

Paper E

Isothermal Gravity/Chemical Equilibrium Calculations *

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ISOTHERMAL GRAVITY/CHEMICAL EQUILIBRIUM CALCULATIONS

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Abstract

We have implemented and tested a computer program which can determine the phase composition and the pressure above and below a given reference depth in a fluid column. The program can also determine whether the oil phase becomes saturated, i.e., whether a gas-oil contact exists within a specified depth range in the reservoir. To do so, the program uses a phase stability test. We have only considered isothermal cases.

As an extension of the above tasks, the program also calculates bubblepoint or dewpoint pressures at the various depths, provided that suitable initial estimates are calculated. The ultimate alternative of generating the entire phase envelope has also been implemented.

The program can be used as a tool for initializing a 3D reservoir simulator at steady state equilibrium. It can also be applied to check if data from different fluid test samples, taken from the same petroleum reservoir at different depths, are in accordance. However, under the current implementation, the program can only do calculations on fluids containing species from a list of 15 components.

This report provides an outline of the thermodynamic relations behind the calculations, and the numerical schemes used for solution of the various equations are presented shortly. Application of the program is also presented, including plots of reservoir pressure versus depth, saturation pressure versus depth, phase composition versus depth and some phase envelopes, all generated by the program.

A copy of the source code of the program is given as an attachment to this report.

1 Introduction

When fluids are at equilibrium in a gravity field, the individual phases are not homogenous. At each depth there exists at most one distinct phase, and

the fluids are subject to pressure and composition gradients in the vertical direction.

The pressure at a given point depends on the mass density of fluids situated above that point. Consequently, pressure increases with depth, and the pressure gradient is larger in an oil (liquid) phase than in a gas (vapour) phase. Heavy components tend to be placed in the lower part of the fluid column, and the largest amounts of light components are found in the upper part.

If both an oil phase and a gas phase exist in a fluid column, the gas is situated on top of the oil. The border between oil and gas can be sharp, in which case we have a distinct so-called gas-oil contact (GOC). As we approach such a GOC from below, we find that the oil phase becomes unable to increase its amount of light components, i.e., the oil becomes saturated.

If, however, the fluids are critical in the region between the gas column and the oil column, it is impossible to specify an exact GOC. As we approach the GOC region from below the oil phase is still able to increase its amount of light components. Such a GOC region is therefore referred to as an undersaturated GOC.

In order to determine the variations in pressure and composition with depth, and to be able to indicate if a gas-oil contact exists, we must perform gravity/chemical equilibrium (GCE) calculations. GCE calculations are based on thermodynamic principles and equations.

1.1 The GCE governing equations

By including the effect of gravity in the first law of thermodynamics, we obtain the so-called fundamental relation:

$$dU = TdS - PdV + \sum_{i=1}^{N_c} \mu_i dn_i - d\left(\sum_{i=1}^{N_c} m_i gD\right), \quad (1)$$

where U is internal energy, T is absolute temperature, S is entropy, P is pressure, V is volume, μ_i is the chemical potential of component i , n_i are the

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moles of component i , m_i is the total mass of component i , g is the gravitational acceleration and D is depth. The number of components in the system is denoted N_c .

The internal energy U is by definition given by

$$U = TS - PV + \sum_{i=1}^{N_c} \mu_i n_i - \sum_{i=1}^{N_c} m_i g D. \quad (2)$$

By comparing the total differential of U ,

$$\begin{aligned} dU &= TdS - PdV + \sum_{i=1}^{N_c} \mu_i dn_i - d\left(\sum_{i=1}^{N_c} m_i g D\right) \\ &+ SdT - VdP + \sum_{i=1}^{N_c} n_i d\mu_i, \end{aligned} \quad (3)$$

to the fundamental relation (1), we obtain the so-called Gibbs-Duhem condition,

$$SdT - VdP + \sum_{i=1}^{N_c} n_i d\mu_i = 0. \quad (4)$$

The second law of thermodynamics implies that an equilibrium state of an isolated system is a stationary point of maximum entropy. Equivalently, but more conveniently, using T, P and \mathbf{n} as the complete set of independent variables, equilibrium corresponds to a minimum of the Gibbs energy G , given by

$$G = U + PV - TS = \sum_{i=1}^{N_c} \mu_i n_i - \sum_{i=1}^{N_c} m_i g D. \quad (5)$$

Consequently, in order for a single phase fluid to remain at equilibrium in a gravity field, we must not be able to decrease the Gibbs energy by moving a differential molar amount δn_i a vertical distance dD .

Assume that moving δn_i corresponds to a change $d\mu_i$ in the chemical potential of component i . Using the relation $m_i = M_i n_i$, where M_i is the molecular weight of component i , we write

$$dG = \sum_{i=1}^{N_c} (d\mu_i - M_i g dD) \delta n_i \geq 0, \quad \forall \delta n_i, \quad (6)$$

which yields the stability condition

$$d\mu_i - M_i g dD = 0, \quad i = 1, 2, \dots, N_c. \quad (7)$$

For an isothermal system, $dT = 0$, the Gibbs-Duhem condition (4) combined with the stability condition (7) gives

$$dP = \rho g dD, \quad (8)$$

where $\rho = \sum_{i=1}^{N_c} M_i n_i / V$ is the mass density of the fluid. Equation (8) is the well-known condition for hydrostatic equilibrium.

1.2 Convenient reformulation

The chemical potential μ_i is conveniently expressed by the relation

$$\mu_i = \mu_i^*(T) + RT \ln f_i, \quad (9)$$

where $\mu_i^*(T)$ is the temperature-dependent ideal-gas contribution, R is the universal gas constant, and f_i is the fugacity of component i . For an isothermal system, equation (7) may therefore be written

$$\frac{1}{f_i} df_i = \frac{M_i g}{RT} dD. \quad (10)$$

This ordinary differential equation has the solution

$$f_i(D) = f_i(D_{\text{ref}}) e^{\frac{M_i g}{RT} (D - D_{\text{ref}})}, \quad (11)$$

where D_{ref} is some reference depth at which we know the pressure and the phase composition (in addition to the uniform temperature), and thereby also the fugacity.

We note that fugacities f_i are often expressed in terms of pressure P , phase composition \mathbf{z} and the fugacity coefficient ϕ_i ,

$$f_i = P z_i \phi_i. \quad (12)$$

The fugacity coefficients are calculated from some thermodynamic model, for example an equation of state model (e.g., Peng-Robinson, Soave-Redlich-Kwong). We refer to Michelsen and Mollerup, [1], for details.

If the GCE calculation is based on an equation of state model, component volumes v_i should, according to Whitson and Berely, [2], be adjusted by the Peneloux correction, $v_{i,\text{corr}} = v_i + c_i$, where c_i is known as the volume shift. Fugacities must then also be corrected:

$$f_{i,\text{corr}} = f_i e^{\frac{c_i P}{RT}}. \quad (13)$$

However, the Peneloux correction has not been used in the calculations presented in this report.

1.3 The possible presence of a GOC: Stability analysis

Equation (11) applies to single phase fluids, both liquid and vapour, and can therefore be used to determine pressure and composition throughout a fluid column at steady state. However, precautions must be made to prevent the GCE calculation from being applied to an unstable (e.g., two phase) composition. Any pressure P and composition \mathbf{z} calculated from (11) must therefore be checked, to see if the proposed solution is a stable single phase.

The single phase stability condition is derived in a similar manner to the gravity/chemical equilibrium condition (7), and may be written

$$\text{TPD}(\mathbf{y}) = \sum_{i=1}^{N_c} y_i (\mu_i(\mathbf{y}) - \mu_i^I(\mathbf{z})) \geq 0, \quad \forall \mathbf{y}. \quad (14)$$

Here \mathbf{y} is the composition of a proposed new phase, and superscript l indicates a single phase of composition \mathbf{z} . Condition (14) is often referred to as the tangent plane distance condition of Gibbs. For computational convenience, we may introduce the modified tangent plane distance measure

$$\begin{aligned} \text{tm}(\mathbf{Y}) &= 1 + \sum_{i=1}^{N_c} Y_i (\ln Y_i + \ln \phi_i(\mathbf{Y}) - e_i - 1), \\ e_i &= \ln z_i + \ln \phi_i(\mathbf{z}). \end{aligned} \quad (15)$$

Here the Y_i are formally treated as mole numbers. We refer to Michelsen and Mollerup, [1], for details.

The application of stability analysis in GCE calculations can be described as follows. If, at some depth, the solution obtained from (11) implies an unstable fluid, i.e., there exists at least one composition \mathbf{y} such that the tangent plane distance condition (14) is violated, we have discovered the existence of a gas-oil contact (a gas-oil contact region).

To proceed with GCE calculations on the other side of the GOC, we may let the \mathbf{y} , corresponding to the most negative minimum, be the initial estimate for a repeated solution of (11), so that we eventually obtain a switch from one single phase state to another.

Moving through an undersaturated GOC region, the stability test will never indicate instability, and no distinct phase switch can be observed. To locate an undersaturated GOC, we must do saturation point calculations.

1.4 Saturation point calculations

Saturation point calculations may serve as an illuminating complement to stability analysis in GCE calculations. At each depth in the liquid column, the difference between the reservoir pressure and the bubblepoint pressure indicates how far we are from the appearance of a vapour phase. Similarly, in a gas column, the difference between the reservoir pressure and the dewpoint pressure indicates how far we are from the appearance of a liquid phase (i.e., condensed vapour).

The dewpoint pressure will also indicate whether we have a so-called retrograde gas condensate. If the dewpoint pressure is below the reservoir pressure, depressurization will lead to condensation of the gas.

In addition, if a GOC exists, the bubblepoint pressure and the dewpoint pressure will be equal at the GOC. If the GOC is saturated, the saturation pressures will also be equal to the reservoir pressure. This is not the case if the GOC is undersaturated. Consequently, saturation point calculations give guidance for characterizing a GOC.

Saturation point calculations are based on the set of equations

$$\ln K_i = \ln \phi_i^l(\mathbf{x}, T, P) - \ln \phi_i^v(\mathbf{y}, T, P), \quad (16)$$

$$\sum_{i=1}^{N_c} (y_i - x_i) = 0. \quad (17)$$

Here \mathbf{x} denotes a liquid composition, \mathbf{y} is a vapour composition and $K_i = y_i/x_i$ is the K-value of component i . Equation (16) requires that the chemical potentials of the liquid and vapor phases are equal, while equation (17) represents the material balance.

In the isothermal case, the task reduces to finding the saturation pressure of a given single phase composition \mathbf{z} at the given temperature T . For bubblepoint calculations, $\mathbf{z} = \mathbf{x}$, equation (17) reduces to

$$g = \sum_{i=1}^{N_c} K_i z_i - 1 = 0, \quad (18)$$

and for dewpoint calculations, $\mathbf{z} = \mathbf{y}$, it reduces to

$$g = 1 - \sum_{i=1}^{N_c} \frac{z_i}{K_i} = 0. \quad (19)$$

Saturation point pressure calculations rely on good initial estimates for pressure and the incipient phase composition. If a saturation point of the same kind as the one we are looking for (bubblepoint or dewpoint) has already been found, this previous point is likely to be a good initial estimate. However, for the calculation of the very first saturation point, we use the Wilson correlation,

$$\ln K_i = \ln \left(\frac{P_{ci}}{P} \right) + 5.373(1 + \omega_i) \left(1 - \frac{T}{T_{ci}} \right), \quad (20)$$

to generate the initial estimate. This approximation is valid at low pressures, as fluids in the low pressure region behave nearly like ideal gases.

We can not expect that saturation point calculations based on initial estimates from the Wilson correlation succeed in a broad pressure range. Then the ultimate solution is to start with an easy saturation point calculation (for instance, a low pressure bubblepoint), and generate the entire phase envelope, including the saturation point(s) we are looking for.

Phase envelope calculations are based on the set of equations (16) and (17), with the relations

$$x_i = \frac{z_i}{1 - \beta + \beta K_i}, \quad y_i = \frac{K_i z_i}{1 - \beta + \beta K_i}. \quad (21)$$

If \mathbf{x} is the liquid phase composition and \mathbf{y} is the vapour phase composition, β is the vapour fraction.

2 Practical Implementation

The implemented computer program requires that a reference pressure P_{ref} and a stable single phase reference composition \mathbf{z}_{ref} at some reference depth D_{ref} is given as input. The temperature T must also be specified, and is kept fixed at all depths.

On user demand, the program should then be able to determine the pressure and fluid composition at other depths D , above and below the reference point. In addition, the program should be able

to indicate whether a gas-oil contact exists within a user-specified depth range. In the case of an undersaturated GOC, the user must identify the GOC from the generated saturation pressure versus depth plot.

2.1 GCE calculations

The gravity/chemical equilibrium part of the program must solve equation (7), or more conveniently, equation (11), in a way so that the Gibbs-Duhem condition (8) is fulfilled. We accomplish this by using a numerical scheme that converges pressure and composition at the same time.

For notational convenience, we define

$$\tilde{f}_i \equiv \tilde{f}_i(D, D_{\text{ref}}) = f_i(D_{\text{ref}}) e^{\frac{M_i g}{RT}(D - D_{\text{ref}})} \quad (22)$$

so that fugacities with a $\tilde{}$ have been gravity corrected with respect to some reference depth D_{ref} . The calculation of all the \tilde{f}_i is the starting point of any GCE calculation in the program.

2.1.1 A Newton-Raphson scheme

We define the vector equation

$$\mathbf{F} = \begin{bmatrix} f_1 - \tilde{f}_1 \\ f_2 - \tilde{f}_2 \\ \vdots \\ f_{N_c} - \tilde{f}_{N_c} \\ \sum_{i=1}^{N_c} z_i - 1 \end{bmatrix} = \mathbf{0}, \quad (23)$$

and the variable set

$$\mathbf{u} = [z_1, z_2, \dots, z_{N_c}, P]^T, \quad (24)$$

where \mathbf{u} is to be determined at a depth D , and $f_i = P z_i \phi_i$ is the fugacity at that depth.

We set up the following Newton-Raphson scheme for solving equation (23):

$$\mathbf{F}'^{(k-1)} \left(\mathbf{u}^{(k)} - \mathbf{u}^{(k-1)} \right) = -\mathbf{F}^{(k-1)}. \quad (25)$$

Here superscript k refers to iteration step k , and $k = 0$ corresponds to an initial estimate.

The Jacobian $\mathbf{F}' = \left\{ \frac{\partial F_i}{\partial u_j} \right\}$ is calculated using the following derivatives:

$$\frac{\partial f_i}{\partial u_j} = \frac{f_i}{P} \frac{\partial P}{\partial u_j} + \frac{f_i}{z_i} \frac{\partial z_i}{\partial u_j} + \frac{f_i}{\phi_i} \frac{\partial \phi_i}{\partial u_j}, \quad (26)$$

$$\frac{\partial P}{\partial u_j} = \begin{cases} 1 & , \quad u_j = P \\ 0 & , \quad u_j \neq P \end{cases}, \quad (27)$$

$$\frac{\partial z_i}{\partial u_j} = \begin{cases} 1 & , \quad u_j = z_i \\ 0 & , \quad u_j \neq z_i \end{cases}, \quad (28)$$

$$\frac{\partial \phi_i}{\partial u_j} = \phi_i \frac{\partial \ln \phi_i}{\partial u_j}. \quad (29)$$

Expressions for the derivatives of the $\ln \phi_i$, are provided by Michelsen and Mollerup, [1].

With a suitable initial estimate \mathbf{u}^0 , the Newton-Raphson approach is quadratically convergent, and the solution \mathbf{u} satisfies the Gibbs-Duhem condition (see Halldórsson and Stenby, [3]).

If the depth where we want to determine pressure and composition is not too far from the reference depth, $\mathbf{u}^0 = [z_{\text{ref}}, P_{\text{ref}}]^T$ provides a good initial estimate for the Newton-Raphson scheme. In addition, if we calculate several subsequent pressures and compositions in some depth range, we may redefine the reference state to increase the quality of the initial estimates.

If we look for a single pressure and composition far away from the reference depth, the reference state may no longer be a sufficiently good initial estimate for the Newton-Raphson scheme. We have therefore also included a successive substitution based approach. Such a scheme is not as dependent on proper initial estimates as the Newton-Raphson scheme. However, many iterations may be required for convergence, especially in near critical regions. The program therefore only switches to the successive substitution approach if the Newton-Raphson scheme fails to converge.

2.1.2 A successive substitution scheme

The successive substitution scheme we have implemented is described by Whitson and Berely, [2]. The scheme is used to solve the equation

$$Q(\mathbf{z}, P) = 1 - \sum_{i=1}^{N_c} z_i \frac{\tilde{f}_i}{f_i} = 1 - \sum_{i=1}^{N_c} Y_i = 0, \quad (30)$$

iteratively with respect to pressure and composition. Each iteration step consists of a Newton-Raphson correction of the pressure,

$$P^{(k+1)} = P^{(k)} - \frac{Q^{(k)}}{(\partial Q / \partial P)^{(k)}}, \quad (31)$$

followed by an update of the variable Y_i ,

$$Y_i^{(k+1)} = Y_i^{(k)} \left[r_i^{(k)} \right]^\lambda, \quad (32)$$

where

$$r_i = \frac{\tilde{f}_i}{f_i} \left(\sum_{i=1}^{N_c} Y_i \right)^{-1}. \quad (33)$$

λ is an acceleration parameter, and $\lambda = 1$ implies an unaccelerated scheme. For acceleration, Whitson

and Berely suggest to calculate λ as an approximation to the dominant eigenvalue of the problem. Acceleration is then performed at every fourth step of the iteration. We have not investigated the effects of this acceleration, and consequently used $\lambda = 1$.

The composition \mathbf{z} is at each step updated by

$$z_i^{(k+1)} = \frac{Y_i^{(k+1)}}{\sum_{j=1}^{N_c} Y_j^{(k+1)}}, \quad (34)$$

and we iterate until convergence. We refer to Whitson and Berely, [2] for more details on the successive substitution scheme.

2.2 Stability tests

To ensure that only GCE calculations on a stable single phase are pursued, and to be able to locate saturated GOCs, the program contains a stability test. The stability test is performed after each proposed solution of the GCE problem. We have implemented the stability test as a simplified search for negative minima of the tangent plane distance. Using the Wilson correlation, the program calculates two initial estimates, one “light” estimate

$$y_i = K_i^{\text{Wilson}} z_i, \quad (35)$$

and one “heavy” estimate

$$x_i = \frac{z_i}{K_i^{\text{Wilson}}}. \quad (36)$$

We then seek (possibly negative) minima of the function (15) by the successive substitution scheme

$$\ln Y_i^{(k+1)} = e_i - \ln [\phi_i(\mathbf{Y}^{(k)})]. \quad (37)$$

Here $Y_i^0 = y_i$ (light estimate) or $Y_i^0 = x_i$ (heavy estimate), and the Y_i are formally treated as mole numbers.

If a negative minimum of the tangent plane distance is discovered, the program reports that a saturated gas-oil contact has been found.

To proceed calculations on the other side of the GOC, the program uses the composition \mathbf{w} corresponding to the most negative minimum as an initial estimate for recalculating the GCE. Consequently, a switch from one single phase state to another eventually is obtained.

2.3 Saturation point calculations

The implemented GCE calculations combined with a stability test yields a computer program capable of determining pressure and composition at depths above and below a given reference depth, and of deciding whether a saturated gas-oil contact exists in a certain depth range. However, to identify any undersaturated gas-oil contacts, procedures for calculating saturation pressures are added. Under the

current implementation, saturation point calculations are only performed when the user specifies a depth range for GCE calculations.

2.3.1 A successive substitution approach

The saturation point calculations are based on a successive substitution approach. With an ideal solution approximation, the compositional dependence in the K-values of equations (18) and (19) are neglected. By using this approximation at the start of each iteration step we may update the saturation pressure by a Newton-Raphson correction,

$$P^{(k+1)} = P^{(k)} - \frac{g^{(k)}}{(dg/dP)^{(k)}}, \quad (38)$$

where the equation $g = 0$ is defined by (18) for bubblepoint calculations, and by (19) for dewpoint calculations. We then update the composition of the incipient phase by

$$y_i^{(k+1)} = z_i \left(\frac{\phi_i^l}{\phi_i^v} \right)^{(k)}, \quad (39)$$

or

$$x_i^{(k+1)} = z_i \left(\frac{\phi_i^v}{\phi_i^l} \right)^{(k)}, \quad (40)$$

for bubblepoints and dewpoints, respectively.

The very first bubblepoint and dewpoint calculations are the most difficult, as no initial estimates of guaranteed quality are given. The program therefore first tries to use an initial estimate from the Wilson approximation. In other words, it solves (18) or (19) with respect to the initial pressure estimate, and finds the incipient phase initial estimate from the relation $K_i^{\text{Wilson}} = y_i/x_i$.

If calculations based on the Wilson initial estimate fail to converge, the program tries to construct the entire phase envelope (see below), thereby most likely generating a sufficiently good initial estimate for the desired saturation point(s).

When the very first dew- and bubblepoints have been determined, these points are used as initial estimates for later saturation point calculations. However, in near critical regions, the successive substitution scheme may still fail to produce a solution in a reasonable number of iterations, in which case the program skips the saturation point calculation in question.

2.3.2 Phase envelope construction

The phase envelope calculation available in the program uses the natural logarithms of pressure, temperature and K-values as primary variables. As we have $N_c + 1$ equations, (16) and (17), in $N_c + 2$ variables, the program may at each stage in the construction process, specify one of the primary variables, say U , as $U = S$.

At each determined point of the phase envelope, the program also calculates the derivatives of all primary variables with respect to the specified S at that point (so-called sensitivities). The sensitivities indicate how much each primary variable will change if S is changed. The program uses this information to provide a suitable initial estimate for a Newton-Raphson calculation of the next saturation point. To control the changes in all the variables, the program automatically chooses to specify the variable that is expected to change the most (i.e., has the largest sensitivity). Based on the number m of Newton iterations required for convergence of the previous point, the steplength (the change in the specified variable U) is either kept fixed ($m = 3, 4$), increased ($m < 3$) or decreased ($m > 4$).

The near critical region should pose no convergence problems for this procedure, as long as at least one of the $\ln K_i$ is kept non-zero in that region. In addition, the program can locate the approximate position of critical points by registering when all the $\ln K_i$ switch sign.

As the first initial estimate, the program uses a low pressure bubblepoint temperature calculation ($P < 1$ MPa). This should be a fairly easy task, as fluids at low pressures behave nearly ideal, and the Wilson correlation gives good K-value estimates. When calculations reach/pass the given reservoir temperature T , the program registers the pressure and the incipient phase composition, and is able to interpret the point as a bubblepoint (if no critical point has been detected) or a dewpoint (if a single critical point has been detected).

We note that the implemented automatic generation of the entire phase envelope may fail, in which case the program ignores the phase envelope calculation, and produces an error message.

Further details on phase envelope construction are found in [1].

2.4 The final program

The final program reads reference data from the file `input.dat` and gives the following user options:

1. Calculate pressure and composition at a specified depth D
2. Search for a gas-oil contact in a specified depth range
3. Generate the phase envelope at a specified depth D
4. Exit program

Option 1 only gives output to screen. Option 2 gives output to screen and generates the matlab-files `plots.m` and `comps.m`, which can be used to obtain plots of reservoir pressure and saturation pressures versus depth, and compositions versus

depth, respectively. Option 3 generates a matlab-file `phaseenv.m`, used for plotting the phase envelope. Note that repeated runs will overwrite the output files.

Note also that, under the current implementation, the user must choose from the following list of components when constructing `input.dat`:

Table 1: List of components

1: C1	2: C2	3: C3
4: iC4	5: nC4	6: iC5
7: nC5	8: nC6	9: nC7
10: nC8	11: nC9	12: H2O
13: N2	14: CO2	15: H2S

This is due to the use of Fortran subroutines provided at the IVC-SEP Summer School 2004. We refer to [4] for details.

A listing of the source code behind the program is given as an appendix to this report.

3 Results

The program has been tested on the reference composition given in Table 2:

Table 2: Fluid reference sample

Component	Molepercent
C1	94.30
C2	2.70
C3	0.74
nC4	0.49
nC5	0.27
nC6	0.10
N2	1.40

We use a uniform temperature of 180.0 K and a reference pressure of 6.0 MPa. The reference depth is set to 4000 m.

The phase envelope at the reference depth is shown in Figure 1, and is generated by choosing option 3 and letting 4000 m be the specified depth.

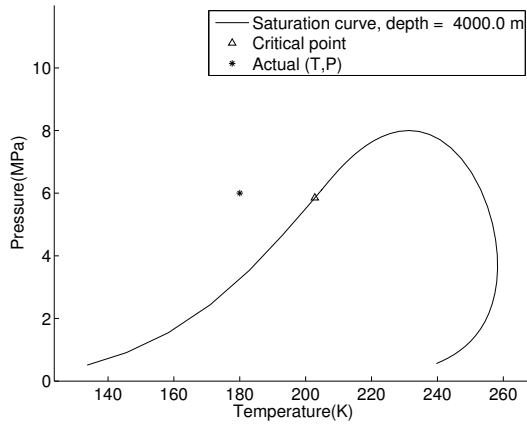


Figure 1: Phase envelope at reference depth

We then perform a search for a GOC in the depth range 4200-2000 m (option 2), specifying that the program should do calculations at 20 depths. The resulting plot is shown in Figure 2. The plot also shows a comparison to results obtained with the simulator SPECS (see [5]).

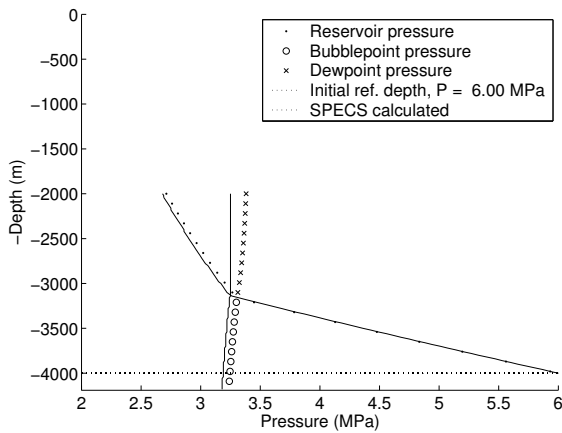


Figure 2: GCE calculations and saturation curves, depth range 4200-2000 m

As we can see, the reservoir pressures calculated by our program seem to be in accordance with the results from SPECS. However, the saturation point calculations show a poorer match. We have not been able to investigate this disagreement, but note that SPECS results are Peneloux corrected.

During calculations, the program reports that a saturated gas-oil contact appears at or near a depth of 3100.0 m. It also reports that the pressure appears to be 3.12 MPa (before recalculation using the stability test generated estimate). The recalculated pressure is reported to be 3.27 MPa. SPECS here reports a gas-oil contact at approximately 3150.0 m. In view of the chosen resolution in our program

(20 points, 110 m per step), we have a satisfactory match in finding the GOC.

We can also get plots of the compositional gradient in the same depth range. These are shown for components 1 (C1) and 6 (nC6) in Figures 3 and 4, respectively.

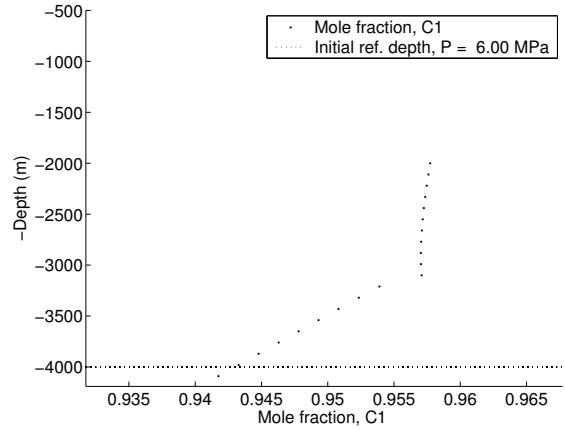


Figure 3: Mole fraction of component 1 versus depth

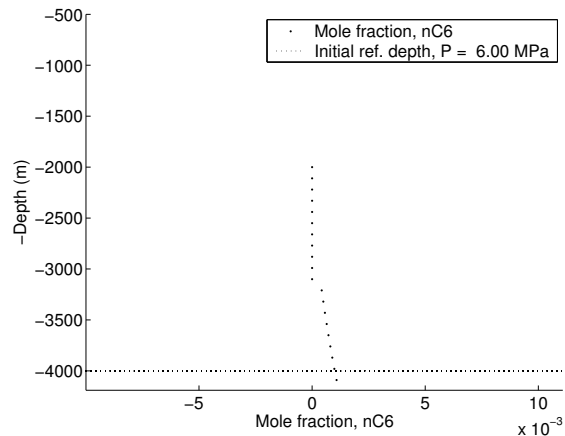


Figure 4: Mole fraction of component 6 versus depth

To investigate what happens near the gas-oil contact, we use option 3 to generate phase envelope plots at depths 3000 m and 3200 m. These are shown in Figures 5 and 6.

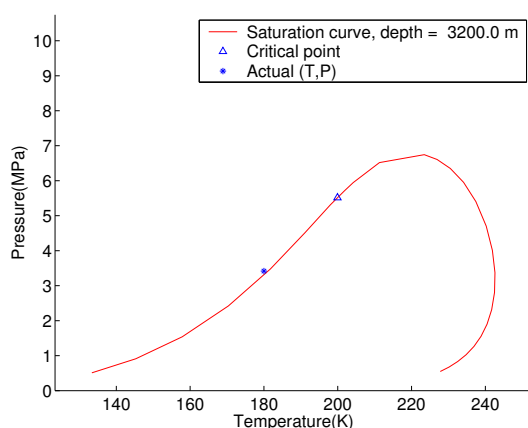


Figure 5: Phase envelope below GOC

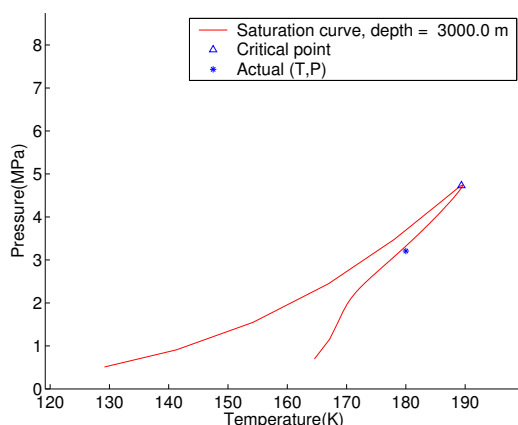


Figure 6: Phase envelope above GOC

The figures confirm that a gas-oil contact appears between 3000 m and 3200 m.

We have also made attempts at introducing up to 22 components, where the C7+ components were lumped in up to 12 pseudocomponents. Component properties were obtained from [2]. However, we were unable to match the results presented in [2]. At present, it is not evident what causes the mismatch, but the necessary altering of IVC-SEP subroutines, [4], appears to be errorprone.

4 Conclusions and Further Work

A program for performing gravity/chemical equilibrium calculations, including searches for a possible gas-oil contact and calculations of saturation points and phase envelopes has been implemented.

The program has only been tested on a narrow range of test cases, but appears to give reasonable results, also measured against available soft-

ware (SPECS). However, we have not been able to test the program on undersaturated GOC problems, and extensive testing is needed to validate the results given by the program.

We have noted in the report that the Peneloux volume correction should be applied for correct results. This is an important subject of further development of the program.

As mentioned, the possibility of including a broader range of components, especially heavier ones, is already under investigation. In addition, it would be interesting to include the effect of thermal gradients in the calculations.

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