INFLUENCE OF THE CRUDE OIL CHARACTERIZATION ON MMP CALCULATION

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INFLUENCE DE LA CARACTÉRISATION D'UN PÉTROLE BRUT SUR LE CALCUL DE LA PRESSION MINIMALE DE MISCIBILITÉ

Dans cet article, nous étudions l'influence de la modélisation des coupes d'un pétrole brut sur la valeur calculée de la pression minimale de miscibilité (MMP). En particulier, il est expliqué quels types de constituants peuvent être regroupés sous forme d'un peusdo-constituant sans pour autant dégrader la valeur de la MMP. La procédure suivie dans cet article est simple : à partir d'un pétrole brut donné, nous utilisons dans un premier temps une représentation par 37 composants, exploitant l'information analytique standard disponible sur ce fluide. La modélisation des fractions lourdes utilisée est celle développée par Avaullée et al. (1997a), dans laquelle nous avons ajusté deux paramètres du résidu de distillation C_{20+} sur les pressions de saturation expérimentales. Sur le fluide étudié, nous mettons en évidence le bon niveau de restitution des grandeurs volumétriques, des données expérimentales de gonflement ainsi que de la MMP mesurée lors d'une expérience de déplacement en tube mince. Dans un deuxième temps, les composés intermédiaires lourds, les intermédiaires moyens et les composants légers font successivement l'objet de regroupement en pseudo-constituant. L'influence de tels regroupements sur la valeur calculée de la MMP est alors analysée.

INFLUENCE OF THE CRUDE OIL CHARACTERIZATION ON MMP CALCULATION

This paper focuses on the influence of the crude oil characterization on minimum miscibility pressure (MMP) calculation. It is shown what kind of compounds may be lumped together in order to calculate the MMP with a good accuracy. In a first step, a selected crude oil is modeled with 37 pure compounds using the characterization procedure developed by Avaullée et al. (1997a) in which two parameters of the distillation residue are fitted on the experimental bubble points. In this context, all the experimental data (PVT, swelling test, slim tube test) are calculated with a very good accuracy. In a second step, the heavy intermediate, the middle intermediate and the light compounds are successively lumped. The influence of such lumping procedure on the calculated MMP is discussed.

INFLUENCIA DE LA CARACTERIZACIÓN DE UN PETRÓLEO CRUDO RESPECTO AL CÁLCULO DE LA PRESIÓN MÍNIMA DE MISCIBILIDAD

En este artículo se estudia la influencia de la modelización de las fracciones de un petróleo crudo con respecto al valor calculado de la presión mínima de miscibilidad calculada (MMP). Básicamente,

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se indica qué tipos de componentes se pueden reunir en forma de un seudocomponente sin por ello degradar el valor de la MMP. El procedimiento seguido para este artículo es sencillo : tomando como punto de partida un petróleo crudo determinado, utilizamos en una primera etapa una representación por medio de 37 componentes, en cuyo caso se utiliza la información analítica estándar disponible en este fluido. La modelización de las fracciones pesadas utilizada es aquella desarrollada por Avaullée y sus colaboradores (1997a), en la cual hemos ajustado dos parámetros del residuo de destilación C_{20+} en las presiones de saturación experimentales. Se hace resaltar, para el fluido estudiado, el correcto nivel de restitución de las magnitudes volumétricas, de datos experimentales de aumento de volumen, así como de la MMP medida con motivo de una experiencia de desplazamiento en tubo delgado. En una segunda etapa, los compuestos intermedios pesados, los intermedios medianos y los componentes livianos, son sucesivamente objeto de reagrupación en seudocomponente. Se analiza entonces la influencia de semejantes reagrupaciones sobre el valor calculado de la MMP.

INTRODUCTION

It is well known from the literature (Johns, 1992) that the miscibility process, when a gas is injected into a crude oil, is controlled by a sequence of nc-1 key tie lines if nc is the number of components present. There is the initial tie line (the tie line that extends through the original oil composition), the gas tie line (the tie line that extends through the injected gas composition) as well as nc-3 intermediate tie lines called crossover tie lines as initially defined by Monroe *et al.* (1990). In this context, the minimum miscibility pressure (MMP) which is a key parameter in a gas injection project design must be defined as the lowest pressure at which any one of these nc-1 tie lines becomes a critical tie-line. However, in softwares currently available in petroleum companies, a crude oil is usually described by a maximum of 10 components or pseudo-components meaning that some hydrocarbons are lumped together in order to reduce computing times. It is obvious that such a lumping procedure makes disappear many key tie lines and may lead to very different values of the MMP. The goal of this study is to test the influence of such lumping procedures on the calculated MMP value.

1 EXPERIMENTAL DATA

A crude oil for which many PVT experiments were performed by the French Petroleum Company *TOTAL SA* was selected. The composition of the reservoir fluid and the results of the True Boiling Point (TBP) distillation are shown in Table 1.

The following experimental data are available:
– Bubble points, total densities and relative volumes measured during constant mass expansions performed at three different temperatures (t_1 = 87.8°C, t_2 = 103.3°C and t_3 = 121.1°C). The reservoir temperature is t_2. In such experiments, the relative volume $\left(V_{tot}/V_{sat}\right)$ is defined as the total cell volume divided by the liquid volume at saturation pressure.
– Liquid densities, compressibility factors of liberated gas and *Bo* measured during a differential vaporization at the reservoir temperature. It is recalled that $Bo = \left(V_{liq}/V_{ref}\right)$ is defined as the liquid volume divided by a reference volume

TABLE 1

Composition of the reservoir oil and TBP distillation results

Components	Molar composition (%)	Components	Molar composition (%)	TBP distillation	
				Molecular weight	Density (kg·m⁻³)
H_2S	1.490	n-octane	0.530		
nitrogen	0.320	i-nonanes	0.570		
carbon dioxide	2.800	aromatics C_8	0.850		
methane	45.300	cyclanes C_9	0.590		
ethane	9.110	n-nonane	0.480		
propane	5.500	i-decanes	1.300		
i-butane	1.060	aromatics C_9	0.450		
butane	3.070	n-decane	0.400		
i-pentanes	1.240	undecanes	1.740	148.0	791.3
n-pentane	1.820	dodecanes	1.420	164.0	798.2
i-hexanes	1.210	tridecanes	1.310	174.0	810.3
n-hexane	1.170	tetradecanes	1.150	188.0	814.0
i-heptanes	0.350	pentadecanes	1.000	203.0	835.5
benzene	0.180	hexadecanes	0.880	218.0	847.7
cyclanes C_7	1.690	heptadecanes	0.760	232.0	850.4
n-heptane	0.620	octadecanes	0.690	249.0	862.6
i-octanes	0.470	nonadecanes	0.620	261.0	874.5
toluene	0.490	eicosanes-plus	6.040	460.0	939.0
cyclanes C_8	1.340				

(liquid volume at the final pressure measured under atmospheric conditions: 15°C, 1 atm). It is thus possible to calculate the relative volume $\left(Bo / Bo_{sat}\right)$ defined as $\left(V_{liq}/V_{sat}\right)$ where Bo_{sat} is the Bo value at the bubble point.

– Bubble points and densities of the reservoir oil swollen with a lean gas at the reservoir temperature (swelling test).
– The minimum miscibility pressure MMP (slim tube test) when the lean gas used during the swelling test is injected into the reservoir crude oil.

TABLE 2

Composition of the injection gas used in the swelling test and in the slim tube test

Components	Molar composition (%)	Components	Molar composition (%)
H_2S	3.81	butane	1.29
nitrogen	0.20	i-pentanes	0.25
carbon dioxide	7.57	n-pentane	0.28
methane	64.89	n-hexane	0.15
ethane	15.03	n-heptane	0.10
propane	5.76	n-octane	0.03
i-butane	0.63		

The composition of the injection gas is shown in Table 2. All the experimental data are summarized in Tables 3 to 6.

TABLE 3

Experimental relative volumes and total densities during constant mass expansions performed on the reservoir crude oil at $t_1 = 87.8$°C and $t_2 = 103.3$°C

Constant mass expansion at $t_1 = 87.8$°C			Constant mass expansion at $t_2 = 103.3$°C		
Pressure/ bar	Relative volume $\dfrac{V_{tot}}{V_{sat}}$	Total density (kg/m³)	Pressure/ bar	Relative volume $\dfrac{V_{tot}}{V_{sat}}$	Total density (kg/m³)
351.4	0.976	671.6	351.8	0.976	659.6
321.3	0.983	666.7	326.3	0.983	655.3
300.2	0.988	663.6	302.2	0.990	650.6
261.0	0.999	656.2	277.4	0.998	645.6
256.4	1.000	655.3	270.0	1.000	643.9
247.2	1.010	649.3	264.2	1.006	640.2
237.6	1.021	641.8	251.6	1.021	630.9
225.4	1.038	631.3	235.3	1.044	617.3
211.7	1.061	617.7	217.9	1.074	599.9

TABLE 4

Experimental relative volumes and total densities during
a constant mass expansion performed on the reservoir
crude oil at t_3 = 121.1°C.

Summary of experimental bubble points

Constant mass expansion at t_3 = 121.1°C			Saturation pressures of the reservoir oil	
Pressure/ bar	Relative volume $\dfrac{V_{tot}}{V_{sat}}$	Total density (kg/m³)	Temperature (°C)	Saturation pressure of the reservoir oil (bar)
400.5	0.966	647.2	121.1	275.0
351.4	0.978	639.4		
311.6	0.988	632.5		
281.3	0.998	626.2	103.3	270.0
275.0	1.000	625.0		
270.0	1.005	621.9		
262.9	1.014	616.5	87.8	256.4
253.7	1.025	609.8		
242.8	1.041	600.6		

TABLE 5

Experimental *Bo*, relative volumes, oil densities
and compressibility factors of liberated gas during
a differential vaporization performed on the reservoir
crude oil at t_2 = 103.3°C

Differential vaporization depletion at t_2 = 103.3°C				
Pressure/ bar	$Bo = \dfrac{V_{liq}}{V_{ref}}$	Relative volume: $\dfrac{Bo}{Bo_{sat}} = \dfrac{V_{liq}}{V_{sat}}$	Oil density (kg/m³)	Compressibility Factor of liberated gas
351.8	1.769	0.9763	359.7	
326.3	1.781	0.9829	655.4	
302.2	1.793	0.9895	650.8	
277.4	1.807	0.9972	645.7	
270.0	1.812	1.0000	644.1	
245.8	1.720	0.9492	651.9	0.880
201.0	1.603	0.8847	672.0	0.857
133.8	1.456	0.8035	702.7	0.854
67.4	1.330	0.7340	734.1	0.889
33.6	1.261	0.6959	753.0	0.920
1.0	1.072	0.5916	796.8	0.998

TABLE 6

Experimental saturation pressures and densities of fluids obtained by
injection of a lean gas (see Table 2)
in the crude oil at t_2 = 103.3°C (swelling test).
Measured MMP by displacement of the reservoir oil by the lean gas

Gaz injection experiments at t_2 = 103.3°C			
Mole (%) of injected gas in the mixture oil + gas	Saturation Pressure (bar) of swollen fluid	Density of swollen fluid at saturation pressure (kg/m³)	Experimental MMP/bar
0.0	270.0	644.0	
30.0	348.0	592.8	
40.0	382.8	574.0	MMP = 327±10
50.0	424.0	552.1	
60.0	515.6	526.0	

2 THE THERMODYNAMIC MODEL

In this paper, the Peng-Robinson (1976) Equation of State (EoS) was used:

$$P = \frac{RT}{v - b} - \frac{a(T)}{v(v + b) + b(v - b)}$$

with $\quad b = 0.07780 \ \dfrac{RT_c}{P_c}$

and $\quad R = 8.31441 \ \text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$

In order to calculate accurate vapor pressures of pure compounds, the following Soave type function, developed by Rauzy (1982) was used for all compounds except for the C_{20+} residue.

$$a(T) = 0.457236 \ \frac{R^2 T_c^2}{P_c} \left[1 + m \left(1 - \left(\frac{T}{T_c} \right)^{0.445075} \right) \right]^2$$

with

$$m = 6.812553 \left[\sqrt{1.127539 + 0.517252\omega - 0.003737\omega^2} - 1 \right]$$

For the C_{20+} residue, the Trebble and Bishnoï (1987) $a(T)$ function, more suitable for heavy hydrocarbons was used:

$$a(T) = 0.457236 \ \frac{R^2 T_c^2}{P_c} \exp \left[m \cdot \left(1 - \left(\frac{T}{T_c} \right)^{0.5} \right) \right]$$

In order to calculate correct densities, the molar volume v, solution of the EoS must be reduced using a volume translation c as proposed by Péneloux *et al.* (1982).

$$v_{correct} = v_{eos} - c$$

with $\quad c = \dfrac{RT_c}{P_c}\Big[0.1153758 - 0.440642Z_{RA}\Big]$

In the previous equation, Z_{RA} is the Rackett compressibility factor appearing in Spencer and Danner's (1973) modification of the Rackett Equation.

For a mixture containing p compounds of mole fraction x_i, classical mixing rules were used:

$$b_m = \sum_{i=1}^{p} x_i b_i \qquad c_m = \sum_{i=1}^{p} x_i c_i$$

$$a_m(T) = \sum_{i=1}^{p}\sum_{j=1}^{p}\Big[\sqrt{a_i(T)\cdot a_j(T)}\; x_i \cdot x_j\big(1 - k_{ij}(T)\big)\Big]$$

with $\quad k_{ij}(T) = \dfrac{E_{ij}(T) - \big(\delta_i - \delta_j\big)^2}{2\delta_i\delta_j}$

and $\quad \delta_i = \dfrac{\sqrt{a_i(T)}}{b_i}$

The binary interaction energies E_{ij} were estimated using the group contribution method developed by Abdoul *et al.* (1992).

3 CRUDE OIL MODELING

According to the EoS described in the previous section, each component of a petroleum fluid is characterized by the following parameters:

critical temperature T_c

critical pressure P_c

acentric factor ω

Rackett compressibility factor Z_{RA}

atomic group fractions allowing the calculation of the binary interaction parameters (bips).

3.1 The light compounds

For light compounds (until C_{10}), all these parameters are known in the literature.

3.2 The intermediate compounds

In this study, each cut from C_{11} to C_{19} was modeled according to the method recently developed by Avaullée *et al.* (1997a). In this approach, each cut is in a first step modeled as a mixture of three pure compounds (one paraffin, one naphtene and one aromatic). The relative amount of these three molecules is determined in order to reproduce the experimental molar weight and density of the cut. The critical properties and the acentric factor of these three pure compounds are estimated using the group contribution method developed by Avaullée *et al.* (1997b). In a second step, these three compounds are lumped together in order to model a given cut by one pseudo-component only. The critical temperature, critical pressure and acentric factor of this pseudo-component are solution of a non-linear three equation system (Avaullée *et al.*, 1997a). The Rackett compressibility factor and the group fraction allowing to estimate the bips are calculated by additivity balanced by the corresponding relative amounts.

3.3 The C_{20+} residue

Once more, the method developed by Avaullée *et al.* (1997a) was used in order to model the C_{20+} residue by a single compound. In order to use the PR EoS, the critical temperature, critical pressure and the shape parameter m must be estimated. Avaullée *et al.* (1997a) developed a specific correlation allowing the calculation of the critical pressure knowing the critical temperature and suggest to tune the critical temperature and the m parameter on the experimental bubble points of the crude oil. Since in this study, three saturation pressures were experimentally determined, this method can be used. The Rackett compressibility factor of the residue is determined so that the density calculated using the cubic EoS matches the experimental one. Moreover, the knowledge of the experimental molar weight and density of the C_{20+} compound allows to determine the group fractions necessary to estimate the bips.

4 CALCULATION OF THE PVT EXPERIMENTAL DATA

Before performing MMP calculations, the crude oil modeling previously described was used in order to check whether it was accurate to reproduce with a good accuracy the experimental data. The evolution of

the relative volume versus pressure for the four depletions, the *PT* phase envelop and the *P-X* diagram corresponding to the swelling test are shown on Figures 1 to 6. Moreover, during the swelling test simulation, the densities of the saturated mixtures of reservoir oil and injected gas were calculated with a 0.8% deviation. The average overall deviation between calculated and experimental total densities obtained during constant mass expansions was 1.6%. During the differential vaporization simulation, the liquid phase densities and the liberated gas compressibility factors deviated respectively of 1.5% and 0.7% from experimental data. In conclusion, the characterization procedure used allows a very satisfactory estimation of the various PVT data.

5 MMP CALCULATIONS

5.1 Results using the complete crude oil compositional model

In a first step, the previous crude oil modeling was used to calculate the MMP when the gas, the composition of which is given in Table 2, was injected in the reservoir crude oil. Before performing such a calculation, it is necessary to determine the process mechanism: pure vaporizing (VGDM), pure condensing (CGDM) or mixed condensing/vaporizing (C/VM).

For the fluids investigated in this study, the mechanism was found to be a mixed C/V mechanism as discovered by Zick (1986). In this case, the MMP may be determined using either a multicell approach developed by Zick but never published, or a classical commercial 1D simulator. The first solution was chosen in this study. The results of the calculations are shown in Table 7 and evidence a very good agreement between experimental and calculated MMP. Indeed, the deviation observed is less than 3% which is the experimental uncertainty in the determination of the MMP using a slim tube.

TABLE 7

Comparison between calculated and experimental MMP using a
37 component characterization for the crude oil

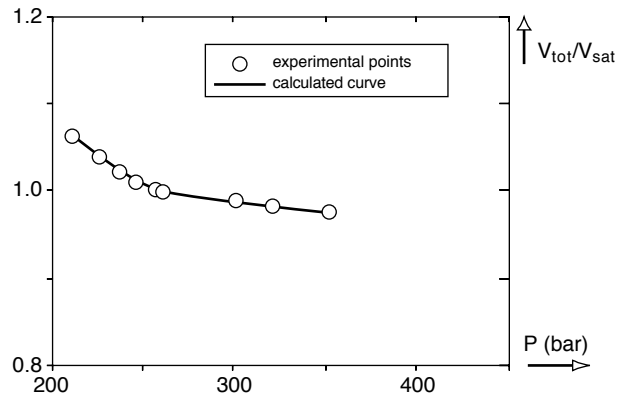| Experimental MMP/bar	Calculated MMP/bar	Deviation
327	319 (reference value)	2.4%

Figure 1

Relative volume V_{tot}/V_{sat} versus pressure during a constant mass expansion performed on the selected crude oil at $t_1 = 87.8°C$.

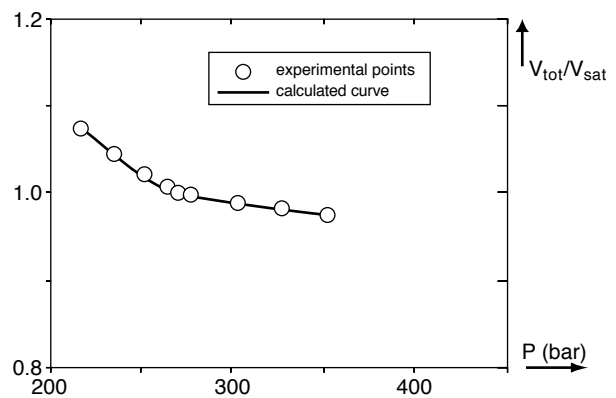Figure 2

Relative volume V_{tot}/V_{sat} versus pressure during a constant mass expansion performed on the selected crude oil at $t_2 = 103.3°C$.

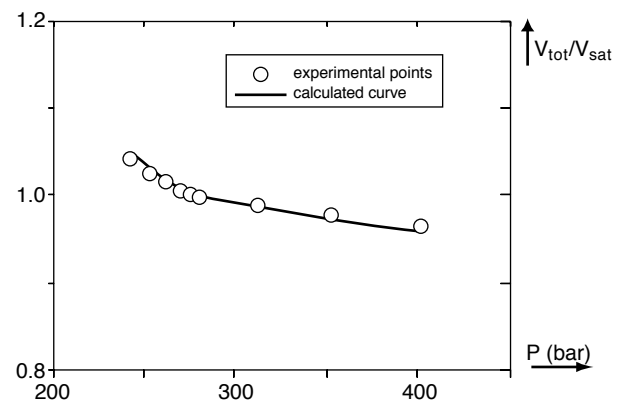
Figure 3

Relative volume V_{tot}/V_{sat} versus pressure during a constant mass expansion performed on the selected crude oil at $t_3 = 121.1°C$.
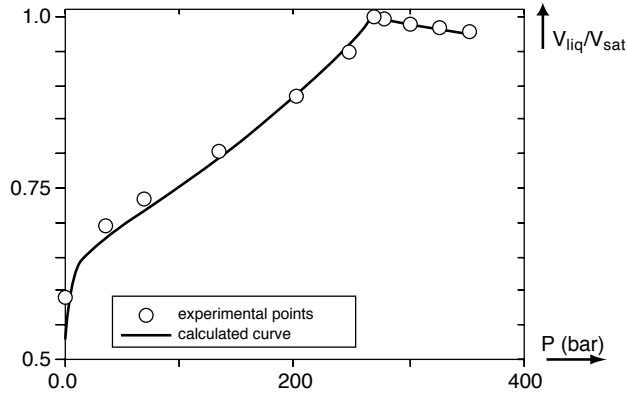
Figure 4

Relative volume V_{liq}/V_{sat} versus pressure during a differential vaporization performed on the selected crude oil at $t_2 = 103.3°C$.
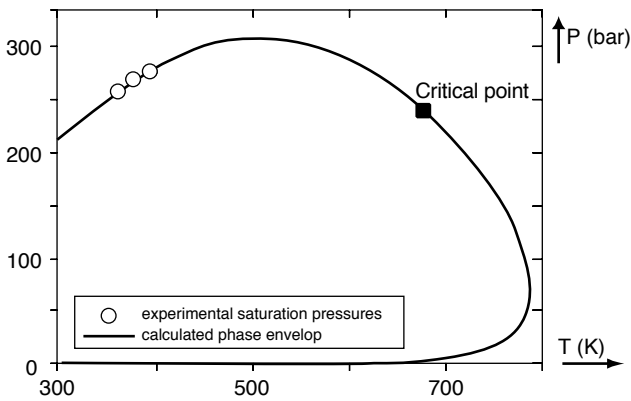

Figure 5

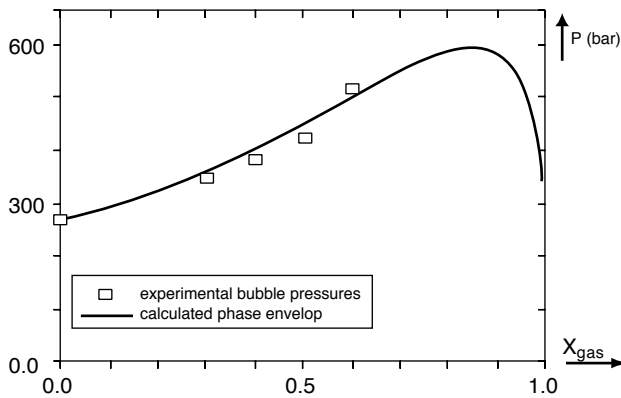*P-T* phase envelop of the selected reservoir crude oil.

Figure 6

P-X diagram resulting of a swelling test simulation.

5.2 Results using different compositional models

In this section it was decided to lump together successively the middle intermediate components (from C_{11} to C_{19}), the light intermediate components (from C_5 to C_{10}), the light hydrocarbons (from C_1 to C_4) and to compute the MMP. A similar lumping procedure was applied to the injected gas composition.

The pseudoization (lumping procedure) used in this paper was the very simple API method. In order to lump together *n* compounds of internal mole fractions x_i in a pseudo-component *k*, the following formulae were used:

$$Vc_k = \sum_{i=1}^{n} x_i Vc_i \text{ with } Vc_i = \frac{RTc_i Zc_i}{Pc_i}$$

(in this study Z_{ci} was merged with Z_{RA_i})

$$T_{c_k} = \frac{\sum_{i=1}^{n} x_i V_{c_i} T_{c_i}}{V_{c_k}}$$

$$\omega_k = \sum_{i=1}^{n} x_i \omega_i$$

$$Z_{RA_k} = \sum_{i=1}^{n} x_i Z_{RA_i}$$

$$P_{c_k} = \sum_{i=1}^{n} x_i P_{c_i} \left[1 - \beta \cdot \left(1 - \frac{T_{c_k}}{\sum_{i=1}^{n} x_i T_{c_i}} \right) \right]$$

with $\beta = 5.808 + 4.93 \omega_k$

On the other hand, atomic groups of pseudo-component *k* were calculated knowing those of compounds *i* and the internal mole fractions x_i.

The complete results are shown in Table 8.

Table 8 clearly evidences that it is not conceivable to lump together the light components to calculate the MMP.

Indeed, the calculated value is very far from the one obtained using the complete modeling of the crude oil and the process mechanism is not the same.

TABLE 8

Effect of various clustering configurations on the calculated MMP

Lumped compounds	Number of compounds used to model the crude oil	Process mechanism	Calculated MMP/ bar	Deviation due to lumping: comparison with reference to the 37 component modeling
from C_{11} to C_{19}	29	C/VM	314	1.6%
from C_5 to C_{10}	21	C/VM	329	-3.1%
from C_1 to C_4	33	VGDM	269	15.7%

Using 37 components a crossover tie line controls the miscibility process whereas the initial oil tie line does control the miscibility when light compounds are lumped together.

On the other hand, lumping together either the compounds from C_5 to C_{10} or from C_{11} to C_{19} gives a calculated MMP close to the one obtained with the complete compositional model. It is interesting to notice that lumping together the middle intermediate compounds makes decrease the MMP whereas lumping together the light intermediate components makes increase the MMP. In a last step, it was decided to model the crude oil with only 12 components introducing simultaneously both pseudo-components "C_5-C_{10}" and "C_{11}-C_{19}". The calculated MMP was thus MMP = 325 bars, what is very close (1.9% deviation) to the reference value. In this later case, the number of components has been reduced by a factor three and computing times by a factor 10.

CONCLUSION

This paper showed that:

– the characterization procedure developed by Avaullée *et al.* is suitable for MMP calculation;
– The MMP may be calculated with the same accuracy, modeling the crude oil with 37 or 12 compounds. To do so, the light intermediate compounds and the heavy intermediate compounds have to be lumped into two pseudo-components;
– Lumping together the light compounds is not suitable to determine the MMP.

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