the model-imposed assumption that reservoir pressure equals dewpoint pressure, $p(z) = p_d(z)$.

Another fluid initialization data might include temperature $T(x,y,z)$. Some black-oil models allow spatial variation of stock-tank oil density, $\gamma_{\mathrm{API}}(x,y,z)$, where black-oil properties are correlated in multidimensional tables as a function of pressure and γ_{API} . Across barriers such as faults and sealing shales, discrete PVT model data may be defined, such as EOS parameters or black-oil tables; such "discontinuous" fluid descriptions may cause physical and model incompatibilities if fluids mix in the reservoir or at the surface.

A typical problem with initialization is that the specified fluid distribution, initial pressure specifications, and fluid contacts lead to fluid movement when the model is turned on (without production or injection). Initial fluid movement may be unimportant without significantly changing the user-specified fluid system; serious inconsistencies may lead to time-zero flow that has an impact on model performance.

Nomenclature

K_i = equilibrium constant for component i
α = mole fraction vapor phase
∇ = potential term

Subscripts

g = gas phase
I = component number, index counter, or initial condition

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