Properly Defining the Classical Vaporizing and Condensing Mechanisms When a Gas Is Injected into a Crude Oil

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In this paper, real crude oils are dealt with which are modeled with an average of 30 components. On the selected examples, neither the initial tie line, i.e., the tie line that extends through the original oil composition, nor the gas tie line, i.e., the tie line that extends through the injected gas composition, controls the miscibility process. In any case, the miscibility process is controlled by one of the \((nc - 3)\) crossover tie lines, if \(nc\) is the number of components in the crude oil. However, it is shown that the miscibility process may be a pure vaporizing gas drive mechanism (VGDM). To be more precise, it is shown that a mixed condensing/vaporizing mechanism may, with increasing pressure, turn into a pure VGDM. This means that the classical definition of a VGDM, i.e., the lowest pressure at which the initial tie line is critical, must be changed. This is the main point of this paper. In the case of a VGDM controlled by a crossover tie line, the MMP (the lowest pressure at which the key crossover tie line becomes critical) may still be computed by a one cell simulation algorithm. Another aim of this paper is to explain what really happens during a one cell simulation and to give proof that such an algorithm may not make critical the initial or the gas tie line.

Introduction

For many years, the mechanisms of development of miscibility have traditionally been simplified and described using ternary phase diagrams. This simplification relied on the apparent similar behavior of real fluids and ternary systems. In this approach, only two key tie lines may control the miscibility process: (1) the initial tie line, i.e., the tie line that extends through the initial oil composition; (2) the injected gas tie line, i.e., the tie line that extends through the injected gas composition. Under these conditions, the miscibility mechanism is respectively a pure vaporizing (VGDM) or a pure condensing (CGDM) gas drive mechanism. As a consequence, if the crude oil is modeled with only 3 pseudocomponents, the minimum miscibility pressure (MMP) may be accurately determined using a classical one cell simulation algorithm. Jensen and Michelsen\(^1\) showed that a negative flash algorithm\(^2\) might also be used for a VGDM.

In 1986, Zick\(^3\) discovered a new combined process called the condensing/vaporizing mechanism (C/VM). This mechanism, which was observed on real petroleum fluids, cannot be explained using the classic ternary approach.

In 1997, Wang and Orr\(^4\) worked on the transport equations of the displacement. A major result of their work was that the flow behavior in slim tube experiments is controlled by a sequence of \((nc - 1)\) key tie lines if \(nc\) is the number of components in the oil. These key tie lines are the initial oil and the gas tie line, as well as \((nc - 3)\) crossover tie lines as initially defined by Monroe et al.\(^5\) Multicontact miscible displacement occurs when the pressure is increased sufficiently so that any one of these key tie lines becomes a critical tie line. That pressure is the MMP. To compute the MMP, Wang and Orr\(^4,6\) on one hand and J.essen et al.\(^7\) on the other have developed very fast algorithms based on location of key tie lines. Jaubert et al.\(^8\) have also developed a simplified multicell approach.

The discovery of the existence of these \((nc - 3)\) crossover tie lines by Professor Orr's research group, as well as the discovery of the mixed condensing/vaporizing mechanism (CVM) by Zick, have profoundly changed the way of explaining the miscibility processes. This means that, a few years ago, many incorrect results were published. This paper seeks to correct some of them.

In this paper, devoted to real petroleum fluids modeled with a realistic \(C_{11+}\) characterization, it is shown that care must be taken in determining what mechanism is controlling the development of miscibility. Indeed, in some papers, it is assumed that the process is (1) a mixed C/VM when a crossover tie line controls the miscibility and (2) a VGDM or a CGDM when the initial or the gas tie line, respectively, controls the process. Such an assumption is unfortunately not...
always true. For the crude oils selected in this study, a crossover tie line different from the initial or from the gas tie line always controls the miscibility process. However, in some cases the process may be a pure VGDM. More precisely, it is shown that a mixed C/VM may, with increasing pressure, turn into a pure VGDM. This means that the classical definition of a VGDM, i.e., the lowest pressure at which the initial tie line is critical, must be changed. A key point of this paper is thus to give a proper definition of the VGDM and CGDM for multicomponent systems.

This paper also comes back to the description of the one cell simulation algorithm which has been used for many years in petroleum companies in order to compute the MMP. In particular, it is shown that (1) such an algorithm may still be used to compute the MMP when a mixed C/VM turns into a VGDM and (2) such an algorithm does not often make critical the initial or the gas tie line but often makes critical the key crossover tie line which controls the miscibility process. In the case of a C/VM, such an algorithm overestimates the MMP but gives a value closer to the true MMP than the use of a negative flash making critical the initial or the gas tie line. Such results agree with those of Jensen and Michelsen, who explained, ignoring the existence of the crossover tie lines, that a negative flash algorithm could lead to wrong MMP values. In other words, this paper also shows the use and limitations of a 1 cell simulator to compute the MMP.

**Visualization of the Key Crossover Tie Line Controlling the Miscibility Process**

For this study, three pairs of oil/gas fluids in the database of the French Petroleum Co. TOTAL SA were selected. The three MMPs were experimentally determined by a slim tube test. These crude oils will be noted O2 to O3 and the associated injection gases I2 to I3. Actually, O2 and O3 are strictly identical, but since two different gases (I2 and I3) were injected, it was found to be easier to understand if the oil had two different names. The molar compositions of all these fluids are summarized in Table 1.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Mole Fractions</th>
<th>Reservoir Temp/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2S</td>
<td>0.003 83</td>
<td>394.25</td>
</tr>
<tr>
<td>N2</td>
<td>0.004 50</td>
<td>387.45</td>
</tr>
<tr>
<td>CO2</td>
<td>0.020 70</td>
<td>370.45</td>
</tr>
<tr>
<td>methane</td>
<td>0.265 76</td>
<td>350.00</td>
</tr>
<tr>
<td>ethane</td>
<td>0.078 94</td>
<td>330.00</td>
</tr>
<tr>
<td>propane</td>
<td>0.067 30</td>
<td>310.00</td>
</tr>
<tr>
<td>butane</td>
<td>0.041 85</td>
<td>290.00</td>
</tr>
<tr>
<td>isobutane</td>
<td>0.039 88</td>
<td>270.00</td>
</tr>
<tr>
<td>and</td>
<td>0.027 90</td>
<td>250.00</td>
</tr>
<tr>
<td>n-pentane</td>
<td>0.017 83</td>
<td>230.00</td>
</tr>
<tr>
<td>n-hexane</td>
<td>0.015 68</td>
<td>210.00</td>
</tr>
<tr>
<td>3-m-hexane</td>
<td>0.005 31</td>
<td>190.00</td>
</tr>
<tr>
<td>benzene</td>
<td>0.005 36</td>
<td>170.00</td>
</tr>
<tr>
<td>cyclohexane</td>
<td>0.022 29</td>
<td>150.00</td>
</tr>
<tr>
<td>n-heptane</td>
<td>0.010 13</td>
<td>130.00</td>
</tr>
<tr>
<td>4-m-hexane</td>
<td>0.012 15</td>
<td>110.00</td>
</tr>
<tr>
<td>toluene</td>
<td>0.010 04</td>
<td>90.00</td>
</tr>
<tr>
<td>methylcyclohexane</td>
<td>0.016 65</td>
<td>70.00</td>
</tr>
<tr>
<td>n-octane</td>
<td>0.008 49</td>
<td>50.00</td>
</tr>
<tr>
<td>ethylbenzene</td>
<td>0.010 43</td>
<td>30.00</td>
</tr>
<tr>
<td>ethylcyclohexane</td>
<td>0.006 20</td>
<td>10.00</td>
</tr>
<tr>
<td>n-nonane</td>
<td>0.002 25</td>
<td>-10.00</td>
</tr>
<tr>
<td>4-m-octane</td>
<td>0.012 67</td>
<td>-27.00</td>
</tr>
<tr>
<td>propylbenzene</td>
<td>0.004 33</td>
<td>-47.00</td>
</tr>
<tr>
<td>n-decane</td>
<td>0.003 33</td>
<td>-67.00</td>
</tr>
<tr>
<td>C15-C19</td>
<td>0.162 30</td>
<td>-87.00</td>
</tr>
<tr>
<td>C20+</td>
<td>0.129 62</td>
<td>-107.00</td>
</tr>
</tbody>
</table>

The C11+ characterization procedure developed by J. Aubert was applied for all the calculations. Previous papers discussed the model's accuracy in predicting, first, the evolution of the relative volume during a constant mass expansion or a differential vaporization and, second, the behavior of the crude oil during a swelling test or a multicontact test. This characterization procedure models the C11+ fraction with two pseudocomponents ("C11-C19" and "C20+"). As the compounds we work with have widely varying volatility, no lumping method was applied. With such a composition model, crude oils are described with 28 or 29 compounds.

In many of their papers, Orr and co-workers have already shown the crossover tie lines in phase diagrams. In this paper another approach is used. Indeed, an easy way to visualize the crossover tie lines is to simulate the slim tube by a series of mixing cells (cell to cell simulation). This approach was initially developed by Cook et al. and then taken further by Metcalf and Pedersen et al. Such a simulation may be summarized as follows: In a first step, the program simulates a number of cells of equal volume in a series. The temperature and the pressure are the same in each cell, and the volume is kept constant. All the cells initially contain the same fluid (the reservoir oil). A specified amount of gas is added to cell 1 (for instance 25% of the cell volume). It is assumed that perfect mixing takes place and that thermodynamic phase equilibrium is reached. This means that the conditions in the cell can be described by a P/T-flash calculation, here based on a modified Peng–Robinson equation of state. After mixing of the injected gas and the cell fluid, the total volume of the cell will be larger than the assumed cell volume. The excess volume is transferred from cell 1 to cell 2. If two phases are present, the gas phase is moved first. If after moving all the gas phase the cell volume is still larger than the initial cell volume, a part of the liquid phase is also moved. In a second step, the excess volume formed in cell 2 is transferred to cell 3 and so on until production is obtained from the last cell. When one batch calculation has been completed, a new injection into cell 1 can take place and the cell to cell transfer calculation is resumed.

To visualize the different crossover tie lines, it is necessary to record in each cell (or in selected cells) a thermodynamic parameter versus time (proportional to the number of batch calculations). Moreover, the visualization of the numerous key tie lines requires good resolution, which can only be provided by a high number of cells. A typical value is 1000. As the simulation goes on, time is measured in terms of the total quantity of gas injected into the first cell since the beginning of the simulation. This quantity is expressed in "pore volume" in reference to the slim tube test. For instance, 4000 batch calculations are equivalent to one pore volume of gas when the tube is modeled with 1000 cells and when the amount of gas added to cell 1 at each batch equals 25% of the cell volume. As it is important to keep track of the simulation history, diphasic cells are characterized with an aggregate parameter that is recorded as a function of time. In this study, the parameter dc,
defined by Zick (unpublished results) and called the critical distance, was used:

\[ dc = \frac{\rho_{\text{liquid phase}} - \rho_{\text{gas phase}}}{\frac{1}{2} (\rho_{\text{liquid phase}} + \rho_{\text{gas phase}})} \quad dc \geq 0 \quad (1) \]

\( \rho_{\text{liquid phase}} \) and \( \rho_{\text{gas phase}} \) are respectively the liquid and gas phase density. If a cell becomes critical, both phases will have exactly the same density; thus, \( dc = 0 \). The closer the critical distance in a cell is to zero, the closer the fluid in this cell is to a critical point.

Figure 1 gives the evolution of \( dc \) versus time in selected cells for the 3 investigated systems. Pressure and temperature are constant in each subplot.

For the three examples selected in this study, at pressures lower than the MMP, the history diagrams are formed by a vaporization and a condensation zone. This does not mean however that the miscibility mechanism is a C/VM. Indeed, in the next section C/VM displacements will be investigated, which, with increasing pressure, turn into a pure vaporizing mechanism. For such displacements, the MMP can easily be calculated with a one cell simulation, even if a crossover tie line controls the miscibility process.
Looking More Closely at the One Cell Simulation

This section aims to explain what really happens during a single cell simulation and considers such a simulation in a new perspective. Indeed, many years of practice on ternary diagrams have blurred many researchers’ understanding of this technique. As an example, it is possible to find written in recent papers the following:

(1) “during a one cell simulation the pressure is increased until either the initial or the gas tie line is a critical tie line”. Proof will be given in the next section that such a sentence is never exact when one works on real petroleum fluids for which a crossover tie line controls the miscibility process.

(2) “the one cell simulation works well as long as it is the oil tie line (vaporizing gas drive) or the injection gas tie line (condensing gas drive) that controls miscibility”. It is obvious that this sentence is both rigorous and exact. However, it will be shown that it is too restrictive since one cell simulations may work well even if a crossover tie line controls the miscibility process.

(1) Results of One Cell Simulations. To find out what tie line is made critical during a one cell simulation and in order to correctly know how to call the corresponding MMP, one cell simulations were performed with the three different systems O1/I1, O2/I2, and O3/I3 in order to determine the MMP_{1cell}. More information on this kind of calculation is given by Jensen and Michelsen2 and by Neau et al.20 In a ternary approach, the displacement mechanism for both O2/I2 and O3/I3 would be a vaporizing gas drive, which involves performing forward contacts. O1/I1 exhibits features of a CGDM; thus, backward contacts were performed. To find out when forward or backward contacts must be simulated, the criterion developed by Novosad and Costain21 was used.

The MMP_{1cell} values along with the mechanism of miscibility in a ternary approach are summarized in Table 2.

Table 2. Mechanism of Miscibility in a Ternary Approach with Value of the Calculated MMP_{1cell} at the Reservoir Temperature

<table>
<thead>
<tr>
<th>Mechanism in a ternary approach</th>
<th>system</th>
<th>O2/I1</th>
<th>O2/I2</th>
<th>O3/I3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of contact</td>
<td>O2/I1</td>
<td>CGDM</td>
<td>VGDM</td>
<td>VGDM</td>
</tr>
<tr>
<td>MMP_{1cell}/bar</td>
<td>312.91</td>
<td>497.21</td>
<td>444.35</td>
<td></td>
</tr>
</tbody>
</table>

Some curves in Figure 2 were computed at pressures that are just 0.01 bar below the MMP_{1cell}. Looking more closely at these plots, it is obvious that neither the initial (Figure 2b,c) nor the gas (Figure 2a) tie line is critical at the MMP_{1cell}. However, the key crossover tie line is critical (at a pressure strictly equal to the MMP_{1cell}, the minimum value of dc is equal to zero).

As a fundamental conclusion, proof was given that (1) a one cell simulation makes critical the key crossover tie line which controls the displacement and (2) during a one cell simulation the pressure is not increased until either the initial or the gas tie line is critical. To make such a tie line critical would require a negative flash algorithm at pressures much higher than the MMP_{1cell} (see Figure 3a–c). As a consequence, a negative flash algorithm may calculate the true MMP only if the initial or the gas tie line controls the miscibility
process, but these two extreme cases have practically
never been observed with real fluids.

Note: As explained previously, in some rare cases (not
shown in this paper), the initial tie line may control the
miscibility process. In such a case, it is obvious that a
one cell simulation makes critical such a tie line (a
ternary behavior is observed).

The paramount question that must be addressed is
"is the MMP\textsubscript{1cell} the true MMP?" or in other words "is
there a pressure lower than the MMP\textsubscript{1cell} at which the
key crossover tie line is critical?" An answer to this
question is given in the next section.

(2) A Proper Definition of the Vaporizing and
Condensing Processes. In Figure 2, at a pressure
strictly equal to the MMP\textsubscript{1cell}, the cell is critical after a
few contacts. At this pressure, the critical distance has
then become a monotonic decreasing function of the
contact number. This means that the MMP\textsubscript{1cell} may be
defined in a general way as the lowest pressure at which
the following holds:

(a) The condensation front(s) have disappeared if
forward contacts are made. Because miscibility is
reached by condensation front(s) only, this pressure
must be called the condensing MMP. Performing
forward contacts: MMP\textsubscript{condensing}. In other words, the condensing MMP must not be defined as the
smallest pressure at which the gas tie line is critical
but as the smallest pressure at which miscibility is
reached by condensation fronts only.

(b) The vaporization front(s) have disappeared if
backward contacts are performed. Because miscibility
is reached by vaporization front(s) only, this pressure
must be called the vaporizing MMP. Performing
backward contacts: MMP\textsubscript{vaporizing}. In other words, the vaporizing MMP must not be defined as the
smallest pressure at which the initial tie line is critical but as the smallest pressure at which miscibility is
reached by vaporization fronts only.

As far as system O\textsubscript{2}/I\textsubscript{1} is concerned, the condensing
MMP may not be regarded as satisfactory. In Figure
2a, one of the curves (P = P\textsubscript{1}) was computed at the
actual MMP. At this pressure, the dc parameter is still
a decreasing–increasing function of the contact number.
In addition, a plot of the density of the liquid and gas
phase in equilibrium in the single cell during a 1 cell
simulation performed at the true MMP is shown in
Figure 4a. From this figure, it is clear that the densities
of the phases in equilibrium in the single cell converge
during the first few contacts and then diverge. This simulation, performed at the true MMP, indicates that the mechanism is a real mixed C/VM. Since at the true MMP, a critical point is not reached in the single cell, a one cell simulator cannot lead to the actual MMP (the 1D simulator made the key crossover tie line critical at a pressure much lower than the MMP_{1cell}).

The result obtained for system O1/I1 is widely applicable. Indeed, working on real petroleum fluids modeled with a realistic number of components, it seems that the condensing mechanism does not exist and is always replaced by a mixed C/VM. Moreover the true MMP (MMP_{C/VM}) is always much lower than the condensing MMP.

O3/I3 is very similar to O1/I1 despite different ternary mechanisms. Figure 2c (P = P1 = true MMP) and Figure 4c exhibit the features of a real C/VM. Nevertheless, the MMP_{1cell} and the true MMP are much closer for O3/I3 than they were for O1/I1. When the displacement mechanism is a C/VM, MMP_{C/VM} is always smaller than MMP_{vaporizing}. However the difference between these two values may be small since when a C/VM mechanism takes place instead of a pure VGDM, condensation often plays a minor role.

The vaporizing MMP for O2/I2 matches the correct MMP even if it was seen before that the miscibility process is controlled by a crossover tie line. The two values coincide because the mechanism is a pure VGDM: in Figure 2b (P = P1), the dc parameter is, as expected, a decreasing function of the contact number. In Figure 4b, the densities of the phases in equilibrium in the single cell close together until they become identical (a critical point is reached). What is fundamental to outline here for system O2/I2 is that at pressures lower than the true MMP (the lowest pressure at which the key crossover tie line is critical) all the condensation fronts have disappeared. To our knowledge the evidence of a pure vaporizing mechanism controlled by a crossover tie line has not been reported previously. Only one example is shown here, but such a process is not uncommon. In this section proof was thus given that a 1 cell simulation might work well even if a crossover tie line controls the miscibility.

Remark: For the three systems investigated the following holds:

(a) A crossover tie line controls the miscibility process. This means that at any pressure lower than the MMP_{1cell}, during a one cell simulation, the densities of the phases in equilibrium in the single cell converge during the first few contacts and then diverge.

(b) In the same way at a pressure strictly equal to the MMP_{1cell}, the densities of the phases in equilibrium in the single cell converge until they become identical.

Table 3. Comparison of the MMP_{1cell} and of the True MMP

<table>
<thead>
<tr>
<th>system</th>
<th>true MMP/bar (1D simulator)</th>
<th>MMP_{1cell}/bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1/I1</td>
<td>275.0</td>
<td>312.91</td>
</tr>
<tr>
<td>O2/I2</td>
<td>497.2</td>
<td>497.21</td>
</tr>
<tr>
<td>O3/I3</td>
<td>429.0</td>
<td>444.35</td>
</tr>
</tbody>
</table>

Figure 3. Evolution of the critical distance when liquid and gas phases are located either on the gas (a) or on the initial tie line (b, c) versus pressure: (a) fluids O1–I1 at T/K = 394.25 (backward contacts are performed); (b) fluids O2–I2 at T/K = 394.25 (forward contacts are performed); (c) fluids O3–I3 at T/K = 387.45 (forward contacts are performed).
The crossover tie line controlling the process has thus become critical (a figure similar to Figure 4b would be observed for the three systems).

However, for systems O₁/I₁ and O₃/I₃ at the true MMP, a critical point is not reached in the single cell, meaning that the process is a CVM whereas for system O₂/I₂ such a critical point is reached, meaning that the process is a pure VGDM controlled by a crossover tie line.

Since MMP_{cell} sometimes equals the true MMP, a fast and reliable algorithm that computes its value is proposed in the next section. A way of easily finding out if such a value matches the true MMP is also explained.

(4) Computation of a Fast One Cell Simulator: Determination of the Miscibility Mechanism. The process mechanism, the value of MMP_{cell}, and the confirmation of whether this value is correct are obtained through the following steps:

Step 1: Calculation of the FCMP (first contact minimum miscibility pressure). The FCMP is defined as the lowest pressure at which the injection gas $G^*$ and the crude oil $L^*$ are first contact miscible. This pressure may be easily determined by simulating a swelling test and locating the stationary point at the top of the P–X diagram as shown in Figure 5. Indeed, the FCMP coincides with the cricondenbar $P_{\text{max}}$ (the maximum two phases pressure).
In such a diagram, the amount of injected gas, noted as $X_{\text{gas}}$, is defined by:

\[
X_{\text{gas}} = \left[ \text{number of moles of gas} \right] / \left[ \text{number of moles of reservoir crude oil} \right]
\]

Once the FCMP is known, a $P$–$T$ flash calculation is to be performed at the reservoir temperature and at a pressure just below the FCMP for a fluid of global composition $Z = X_{\text{FCMP}}G° + (1 - X_{\text{FCMP}})L°$. In the previous expression, $X_{\text{FCMP}}$ is the cricondenbar abscissa in the $P$–$X$ diagram. Such a point is represented by a square in Figure 5. The output of this two phase flash calculation reveals whether the cricondenbar is located on the bubble curve (the amount of liquid is close to 100%) or on the dew curve (the amount of gas is close to 100%). Indeed, in 1988, Novosad and Costain demonstrated the following:

If the cricondenbar ($P_{\text{max}}$) is located on the bubble curve (see Figure 5a), the process is a CGDM rather than a VGDM. Under these conditions, backward contacts must be performed to determine the MMP$_{1\text{cell}}$, and in such a case MMP$_{1\text{cell}} = \text{MMP}_{\text{condensing}}$. As previously explained, working on real petroleum fluids, such a MMP is never the true MMP and in such a case the process is always a mixed C/VM. The correct MMP, always smaller than the MMP$_{\text{condensing}}$, must be determined by a 1D simulator or by the key tie line intersection approach.

If the cricondenbar is a dew point (see Figure 5b, c), the process is a VGDM rather than a CGDM. Forward contacts must be performed to determine the MMP$_{1\text{cell}}$ and in such a case MMP$_{1\text{cell}} = \text{MMP}_{\text{vaporizing}}$. Such a MMP may be the correct one (see below).

In all cases MMP$_{1\text{cell}} < \text{FCMP}$.

Notes: (1) If the cricondenbar is found on the bubble curve and if forward contacts are simulated, the MMP$_{1\text{cell}}$ will always equal the FCMP. Symmetrically, if the cricondenbar in the P–X diagram is located on the dew curve and if backward contacts are simulated, MMP$_{1\text{cell}} = \text{FCMP}$ should always be computed. This remark applies whatever the fluids and the displacement mechanism. If the cricondenbar and the critical point in the P–X diagram are merged, MMP$_{1\text{cell}} = \text{MMP}_{\text{condensing}} = \text{FCMP}$ will be observed. (2) The relative position of the initial and gas tie lines on the history diagram (as in Figure 1) may be misleading if one wants to find out if the process is rather a VGDM or a CGDM. Examples were found for which $d_{\text{gas tie line}} < d_{\text{initial tie line}}$, and MMP$_{V\text{GDM}} < \text{MMP}_{\text{CGDM}} = \text{FCMP}$.

Step 2: Isothermal forward or backward contacts are to be simulated at pressures lower than the FCMP. For a given pressure, after each contact the value of the critical distance $dc$ in the cell (compulsory diphasic) is to be recorded versus time (i.e. versus the contact number).

Different cases may appear as follows.

Case 1: At the working pressure, after a few contacts, the cell remains monophasic whatever the quantity of fluid that is added (original oil for forward contacts or injection gas for backward contacts). The critical distance will always be a decreasing function of the contact number which shows that either a vaporization front (forward contacts) or a condensation front (backward contacts) is being simulated. In this case, the pressure is higher than the MMP$_{1\text{cell}}$ and a new lower pressure must be chosen.

Case 2: The critical distance first decreases, then reaches a minimum, and finally increases until it hits the initial or the gas tie line (depending on the contact type). In such a case, a crossover tie line controls the miscibility process. As soon as the dc function starts increasing, the simulation can be stopped because the working pressure is lower than the MMP$_{1\text{cell}}$. A higher pressure has to be chosen for the next simulation.

Case 3: The dc function is a monotonic decreasing function of the contact number, and after many contacts, the composition of both phases in equilibrium in the cell remains the same (dc is constant). In this case if forward contacts are performed, the mechanism is a vaporizing process and the initial tie line controls the miscibility process (rarely observed), or if backward contacts are performed, the mechanism is a condensing process and the gas tie line controls the miscibility process (never observed with the fluids of our database).

The MMP$_{1\text{cell}}$ will be the correct MMP. A direct tie line approach like a negative flash algorithm may also be used to compute the MMP.

Step 3: Once a pressure higher (step 2, case 1) and a pressure lower than the MMP$_{1\text{cell}}$ (step 2, case 2 or 3) have been found, a simple dichotomy makes it easy to find the MMP$_{1\text{cell}}$. In all cases, it will be found that MMP$_{1\text{cell}} < \text{FCMP}$.

Notes: (1) It was observed that pressure does not affect the relative position of the key crossover tie lines. Increasing pressure, a pure VGDM that is controlled by a crossover tie line, will never turn into a VGDM that would be controlled by the initial tie line. (2) In the case where MMP$_{1\text{cell}} = \text{MMP}_{\text{vaporizing}}$, a 1-D simulator may be used to check if the value is correct. It is recommended that a simulation at $P = 0.97\text{MMP}_{\text{vaporizing}}$ be run first. By the end of the computation, if the dispersion-free recovery factor is close to 100%, then the mechanism is a mixed C/VM. On the other hand, if the dispersion-free recovery factor is significantly less than 100%, the process is a pure VGDM and the MMP$_{1\text{cell}}$ is the correct value. This means that if a 1D simulator is normally used to compute the MMP, it is advised to first compute the MMP$_{1\text{cell}}$ with the proposed algorithm (a few seconds are needed) and to make a single run at $P = 0.97\text{MMP}_{\text{vaporizing}}$. By the end of this single run, it will be possible to determine whether the MMP$_{1\text{cell}}$ is the correct one. If this is the case, further 1D simulator runs at different pressures will not be necessary.

If an algorithm based on location of key tie lines is normally used to determine the MMP, it will be only necessary to make a one cell simulation at this pressure to determine the correct mechanism (see the discussion relative to Figure 4).

Significant acceleration of the one-cell simulator could be achieved if the MMP$_{1\text{cell}}$ did not depend on the mixing proportions. The next paragraph addresses this issue.

When a vaporizing process is simulated, the cell is full of saturated gas from the previous contact. At each new contact, a given amount of original oil is added so that a new diphasic fluid may form. If the oil addition is very small compared with the gas quantity, the new fluid will be close to a dew state (the result of the flash calculation will indicate that the cell is essentially formed by a gas phase in equilibrium with a very small amount of liquid phase). Such contacts are called nonoptimized contacts in the following text. Another option is to add as much oil as possible so that the cell gets very close to a bubble state (the flash calculation...
Numerous simulations were performed on real petroleum fluids in order to determine if the type of contact could influence the value of MMP\(\text{1cell}\). It was found that the type of contact hardly changed the MMP\(\text{1cell}\). The optimized contacts overestimate the MMP\(\text{1cell}\) by less than 0.5% when the displacement is controlled by a crossover tie line and do not have any influence at all when either the initial or the gas tie line controls the miscibility process.

Figure 6 is representative of the results obtained. In this study, a separator gas was injected into a real crude oil. Optimized contacts were made first and the calculated vaporizing MMP was 490 bar (see the left of Figure 6). In a second step, nonoptimized contacts were performed: each time the quantity of original oil that was added was close to zero. The MMP\(\text{1cell}\) that came out was 487.4 (see the right of Figure 6). Finally, all the intermediate situations were described to get the quasi continuous curve in Figure 6.

Since, when forward contacts are performed, the influence of the quantity of oil added may be neglected, it is advised, to reduce considerably calculation time (the number of contacts, at a given pressure), to perform optimized contacts i.e., to always inject the maximum quantity of original oil (forward contacts) or the maximum quantity of injection gas (backward contacts) in order to obtain a diphasic fluid. The difference in calculation time when performing optimized or non-optimized contacts may be higher than a ratio of one thousand.

Conclusion: Optimized contacts vastly reduce the time required to compute MMP\(\text{1cell}\). It takes only few seconds on a PC with a Pentium II processor whereas it can still be a matter of hours with nonoptimized contacts.

**Conclusion**

This study devoted to multicomponent fluids has demonstrated different key points which are summarized below:

In all the studied cases, a crossover tie line different from the initial or the gas tie line controls the miscibility process. As a consequence, it is never possible to use a direct tie line approach based on a negative flash algorithm to determine the true MMP. Indeed such an algorithm would make critical the initial or the gas tie line and would overestimate the MMP.

The process was found to be either a pure VGDM or a mixed C/V. This means that, contrary to what is currently explained in the literature, a pure VGDM may develop even when the initial tie line does not control the miscibility process. In such a case, a one cell simulation algorithm is sufficient to calculate the true MMP.

The definition of the pure VGDM or pure CGDM, currently available in the literature, i.e., the lowest pressure at which the initial oil or gas tie line, respectively, is critical, needs to be changed. Being conscious that, when working on multicomponent systems, a crossover tie line usually controls the miscibility process, a new definition of both of these mechanisms was given.

When a vaporizing mechanism controlled by a crossover tie line takes place: condensation and vaporization fronts are observed during a one cell simulation at pressures lower than the true MMP. At a pressure strictly equal to the true MMP, all the condensation fronts have disappeared, meaning that in all cases a C/V has turned into a pure vaporizing process.

Contrary to what may be found in the literature, it was shown that during a static (one cell) multicontact process, if the pressure is increased to the first point where the process leads to a miscible condition, neither the injection gas nor the crude oil is on a critical tie line extension. This means that in the one cell simulation it is the key crossover tie line that is made critical and not the initial or the gas tie line. To be very precise, it is recalled that if the initial or the gas tie line effectively controls the miscibility process, a 1 cell simulator obviously makes such a tie line critical. Such a ternary behavior is however very rare (not observed with the fluids used in this study).

A single cell multicontact algorithm may be a helpful tool to determine the miscibility mechanism. In particular, if the MMP is normally computed with an algorithm based on the location of the key tie lines, a single cell simulation performed at the MMP will indicate easily the process mechanism.

If the MMP is normally computed with a 1D simulator, a single run at \( P = 0.97 \times \text{MMP}_{\text{vaporizing}} \) will indicate whether the MMP\(\text{1cell}\) determined using a single cell simulator is the correct one. In doing so, further runs at different pressures with the 1D simulator will not be necessary.

Using a realistic modeling of the different fractions, the pure CGDM was never observed (it probably does not exist).

The mixed C/V process may replace either a pure CGDM or a pure VGDM. It is the most common mechanism.

If the displacement mechanism is a pure VGDM, it is always observed that \( \text{FCMP} > \text{MMP}_{\text{1cell}} = \text{MMP}_{\text{vaporizing}} \). If the process is a mixed C/V mechanism, it is always observed that \( \text{FCMP} > \text{MMP}_{\text{1cell}} > \text{MMP}_{\text{C/V}} \) (true MMP). In the latter case a 1D simulator, a multicell approach\(^6\) or an algorithm based on location of key tie line must be used to compute the MMP.

The only way to know whether a displacement mechanism is rather a pure VGDM than a pure CGDM is to locate the cricondenbar in the \( P-X \) diagram. For example, if \( \text{MMP}_{\text{vaporizing}} < \text{MMP}_{\text{condensing}} \), it does not mean that the critical distance corresponding to the
initial tie line is smaller than the one of the gas tie line. Using a ternary approach, i.e., focusing only on the initial and on the gas tie line, if such case appeared (initial tie line “less critical” than the gas tie line), it would be concluded that the mechanism is rather a CGDM than a VGDM, which may be incorrect.

Another important conclusion of this paper is that when working on multicomponent systems, it is necessary to forget the ternary systems and diagrams. The essential reason is that when working on ternary systems, only the initial or the gas tie line may control the miscibility process, whereas working on real fluids neither of these key tie lines are generally helpful.

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Nomenclature

dc = critical distance
P = pressure
P_{max} = cricondenbar in the P–X diagram
T = temperature
X_{gas} = relative amount of injected gas

Greek Letters

\rho = density

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