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Compositional Grading – Theory and Practice Lars Høier, SPE, Statoil and Curtis H. Whitson, SPE, NTNU/Pera

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Abstract

This paper quantifies the potential variation in composition and PVT properties with depth due to gravity, chemical, and thermal forces. A wide range of reservoir fluid systems have been studied using all of the known published models for thermal diffusion in the non-isothermal mass transport problem.

Previous studies dealing with the combined effect of gravity and vertical thermal gradients on compositional grading have either been (1) of a theoretical nature, without examples from reservoir fluid systems, or (2) proposing one particular thermal diffusion model, usually for a specific reservoir, without comparing the results with other thermal diffusion models.

We give a short review of gravity/non-isothermal models published to date. In particular, we show quantitative differences in the various models for a wide range of reservoir fluids systems. Solution algorithms and numerical stability problems are discussed for the non-isothermal models which require numerical discretization, unlike the exact analytical solution of the isothermal gradient problem.

A discussion is given of the problems related to fluid initialization in reservoir models of complex fluid systems. This involves the synthesis of measured sample data and theoretical models. Specific recommendations are given for interpolation and extrapolation of vertical compositional gradients. The importance of dewpoint on the estimation of a gas-oil contact is emphasized, particularly for newlydiscovered reservoirs where only a gas sample is available and the reservoir is near saturated.

Finally, we present two field case histories – one where the isothermal gravity/chemical equilibrium model describes measured compositional gradients in a reservoir grading

continuously from a rich gas condensate to a volatile oil; and another example where the isothermal model is grossly inconsistent with measured data and convection or thermal diffusion has apparently resulted in a more-or-less constant composition over a vertical column of some 5000 ft.

Introduction

Composition variation with depth can result for several reasons:

- 1. Gravity segregates the heaviest components towards the bottom and lighter components like methane towards the top 33,34,39 .
- 2. Thermal diffusion (generally) segregates the lightest components towards the bottom i.e. towards higher temperatures and heavier components towards the top (towards lower temperatures)^{3,39}.
- 3. Thermally-induced convection creating "mixed" fluid systems with more-or-less constant compositions, often associated with very-high permeability or fractured reservoirs ^{10,18,31}.
- Migration and "equilibrium" distribution of hydrocarbons is not yet complete, as the times required for diffusion over distances of kilometers may be many 10's of millions of years.⁴⁰
- 5. Dynamic flux of an aquifer passing by and contacting only part of a laterally-extensive reservoir may create a sink for the continuos depletion of lighter components such as methane.
- 6. Asphaltene precipitation (a) during migration may lead to a distribution of varying oil types in the high- and low-permeability layers in a reservoir ³⁶; and (b) in the lower parts of a reservoir ("tar mats") caused by non-ideal thermodynamics and gravitational forces ^{14,32}.
- 7. Varying distribution of hydrocarbon types (e.g.paraffin and aromatic) within the heptanes-plus fractions.^{34,41}.
- 8. Biodegredation varying laterally and with depth may cause significant variation in, for example, H₂S content and API gravity.
- Regional (10-100's km) methane concentrations that may lead to neighboring fields having varying degrees of gas saturation, e.g. neighboring fault blocks which vary from saturated gas-oil systems to strongly-undersaturated oils.
- 10. Multiple source rocks migrating differentially into different layers and geological units.

These conditions and others, separate or in combination, can lead to significant and seemingly-uncorrelateable variations in fluid composition – both vertically and laterally. For a given

reservoir it is impossible to model numerically most of these complex phenomena because (a) we lack the necessary physical and chemical understanding of the problem; (b) boundary conditions are continuously changing and unknown, and (c) we do not have the physical property data and geological information necessary to build even the simplest physical models.

One purpose of this paper is to evaluate simple onedimensional models of vertical compositional gradients due to gravity, chemical, and thermal effects – with the fundamental simplifying assumption of zero component mass flux defining a "stationary" condition.

We show that the gravitational force usually results in maximum compositional variation, while thermal diffusion tends to mitigate gravitational segregation. Published field case histories^{4,21,24,37,42} and a number of

Published field case histories^{4,21,24,37,42} and a number of fields where we have studied vertical compositional gradients show that (a) the isothermal model describes quantitatively the compositional variation in some fields; (b) some fields show almost no compositional variation, even though the isothermal model predicts large variations; (c) a few fields have compositional variations that are larger than predicted with the isothermal model; and (d) some fields show variations in composition that are not at all similar to those predicted by zero-flux models.

Another purpose of this study was to quantitatively compare the various thermal diffusion models for a wide range of reservoir fluid systems. Such a comparison was not available, and we were unsure whether the available models showed significant differences.

Finally, we wanted to give guidelines for how to use measured field data for defining initial fluid distribution, and how simple gradient models can be used to assess measured data, as well as extrapolating compositional trends to depths where samples are not available.

Compositional Grading – Zero-Mass-Flux Model

Calculating the variation of composition with depth is usually based on the assumption that all components have *zero mass* flux – existing in a "stationary" state^{1,7,27,28} in the absence of convection.

To satisfy the condition of zero component net flux, a balance of driving forces or flux equations are used. The driving forces considered include:

- 1. Chemical energy.
- 2. Gravity.
- 3. Thermal gradient.

The general equation to be satisfied is, for all but one component:

$$F_{Gi} = (M_i - \rho V_i)g$$
(2)

where μ_i is the chemical potential, x_i is mole fraction, V_i is the partial molar volume, M_i is the molecular weight of component i, ρ is mass density, and g is the acceleration due to gravity. F_{Ti} is the term used to compute the flux due to thermal diffusion of component i. Several models for estimating F_{Ti} are found in the literature, and below we quantify differences in these models when applied to the compositional gradient problem. What should be noted about F_{Ti} is that (a) it is know with very little certainty and (b) its prediction generally counteracts gravity, resulting in smaller compositional gradients. The most-referenced thermal diffusion models^{12,13,19} are:

$$F_{Ti} = \frac{1}{V_m} \cdot (V_i H_m - V_m H_i) \qquad (Kempers) \dots (4)$$

$$F_{Ti} = -\frac{1}{2\overline{V}} \cdot (V_i \Delta U_m^* - V_m \Delta U_i^*) \quad \text{(Belery-da Silva)(5)}$$

The Belery-da Silva² model is an extension of the Dougherty-Drickamer⁶ model from binary to multicomponent systems. Mixture properties are defined as

$$M_{m} = \sum_{i} x_{i} M_{i}$$
 (9)

where H_i is the partial molar enthalpy. Both H_i and V_i are computed from an equation of state²⁶, and H_i requires an estimate of component- and temperature-dependent ideal heat capacities²⁰ C_{pi,id}.

The "partial molar activation energy" for component i is given by

where n is the number of moles. The term ΔU_m^* is a function of the viscosity-to-density ratio, defined by

$$\Delta U_{m}^{*} \equiv R[(\frac{\partial \ln(\mu/\rho)}{\partial(1/T)})_{p,x_{i}} - pT(\frac{\partial \ln(\mu/\rho)}{\partial p})_{T,x_{i}}] \dots (11)$$

As chemical potential is a function of pressure, mole fraction and temperature, applying the chain rule gives:

$$\nabla \mu_{i} = \left(\frac{\partial \mu_{i}}{\partial p}\right)_{T,x} \nabla p + \sum_{k=1}^{n-1} \left(\frac{\partial \mu_{i}}{\partial x_{k}}\right)_{p,T,x_{k\neq j}} \nabla x_{k} + \left(\frac{\partial \mu_{i}}{\partial T}\right)_{p,x} \nabla T$$
$$= \nabla_{i} \rho \cdot g + \sum_{k=1}^{n-1} \left(\frac{\partial \mu_{i}}{\partial x_{k}}\right)_{p,T,x_{k\neq j}} \nabla x_{k} - S_{i} \nabla T \qquad (12)$$

where S_i = partial molar entropy, $S_i = -\partial \mu_i / \partial T$. Eq. 12 also assumes hydrostatic equilibrium, $\nabla p = \rho g$. Combining Eqs. 1-2 and 12 gives:

Simplifying assumptions which can be used in Eq. 13 are:

- 1. Isothermal gravity chemical equilibrium calculations $(\nabla T = 0)$
- 2. "Passive " thermal diffusion ($F_{Ti} = 0, \nabla T \neq 0$)

Isothermal Gravity/Chemical Equilibrium ($\nabla T = 0$)

In the absence of thermal gradients, a formal solution to compositional grading was given by Gibbs, who defined the conditions of a system in thermodynamic equilibrium under the influence of external forces. For the *isothermal* assumption:

where

$$\mu_i = RT \ln f_i + \lambda_i \quad \dots \quad (15)$$

Eq. 14 integrates from reference depth, h^0 to depth h to yield

$$f_i(h) = f_i(h^0) \exp(-\frac{M_i g(h - h^0)}{RT})$$
(16)

As pointed out by Whitson and Belery³⁹, when using volume shift³⁰ c in the equation of state, the fugacity and fugacity derivatives must be modified using $f_i exp[c_i(p/RT)]$ instead of f_i .

"Passive" Thermal Diffusion ($F_{Ti} = 0, \nabla T \neq 0$)

"Passive thermal diffusion" can be used to describe a hypothetical situation where a thermal gradient exists but thermal diffusion is neglected. Given ∇T and a reference temperature, T(h) is known. Under these conditions our approach has been to solve Eq. 1 numerically, setting $F_{Ti} = 0$, but including the temperature dependency of all other terms. The resulting equation is solved numerically by integrating with depth discretization.

A simplified approach is suggested by Padua²⁹ who makes

additional simplifications for the case where $F_{Ti} = 0$, resulting in the relation

$$f_i(h) = f_i(h^0) \exp(-\frac{M_i g(h - h^0) + S_i \cdot (T - T^0)}{RT})$$
(17)

Padua uses the solution technique proposed in Ref. 39 for isothermal calculations. This approach is *only* valid if both conditions (a) $S_i(T-T^0)$ =constant and (b) $d\lambda_i/dT$ or $d\lambda_i/dh=0$ are satisfied. Unless these two assumptions are known to be valid, numerical integration of Eq. 1 is recommended.

Soret Effect ($F_{Gi} = 0$)

In the absence of gravity, a temperature gradient may induce a compositional gradient by thermal diffusion. This effect is often referred to as the Soret effect, where Eq. 1 simplifies to

Historically^{7,15}, thermal diffusion is expressed in terms of the dimensionless thermal diffusion ratio k_{Ti} , defined by

which represents a balance of fluxes resulting from a compositional gradient governed by Fick's law and thermal diffusion. Another relation for Fick's law using $\nabla \mu_i$ as the driving potential instead of ∇x_i requires a consistent transformation of the traditional molecular diffusion coefficients based on concentration driving potential.

Gradient Solution Algorithms

Gradient calculations always require the following data at a specific reference condition:

- 1. depth
- 2. fluid composition
- 3. pressure
- 4. temperature

For non-isothermal systems, the temperature gradient dT/dh must also be specified. Results of the gradient calculation include composition and pressure at any user-specified depth. It may also is possible to solve for the location of a gas-oil contact (GOC).

Thermodynamic calculations required by the gradient model are made with a valid equation of state model, preferably tuned to measured PVT data for a wide range of fluid samples in the given reservoir.

Isothermal Solution. Eq. 16 can be solved analytically for the isothermal assumption, as outlined by Whitson and Belery. This allows direct calculation of the solution at any depth away from the reference depth – even if the specified depth is on the other side of a gas-oil contact from the reference depth.

An efficient solution algorithm for the isothermal case is successive substitution accelerated with the General Dominant Eigenvalue Method ⁵ (GDEM) for compositions, and Newton-Raphson for pressure.

Non-Isothermal Solution. Integration of Eq. 1 must be solved numerically in depth for a system with temperature gradient. This makes the solution of the non-isothermal problem slower computationally, and prone to discretization error.

Our approach to the non-isothermal problem uses successive substitutions accelerated with GDEM⁵ for composition, and successive substitution for pressure. Gaussian elimination is applied in the inversion process to calculate ∇x_i .

Stability Test. At each depth the converged solution is tested for thermodynamically stability using Michelsen's stability test²⁵. A stable solution at one depth is used to initialize the search for the solution at a new depth.

If an unstable condition is detected then a saturation pressure calculation is performed and the incipient phase is used to restart the gradient calculation. A search for the gas-oil contact can also be initiated at this point, knowing that the phase type has changed in the interval h to $h+\Delta h$.

Gas-Oil Contact Calculation. A general definition of gas-oil contact is the depth where the fluid system changes from a mixture with bubblepoint to a mixture with dewpoint. This may occur at a saturated condition where the GOC gas is in thermodynamic equilibrium with the GOC oil, and reservoir pressure equals the bubblepoint of the GOC oil which equals the dewpoint of the GOC gas. An "undersaturated GOC" may also occur, where the transition from dewpoint gas to bubblepoint oil occurs through a mixture that has a critical point; the critical pressure is lower than the reservoir pressure at the GOC, and consequently the term "undersaturated GOC".

A simple procedure for calculating either type of GOC is to use interval halving, based only on saturation type, as suggested by Whitson and Belery. This method, though slow, is reliable if the saturation pressure algorithm is reliable.

A more efficient approach³⁸ minimizes (forces to zero) the function $f(h_{GOC}) = \Delta_p \times \Delta_K$, where $\Delta_p = (p_R - p_s)/p_R$,

 $\Delta_{K}=\sum_{i}(\ln K_{i})^{2}$, p_{R} is the reservoir pressure, and K_{i} are

evaluated at saturation pressure p_s . The term $\Delta_p=0$ for a saturated GOC, and $\Delta_K=0$ for an undersaturated GOC. A Newton-Raphson solution with step-length control for $f(h_{GOC})=0$ is efficient, particularly for saturated GOC's.

Quantitative Comparison of Different Models

In this section we *quantify* the differences in the various gradient models, with and without thermal diffusion, for a wide range of reservoir fluid systems. In particular, we compare the methane and C_{7+} content, single-stage gas-oil ratio, fluid density, and saturation pressure versus depth.

The four fluid systems given by Whitson and Belery are

used: (1) a saturated low-GOR black oil (BO) with a very-lean gas cap, (2) a saturated slightly volatile oil (SVO) system with a moderately-lean gas cap, (3) an undersaturated volatile oil (VOA) with continuous transition from the high-GOR oil to a rich gas condensate through a "critical" mixture, and (4) a near-critical oil (NCO) with a saturated transition to a rich gas condensate. These systems represent a wide range of realistic petroleum fluid systems. Vertical fluid communication over large depth intervals has been assumed.

Isothermal Gravity/Chemical Equilibrium

Isothermal gravity/chemical equilibrium (GCE) calculations are characterized by increasing C_{7+} mole fraction and dewpoint pressure with depth, while C_1 mole fraction, GOR and bubblepoint pressure decrease with depth. Compositional gradients decrease with increasing degree of undersaturation. Composition and most phase properties are more-or-less linear with depth unless the reservoir fluids are "near critical" (GORs ranging from about 500 – 800 Sm³/Sm³).

Compositional gradients predicted by the isothermal GCE model can be particularly large if (1) the partial derivatives of chemical potential with respect to composition are small³³ (e.g. close to critical conditions), or (2) the gravity term F_{Gi} is large (e.g. if asphalthenes are present in substantial amounts¹⁴).

Figs. 1 and **2** show the derivative of composition with respect to depth for C_1 and C_{7+} , respectively, plotted relative to the gas-oil contact. The maximum compositional variation is found at the gas-oil contact (GOC) for the near-critical reservoir fluid system; for all fluid systems, the maximum compositional variation occurs in the vicinity of the gas-oil contact.

The volatile oil system is somewhat undersaturated and, as shown in Figs. 1 and 2, has less compositional variation near its GOC. Still, the compositional gradients are significant because the oil is quite volatile. The slightly-volatile oil and black-oil fluids both show smaller and approximately linear compositional gradients, both in the gas zone and the oil zone, and with a distinct discontinuity at the saturated GOC.

Dewpoints are very sensitive to the amount and properties of C_{7+} , while bubblepoints are very sensitive to the amount and K-value of methane. Given the compositional variations of C_1 and C_{7+} shown in Figs. 1 and 2, we find similar gradients for saturation pressures. Whitson and Belery present the variation in saturation pressures for the same four fluid systems, expressed as a cumulative change in saturation pressure from the GOC value (**Fig. 3**). This figure can be used to provide "rules of thumb" for expected saturation pressure gradients based on isothermal GCE calculations – usually ranging from a minimal gradient of 0.025 bar/m to a maximum of about 1 bar/m in the vicinity of the gas-oil contact for nearcritical systems.

Figs. 4 and **5** show the methane and C_{7+} variation with depth based on the isothermal gradient model for a wide range of fluid types. Depth is plotted relative to the GOC. All systems except the volatile oil have a saturated GOC, while the VOA fluid is about 60 bar undersaturated at the GOC. For saturated systems, the general observation is made that low-

GOR oils have lean (high-GOR) gas cap fluids; for more volatile oils, the gas cap contains a richer mixture.

Gravity/Chemical/Thermal Models

Basically, two types of non-isothermal gradient models exist – estimating thermal diffusion with a "thermodynamic-based" or "viscosity-based" model. The Haase and Kempers models are the most well-known *thermodynamic-based* models. The Doughtery-Drickamer (Belery-da Silva modification) model is based on "activation energy" which is estimated from a viscosity correlation¹⁷. The Shukla-Firoozabadi³⁵ and Ghorayeb-Firoozabadi¹¹ non-isothermal models require an empirical term relating the relative energies of vaporization and viscous flow.

Based on Eq. 1, we have found that compositional gradients are consistently reduced when compared with the isothermal model, for both thermal diffusion models based on thermodynamic expressions (Haase and Kempers). This behavior is illustrated in **Fig. 6** using the variation of solution GOR with depth. A temperature gradient of -0.035 °C/m has been used for the slightly volatile oil. The predicted Belery-da Silva thermal diffusion factors are multiplied by 0.25. The larger bubblepoint variation predicted by the Belery-da Silva model results in a deeper GOC. In contrast, the Haase model reduces the compositional, GOR and bubblepoint variation, resulting in a predicted GOC some 200 m higher than the isothermal GOC!

This example demonstrates the significant differences between the various thermal diffusion models for oil systems far from a critical condition.

"Near" a critical condition, the Belery-da Silva model generally counteracts gravity, as shown in **Fig. 7** for the volatile oil example. For this system, the predicted mixtures at depths less than about 3000 m show a more-or-less constant composition with depth. As the system becomes more removed from critical conditions (at greater depths), the model tends to exaggerate the gradients beyond what the isothermal model predicts. Whitson and Belery note that for this system there is a sign change in the thermal diffusion ratio of the heaviest components and methane at approximately 3000 m.

When thermal diffusion counteracts gravity, we have found several examples where the thermal effect strongly opposes gravity segregation and potentially results in a mechanically unstable condition that would naturally induce convection. In the event of convection^{9,10}, a one-dimensional formulation such as the component zero-mass-flux model can no longer be used.

Fig. 8 shows calculated C_{7+} mole fraction versus depth for the near-critical oil system, applying a temperature gradient of -0.037 °C/m. In this example all thermal models predict a thermal contribution that opposes the gravity effect throughout the depth interval investigated. As seen from **Fig. 9** the sign of the predicted methane thermal diffusion ratios is negative over the entire depth interval, reaching its minimum or maximum at the gas-oil contact. The resulting C_1 mole fraction variations with depth (**Fig. 10**) are largest in the case of isothermal calculations. In this fluid system the Haase model predicts larger thermal effects than the Kempers model over the entire depth interval studied. As the reference conditions are taken from the oil zone, the Haase model predicts the highest gas-oil contact, whereas the isothermal model predicts the lowest GOC, as seen in **Fig. 11**.

The thermal diffusion factor calculated by the Belery-da Silva method has consistently been reduced to 2% of its predicted values in the NCO example, leading to similar results as the predictions by the Kempers model shown in **Fig. 12**. Without this severe reduction the thermal diffusion effect predicted by the Belery-da Silva model *totally* dominates the gravity term and probably results in mechanically unstable solutions (where convection results). We have found this to be true for a number of near-critical reservoir fluid systems using the Belery-da Silva model.

Firoozabadi and Ghorayeb⁸ recently proposed a new method for calculating thermal diffusion factors in multicomponent systems. Application of the Firoozabadi-Ghorayeb model to the Ekofisk field has been made available to this study by the operator Phillips Petroleum Company. The Firoozabadi-Ghorayeb study reports that in four field applications of the their model, that thermal diffusion always counteracts gravity. We tested the Haase, Kempers, Belery-da Silva models for the same field example (using the same EOS and reference conditions and a temperature gradient of -2.0°F/100 ft). The isothermal and "passive" thermal gradient models were also used, and as seen previously for the nearcritical system (and most other systems), the passive thermal diffusion model is very similar to the isothermal predictions. Figs. 13-15 show results of this comparative study for this example.

Figs. 13 and 14 show predicted variations in C_{7+} and C_1 mole fraction, respectively. Here the Haase, Kempers, and Firoozabadi-Ghorayeb models are similar; all models consistently counteract gravity over the depth interval investigated. The Firoozabadi-Ghorayeb model predicts slightly larger thermal effects than the two other models. This is also seen in Fig. 15, showing predicted GOR variations. The Belery-da Silva model predicts enhancement of the compositional variations in the lower part of the reservoir, and reduces the compositional variations in the upper parts of the reservoir.

In summary, based on the discussion above and experience from other reservoir fluid systems the following observations are given:

- 1. For normal thermal gradients, implementation of the "passive" thermal gradient model does not change the *compositional* variation with depth significantly when compared to isothermal results.
- 2. The Haase and Kempers models predict a thermal effect that opposes the effect of gravity in both gas-like and oil-like systems.
- 3. The Belery-da Silva model typically (a) reduces compositional variations in gas-like systems, (b) enhances compositional gradients in oil-like systems far removed from critical conditions, and (c) counteracts gravity for

near-critical systems, typically resulting in non-physical (mechanically unstable) solutions.

4. For the Ekofisk example, the Firoozabadi-Ghorayeb model predicts similar compositional variations with depth as the Haase and Kempers models – all counteracting gravity.

Fluid Initialization in Reservoir Models

An important task in building a reservoir model is the initialization of fluids, defining gas/oil contacts (if they exist), and estimating the variation of composition with depth for each reservoir unit (e.g. in non-communicating geologic layers and fault blocks). The fluid initialization process defines the initial stock-tank oil and initial sales gas in place. Recoveries may also be affected by initial fluid distributions – e.g. variation in minimum miscibility pressure, as shown by Høier and Whitson 16,17 .

Another important task is quantifying the uncertainty in the initial fluid distribution. Together with uncertainties in other reservoir parameters such as permeability, reservoir unit volumes, reservoir unit communication, relative permeabilities, etc., engineers are expected to generate "cases" that define limits of probable production forecasts – so-called "P10", "P50", and "P90" cases. We address the issue of quantifying uncertainties in initial fluids distribution.

The ability to define an accurate fluid initialization requires a combination of (1) obtaining measured fluid compositions and (2) using models to analyze, interpolate, and extrapolate the measured fluid data.

Our recommendations for fluid initialization, as outlined below, are based on numerous field case histories and the ability of available compositional gradient models to describe observed fluid variations in those fields.

We are keenly aware of the significant uncertainty associated with models for estimating compositional gradients with depth. An important aspect of this study was to quantify differences in predictions between the various models. Furthermore, we doubt that *most* petroleum reservoirs satisfy the many conditions and fundamental assumptions associated with theoretical gradient models.

Zero-Mass-Flux Assumption. The condition of zero component flux and a stationary state is one of several conditions that can be assumed in solving for compositional gradients. Petroleum reservoirs are three-dimensional heterogeneous systems formed in geologic time, experiencing dynamic aquifers, non-communicating layers and fault blocks, and with temperature gradients that change in time and direction. It is probable that many reservoir systems have not yet reached a "stationary state" where component fluxes are "zero".

Furthermore, the dynamics of petroleum generation can lead to severe compositional variations – e.g. local variations in composition due to varying biodegredation, solids precipitation in the more-permeable layers where migration occurs first, and multiple source rocks. These factors and others can lead to complex compositional gradients which are impossible to describe and have little to do with the theoretical considerations discussed above.

The simple one-dimensional zero-mass-flow stationary model, as summarized in this paper and commonly used, should *only* be applied when:

- 1. Field data are lacking and "cases" are needed for defining the uncertainty in fluids in place; or
- 2. Field data are available to "tune" a gradient model, where the tuned model is used for extrapolation to depths where field data are not available.

Field Data

The best fluid initialization results from the judicious use of:

- 1. All PVT samples (bottomhole, surface, and open-hole RFT/MDT) with reported compositions and particularly the C_{7+} content,
- 2. Pressure-depth (RFT/MDT/buildup) data,
- 3. Producing GOR data, and
- 4. A tuned EOS model.

By "judicious" we mean that the uncertainties in each type of data is *quantified* and used to assess each data's value to the initialization. For example, a long-term stable producing GOR from an early production well may be more important than an expensive isokinetic PVT sample collected in an exploration well.

Quantification of initial fluid uncertainty can be defined using plots of data with error bars in depth (perforation interval) *and* composition. Compositional error bars can be estimated from

- 1. GOR variations prior to and during sampling;
- 2. Variation of separator conditions during testing and the possible misuse of constant separator oil shrinkage factors; and
- 3. Estimating the uncertainty of reported C_{7+} molecular weight using a M_{7+} versus γ_{7+} consistency plot for the reservoir(s).

Recommended Initialization Procedures

"Oil-in-Place" Plot. We recommend plotting either C_{7+} content versus depth or, in terms of black-oil PVT properties, "1/B_o" versus depth. The term $1/B_o$ expresses the surface oil produced per reservoir oil volume in place for reservoir oils. For gas condensate fluids, the equivalent expression for "1/B_o" is r_s/B_{gd} , representing the surface condensate produced per reservoir gas volume. In terms of composition, using C_{7+} is more-or-less equivalent to using $1/B_o$ and r_s/B_{gd} (see Figs. 20 and 21).

The oil-in-place plot can be integrated visually, where the area under the curve is proportional to the initial surface oil in place – albeit assuming that reservoir area is constant with depth. If area versus depth is also plotted on this figure, then the oil-in-place variation can be weighed with area to identify the true vertical variation of oil in place.

Define Trends in Compositional Variation. Use all sample data to define trends in compositional variation. Samples considered more insitu-representative are given more "weight" in trend analysis. Still, all data should be plotted and used in the trend analysis because any sample's value in

establishing a trend is automatically defined by inclusion of the samples error bars in depth and composition.

Isothermal Gradient Calculations. For each and every sample falling generally within the trend and which are considered more-or-less insitu representative, an isothermal gradient calculation is performed. The predicted curves (C_{7+} versus depth) are used to identify common behavior and consistency amongst the samples.

The isothermal gradient calculations may deviate substantially from one sample to another. This does not necessarily indicate that the samples are not in a common fluid system. The calculated gradients can be very sensitive to the reference composition and, accordingly, to the uncertainty in reference composition. This is shown in **Figs. 16** and **17** for the near-critical oil system, where a 5% uncertainty in recombination GOR is evaluated.

The composite behavior of measured and gradientcalculated C_{7+} versus depth is studied to assess which fluids are (a) probably in fluid communication and (b) insitu representative and should be used for fluid initialization.

Clearly, with only a few samples, the use of theoretical gradient models can have a significant impact on fluid initialization. Our experience is that the isothermal model usually predicts the largest gradients, and therefore represents one "extreme". Using the constant-composition case covers the other extreme. Both models have field case histories which substantiate their validity.

Interpolation. If clear trends exist in the measured data, we use them directly with linear interpolation between the samples. Care must be taken to check that the resulting saturation pressure versus depth trend, and density versus depth are physically meaningful. Special treatment around the gas-oil contact may be necessary to ensure consistency with observed contacts.

Extrapolations. Two extrapolations are used for estimating fluids beyond the range of measured data – above the uppermost insitu-representative sample and below the lower-most insitu-representative sample: (1) isothermal gradient prediction using the outer-most selected samples as reference samples, and (2) assuming the compositions are constant and equal to the outer-most selected samples. These two assumptions normally define maximum uncertainties in fluid initialization.

The choice of these two assumptions for defining the *probable uncertainty* in initial fluids in place lies in the observation that (a) several field-case histories indicate that the isothermal model gives a reasonable representation of observed gradients, (b) the isothermal model generally predicts a maximum gradient compared with non-isothermal models, (c) some reservoirs where the isothermal model predicts a strong compositional gradient show very little compositional grading (possibly due to convective mixing).

Defining uncertainties with a non-isothermal gradient model that predicts gradients larger than the isothermal model – e.g. the Belery-da Silva model for near-critical nearsaturated systems – is not recommended. We do not feel that the theoretical foundation for such models (thermal diffusion transport equations, thermal diffusion constants, and boundary conditions assumed to solve the zero-mass-flux problem) are known with enough certainty to take these calculations "to the bank".

GOC Sensitivity to Saturation Pressure. The approximate location of a gas-oil contact can be estimated from the reference sample pressure gradient ($\nabla p_R = \rho g$) and reference sample saturation pressure gradient ∇p_s (based on a gradient calculation),

$$h_{GOC} = h^{o} - \frac{p_{s}^{o} - p_{R}^{o}}{\nabla p_{s} - \nabla p_{R}}$$
....(20)

This relation assumes the saturation pressure and reservoir pressure gradients are approximately constant from the reference depth to the GOC.

An important consequence of this relation is the extreme sensitivity of the predicted GOC to the reference sample saturation pressure. Often a new field is discovered by drilling into gas at a structurally-high location. A major question will be the possibility of an underlying oil zone. An estimate of the GOC can be made using an EOS model tuned to the gas sample and, for example, the isothermal gradient model. This calculation will also provide the values of ∇p_R and ∇p_s .

The impact of uncertainty in reference-sample dewpoint, δp_d^o , on estimated oil-column thickness, δh_{oil} , is given by

$$\frac{\delta h_{oil}}{\delta p_d^o} = \frac{\delta h_{GOC}}{\delta p_d^o} = \frac{1}{\nabla p_s - \nabla p_R}$$
(21)

A "typical" gas condensate discovery might have $\nabla p_R=0.03$ bar/m and $\nabla p_s=0.1$ bar/m, yielding a sensitivity in oil column thickness of 15 m per bar uncertainty in dewpoint pressure of the reference sample. For a leaner reservoir gas with $\nabla p_s=0.05$ bar/m, the uncertainty is 50 m oil column thickness per bar uncertainty in dewpoint of the reference sample!

The strong sensitivity of estimated oil column thickness to reference-sample dewpoint leads us to recommend that every effort should be made to measure accurately *and model accurately* dewpoint pressure of samples in reservoirs showing this type of sensitivity.

History Matching. One attractive feature of our recommended initialization procedure is that the fluid initialization guarantees a near-perfect match of the initial surface oil and surface gas in place and producing GOR for the samples selected for defining the composition versus depth trend.

Updating the composition versus depth trend used in a reservoir model may continue as new wells come on production. This requires that the reservoir remains undersaturated, injection gas has not reached the new producers, and that water movement has not displaced insitu fluid distributions.

New wells and samples may not fall in line with the current fluid initialization. Assuming this data is not affected by depletion or displacement processes, other factors must be considered - e.g. geological segmentation in layers or fault

blocks; lateral methane and temperature variations; regional differences in petroleum generation and migration.

When only one or a few samples are available, then we always recommend evaluating the two most probable extreme cases – (a) variation given by the isothermal gradient model, and (b) constant-composition extrapolation. Both types of behavior have been found in petroleum reservoirs. Management must be warned, however, that only additional samples (delineation wells) can reduce the uncertainty in fluid definition (see the Cupiagua example below). "Putting oil in the ground" with a gradient model, based only on gas samples, *is highly uncertain*, and should be treated as such.

Field Case Histories

In this section we present two field case histories which illustrate some of the issues discussed earlier.

Smørbukk Field, Åsgard

This field produces gas condensate and volatile oil fluids from several non-communicating geologic layers. Most of the layers appear to contain different fluid systems. This can be seen clearly by plots of C_{7+} content versus depth, where separate fluid systems show clear and separate trends.

The example given here is from a geologic layer containing an undersaturated gas condensate, with six samples collected from several wells and test intervals. Each sample is plotted in **Fig. 18** as C_{7+} content versus depth. The perforation intervals are shown as vertical error bars. Some samples have the uncertainty of recombination GOR shown as a horizontal error bar.

As recommended earlier, an isothermal gradient calculation is made for each sample separately. The EOS model used in the gradient calculations was developed for the entire field (seven fluid systems) using more than 70 samples with extensive PVT data covering a wide range of fluid types from medium-to-lean gas condensates to volatile oils.

The "suite" of isothermal gradient predictions for C_{7+} content versus depth do not overlay. Only one of the gradient curves (Well A, DST1 sample) seems to match the compositional gradient defined by the six samples. Still, all of the gradient curves give a similar near-critical behavior, with transition from gas condensate to oil through an undersaturated GOC (critical point).

For this particular reservoir, we recommend using five of the six samples for defining composition versus depth, with linear interpolation amongst these samples. For extrapolation, we suggest using the isothermal gradient predictions downwards for the lowermost sample and upwards for the uppermost sample.

Because the isothermal gradient calculation for the Well A DST1 sample matches reasonably well all of the other samples, it would be acceptable to use its predicted gradient for initializing the entire geologic unit.

Either approach described above would define the P50 case for fluid initialization. The suite of other isothermal gradient curves, together with constant-composition assumption above the uppermost sample and below the lowermost sample can be used to define the P10 and P90 cases for fluid initialization – cases which (1) honor approximately the measured sample data and (2) define the extremities of calculated initial oil in place (minimum and maximum).

In summary, this example shows that the isothermal gradient model quantitatively describes the measured compositional variation of a near-critical gas condensate / volatile oil system Similar results were found for most of the other reservoir units in this field (though most of the units had fewer samples and less compositional variation).

Cupiagua

The Cupiagua field²² in Colombia is an unusual fluid system containing a rich gas condensate showing little variation in composition and properties over a structural depth of almost 5000 ft (10500 to 15000 ft subsea). Dewpoint pressures vary little, 5350 ± 50 psia, with a temperature ranging from 240 to 300 °F. Reservoir density is almost invariant throughout the reservoir 28.5-30.5 lb/ft³ (0.198-0.211 psi/ft), at pressures ranging from about 6200 psia to 7100 psia.

One of the first samples collected in the Cupiagua field was from a top-structure well at about 10750 ft subsea. Using a tuned EOS model, the isothermal gradient calculation with this top-structure sample predicts a gas-oil contact at 11040 ft subsea (**Fig. 19**) – i.e. a 4000 ft of oil column!

Calculation of the initial oil in place is given in **Fig. 20**, where surface oil volume per HC pore volume $(r_s/B_{gd} \text{ and } 1/B_o)$ is plotted versus depth; results come from an EOS-model initialization using constant area with depth. Comparing (a) the current fluid model based on available samples and showing little fluid property variation and (b) the isothermal calculation based only on the initial top-structure gas sample, the isothermal gradient model overpredicts initial oil in place by more than a factor of 3. **Fig. 21** shows C_{7+} variation with depth, where the behavior is strikingly similar to the "oil-in-place" behavior seen in Fig. 20.

It should be clear from this example that the uncertainty in initial fluids can be significant, and particularly when limited (gas) samples are available.

Conclusions and Recommendations

- 1. Thermal diffusion generally counteracts gravity, resulting in compositional gradients with depth which are smaller than predicted with the isothermal gradient model.
- 2. For near-critical, near-saturated systems, thermal diffusion may be so large, compared with gravitational-segregating forces, that convection is initiated and a "mixed" system with more-or-less constant composition with depth results.
- 3. Field observations have shown that some reservoirs follow reasonably well the isothermal gradient model. We suggest that the isothermal model be used to extrapolate fluid compositions beyond the limits of where insitu-representative samples are available.
- 4. Other reservoirs exhibit nearly-constant compositions with depth sometimes over thousands of feet even

9

when the isothermal model predicts large compositional gradients. This observation leads us to suggest that constant-composition extrapolation should be used beyond the limits where insitu-representative compositions are available. Constant-composition extrapolation in depth will define another uncertainty case.

- 5. Other reservoirs exhibit compositional gradients that are larger than predicted by the isothermal model, though few well-documented cases are available in the literature. Gradients larger than predicted by the traditional EOS-based isothermal gradient model may result for many reasons, none of which can be readily modeled with any quantitative certainty.
- 6. The many assumptions used by the zero-component-massflux models, with and without thermal diffusion, may be inappropriate. Many reservoirs may not have reached a "stationary state" of zero component mass flux. We caution the indiscriminate use of these simplified gradient models to describe initial fluid distributions. Instead, measured samples should be used to define compositional trends, where gradient models are used *only* for extrapolating measured trends and defining "possible" fluid distributions.

Nomenclature

\mathbf{B}_{gd}	= formation volume factor of dry gas
Bo	= formation volume factor of oil
ci	= volume shift parameter, component i
C _{pi,id}	= ideal heat capacity, component i
C ₇₊	= heptanes and heavier components
f(h)	= function equal to zero at the gas-oil contact
\mathbf{f}_{i}	= fugacity, component i
F _{Gi}	= gravity term, component i
F_{Ti}	= term including model for thermal diffusion,
	component i
g	= gravitational acceleration
h _{GOC}	= gas-oil contact depth
\mathbf{h}^0	= reference depth
h	= depth
H_i	= partial molar enthalpy, component i
H_{m}	= mixture enthalpy
\mathbf{k}_{Ti}	= thermal diffusion ratio, component i
Ki	= equilibrium ratio (K-value), component i
M_i	= molecular weight, component i
M_{m}	= mixture molecular weight
n _i	= moles of component i
n	= total number of moles; number of components
p _R	= reservoir pressure
p_R^0	= reservoir pressure at reference depth
ps	= saturation pressure
p_{s}^{0}	= saturation pressure at reference depth
р	= pressure
rs	= solution oil-gas ratio
R	= the universal gas constant
Si	= partial molar entropy, component i

 $T_{i} = partial motar$ $T_{i} = temperature$

- ΔU_i^* = partial molar activation energy, component i
- ΔU_m^* = viscosity-to-density ratio dependent term used to calculate ΔU_i^*
- V_i = partial molar volume, component i
- V_m = mixture molar volume
- x_i = composition, mole fraction component i
- $\nabla f = df/dh$
- γ_{7+} = C₇₊ specific gravity
- $\Delta_{\rm K}$ = term equal zero at the undersaturated GOC
- Δ_p = term equal zero at the saturated GOC
- λ_i = temperature dependent term in expression for chemical potential, component i
- δh_{oil} = uncertainty in estimated oil-column thickness
- δp_d^0 = uncertainty in reference dewpoint pressure
- μ = viscosity
- μ_i = chemical potential, component i
- ρ = density

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Fig. 18— Measured and calculated C₇₊ variations with depth for a reservoir in the Smørbukk Field, Åsgard. Isothermal GCE calculations made for each sample separately. Recommended interpolations shown as dashed line.



Fig. 19 — Current field-data based initialization with approximately constant saturation pressure variation with depth in the Cupiagua Field, compared to isothermal GCE predictions based on top structure gas sample.







Fig. 21 — Current field-data based initialization for C_{7*} variation with depth in the Cupiagua Field (density is approximately constant with depth), compared to isothermal GCE calculations based on top structure gas sample