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EOS PARAMETERS ADJUSTMENT FOR MINIMUM MISCIBILITY PRESSURE EXPERIMENTAL DATA

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Abstract. *Minimum Miscibility Pressure (MMP) data is one of the key information needed for the study of miscible gas enhanced oil recovery (EOR) processes. However, difficulties in obtaining accurate and reproducible experimental data have given estimation methods a higher importance, thus leading to a series of evaluation techniques. This paper presents the implementation of an EOS parameter tuning software to match computed data from CMG Winprop and from experimental data, with special focus on the adjustment of MMP data. The quasi-Newton method, expanded to the second-order term, was chosen to achieve the fit of the parameters. CMG Winprop is executed within the software to perform the calculation for the PVT data. This technique takes advantage of the CMG Winprop calculation capabilities, and adds a new functionality, avoiding a slow repetitive process to adjust MMP data. Furthermore, saturation pressure and saturation temperature experiments were implemented, aiming a better fit for the experiments. The method was later tested against available data from the literature.*

Keywords: *MMP, tuning EOS parameters, CMG Winprop software*

1. INTRODUCTION

Studies on enhanced oil recovery processes have been developed and applied for many years in order to improve productivity in petroleum reservoirs, as described in Christensen *et al.* (2001). Some of the oil recovery techniques, such as water alternate gas processes (WAG), are based on the premise of miscible gas injection. In order to determinate whether a process is miscible or not, it is necessary to evaluate the Minimum Miscibility Pressure (MMP), defined as the minimum pressure required to attain miscibility between the injected gas and the in-place oil reservoir. The miscibility is not only a function of the injected pressure, but also of the reservoir temperature and the composition of the injected gas.

As reported by Kechut *et al.* (1999), a series of experiments were designed to compute the MMP of reservoir oils. The most accepted and applied of these techniques is the slim-tube experiment, which consists of a packed bed narrow tube saturated with oil (Elsharkawy *et al.* 1992; Orr *et al.* 1982). This tube is then injected with gas, and the MMP is determined through the analysis of oil recovery. However, as reported in Elsharkawy *et al.* (1992), there are many issues associated with the reliability and reproducibility of results from slim-tube experiment. Other experiments have been developed and applied to MMP calculation, such as the multiple-contact experiment (Bryant and Monger, 1998), the rising bubble experiment (Christiansen and Haines, 1987) and the vanishing interfacial tension (VIT) experiment (Rao, 1997). However, all the mentioned methods present practical issues and restrictions which impose certain limitations for their uses. Therefore, the evaluation of MMP data trough numerical evaluation techniques has gained great importance for practical uses. One of these approaches is the evaluation of MMP data through the use of correlations. Several correlations to evaluate the MMP have also been proposed in the literature (Johns and Orr, 1996; Wang and Orr, 1998; Jenssen *et al.*, 2001, Ghomian, 2008).

This paper proposes the utilization of an EOS parameter tuning software in order to achieve a satisfactory fit for MMP experimental data set. Agarwal *et al.* (1990) used the quasi-Newton method with the iterative tuning of PVT data for adjusting parameters of EOS, like saturation pressure, liquid dropout factor, and swelling factor. Therefore, we will use the same approach in order to adjust the EOS parameters for the Minimum Miscibility Pressure. In order to accelerate the convergence rate of the quasi-Newton method the linearization the second order term was added to the iterative procedure. The commercial CMG Winprop package is used within the tuning program developed in order to perform the calculation of the PVT data, taking advantage of the features and capabilities of the Winprop package. In addition to the MMP experiment, other two calculation options were implemented: saturation pressure and saturation temperature. These two experimental parameters were included as a way to achieve better results by increasing the number of regression parameters available.

2. REGRESSION TECHNIQUE

The quasi-Newton algorithm implemented is defined by the minimization of the required function and the extension to the second-order term. The method as proposed by Agarwal *et al.* (1990) starts the process, minimizing the following function:

$$\min_{x\to} f(\vec{x}) = \vec{r}(\vec{x})^T \vec{r}(\vec{x}) , \tag{1}$$

where $\vec{r}(\vec{x})$ is the residual error. For this case, it is worthwhile to simplify the regression process establishing a simplified quadratic model, q, for the function f. The expansion of the Taylor series up to the second-order term for f is then performed. The resulting expression is given by

$$q_K(\vec{x})^S f(\vec{x}_K) = \nabla f(\vec{x}_K)^T \Delta\vec{x}_K + \frac{1}{2}\Delta\vec{x}_K^{\,T} \nabla^2 f(\vec{x}_K)\Delta\vec{x}_K . \tag{2}$$

Considering, $\Delta\vec{x}_K$ in Eq. (2), defined by $\Delta\vec{x}_K = \vec{x} - \vec{x}_K$, the first and the second derivatives are defined by

$$\nabla f(\vec{x}_K) = 2\,\mathrm{J}(\vec{x}_K)^T \vec{r}(\vec{x}_K) , \tag{3}$$

$$\nabla^2 f(\vec{x}_K) = 2[\mathrm{J}(\vec{x}_K)^T\,\mathrm{J}(\vec{x}_K) + \mathrm{S}(\vec{x})] , \tag{4}$$

where the Jacobian matrix **J** is defined as

$$\mathrm{J}(\vec{x}_K)_{ij} = \partial r_i(\vec{x}_K) / \partial(\vec{x}_K)_j . \tag{5}$$

The second-order term, **S**, cannot be easily evaluated and has uncertain influence on the regression process. However, for large residuals, its presence is deemed important. Therefore, the **S** term, which is also included for accelerating the fitting procedure, is defined by

$$\mathrm{S}(\vec{x}_K) = \sum_{i=1}^{n} r_i(\vec{x}_K) . \nabla^2 r_i(\vec{x}_K) . \tag{6}$$

Combining Eqs. (2) through (4), the resulting quadratic model is given by

$$q_K(\vec{x})^S = \overrightarrow{r_K}^T \overrightarrow{r_K} + 2\overrightarrow{\Delta x_K}^T \mathrm{J}_K^T \overrightarrow{r_K} + \overrightarrow{\Delta x_K}^T (\mathrm{J}_K^T \mathrm{J}_K + \mathrm{S}_K)\overrightarrow{\Delta x_K} . \tag{7}$$

The subscript k represents values evaluated at the *k-th* iteration. The minimization of the quadratic model results in the following linear system:

$$(\mathrm{J}_K^T \mathrm{J}_K + \mathrm{S}_K)(\vec{x}_{K+1} - \vec{x}_K) = -\mathrm{J}_K^T \vec{r}_K \tag{8}$$

If the second term is kept in Eq. (8) in the first iteration and $\mathbf{S}_0$ is set to 0 for the next iterations, $\mathbf{S}_K$ is computed through a secant approximation. This scheme is repeated until a desired tolerance is met or a maximum number of steps are reached. Further details of the present formulation can be found in Coats and Smart (1986) and Agarwal *et al.* (1990).

3. RESULTS

The validation of the implemented method was carried out by the comparison of values obtained by the present formulation with the numerical and experimental data of three cases available in the literature. The regression variables chosen for all the investigated cases were critical temperature (Tc), critical pressure (Pc), and acentric factor (ω) of the heaviest component. For all cases investigated, the injected fluid was composed only of CO_2.

The first case study, presented by Ligero *et al.* (2011), is characterized by 6 hydrocarbon components and is mainly composed of light fractions of petroleum. Table 1 presents the components and the mole fractions of each component.

Table 1. Fluid composition for case study 1.

Component	Composition (Mole %)
$C1/N_2$	45.90
$C2/CO_2$	9.03
C3	3.70
C4	2.35
C5	1.60
C6+	37.42

For case study 1, MMP and saturation pressure were available, as listed in Table 2. The temperature at which the data were obtained is also given in the table

Table 2. Numerical data for case study 1.

MMP (MPa)(1)	17.399
Saturation Pressure (MPa)(1)	26.789

(1) measured at 365.950 K

The second case study is an 11-component fluid mixture presented by Ayirala *et al.*, (2003). Table 3 shows the fluid compositions presented into the reservoir.

Table 3. Fluid composition for case study 3.

Component	Composition (Mole %)
CO_2	0.15
N_2	0.69
C1	45.06
C2	5.37
C3	5.44
i-C4	0.98
n-C4	2.85
i-C5	1.24
n-C5	1.80
C6	9.13
C7+	27.29

For the second case study, the saturation pressure and the MMP data are given in Table 4.

Table 4. Experimental data for case study 2.

MMP (MPa)(1)	57.799
Saturation Pressure (MPa)(1)	24.786

(1) measured at 373.150 K

The third case study is a 12-component fluid mixture in which one of the components is hydrogen sulfide. The data set for this case study was also presented by Ayirala *et al.* (2003). The fluid composition presented into the reservoir is given in Table 5.

Table 5. Fluid composition for case study 3.

Component	Composition (Mole %)
H_2S	1.37
CO_2	0.82
N_2	0.57
C1	35.13
C2	10.15
C3	6.95
i-C4	1.10
n-C4	3.16
i-C5	2.29
n-C5	1.74
C6	3.68
C7+	33.04

The experimental data for both MMP and saturation pressure are given in Table 6.

Table 6. Experimental data for case study 3.

MMP (MPa)(1)	17.399
Saturation Pressure (MPa)(1)	26.789

(1) measured at 365.950 K

In order to validate the adjustment program developed, we first simulated case studies 1 and 2 to saturation pressure and then we compared the results with the ones obtained by the WinProp simulator. For each case study, the critical temperature and pressure and acentric factor were separately tuned. Table 7 presents results obtained with the proposed adjuster software and the ones obtained using Winprop for case study 1. The values of the tuned parameters are also shown in this table.

Table 7. Comparison of saturation pressure with the present work and Winprop - case study 1.

Variable	Original Value	Final Value	Saturation Pressure (MPa) (1)	Error (%)	Saturation Pressure (MPa) (2)	Error (%)
Tc (K)	728.500	801.181	26.525	0.99	26.790	0.00
Pc (MPa)	1.898	2.219	27.063	1.02	26.792	0.00
ω	0.7172	0.9171	27.090	1.12	25.769	3.81

(1) regression solver data
(2) CMG Winprop data

From Table 7, it is possible to infer that the results, in terms of saturation pressure, tuned using the present formulation are in good agreement with the ones from the literature and the ones obtained through the Winprop software.

The results in terms of saturation pressure for case study 2 are presented in Table 8. From this table, we can again see a good match among results obtained by the present formulation, literature, and Winprop software. At least for these two case studies, we can say that the presented formulation has been validated. Now we explore the present formulation for the calculation of the MMP.

Table 8. Comparison of saturation pressure of the present work and Winprop - case study 2.

Variable	Original Value	Final Value	Saturation Pressure (MPa) (1)	Error (%)	Saturation Pressure (MPa) (2)	Error (%)
Tc (K)	1014.600	1072.749	24.804	0.07	24.805	0.07
Pc (MPa)	0.945	1.001	24.582	0.27	24.786	0.00
ω	1.2095	1.3038	24.873	0.35	24.786	0.00

(1) regression solver data
(2) CMG Winprop data

Table 9 presents the results for case study 1, when the parameters were tuned to adjust both MMP and saturation pressure. From Table 9, we can verify that when the proposed formulation is applied to both MMP and saturation pressure, the results are in good agreement with the ones presented in the literature no matter which parameter was tuned.

Table 9. Results for MMP and Saturation Pressure – case study 1.

Variable	Original Value	Final Value	Saturation Pressure (MPa)	Error (%)	MMP (MPa)	Error (%)
Tc (K)	728.500	806.643	26.951	0.61	17.788	2.23
Pc (MPa)	1.898	2.175	26.797	0.03	16.530	4.98
ω	0.7172	0.9229	27.289	1.87	17.478	0.45

Table 10 presents the results for case study 2, in terms of saturation pressure and MMP.

Table 10. Results for MMP and Saturation Pressure – case study 2.

Variable	Original Value	Final Value	Saturation Pressure (MPa)	Error (%)	MMP (MPa)	Error (%)
Tc (K)	1014.600	1015.506	23.115	6.74	62.438	8.02
Pc (MPa)	0.945	0.961	23.561	4.94	63.638	10.10
ω	1.2095	1.2044	23.014	7.14	62.025	7.31

We can infer from Table 10 that the errors are amplified when the parameters are tuned to adjust both MMP and saturation pressure. There was no single parameter that could simultaneously improve the calculation for adjusting both physical parameters. However, the errors are still acceptable.

The results in terms of MMP and saturation pressure for case study 3 are presented in Table 11.

Table 11. Results for MMP and Saturation Pressure –case 3.

Variable	Original Value	Final Value	Saturation Pressure (MPa)	Error (%)	MMP (MPa)	Error (%)
Tc (K)	703.135	708.134	14.316	16.50	16.530	11.69
Pc (MPa)	1.986	1.946	14.329	16.42	16.582	12.04
ω	0.63165	0.57557	14.309	16.54	16.530	11.69

From Table 11 it is possible to verify that the errors are larger compared to the results obtained for case studies 1 and 2, especially the ones obtained for the saturation pressure. The last test that we performed was to adjust only the MMP for case study 3. The results of this last investigation are presented in Table 12.

Table 12. Results for MMP – case study 3.

Variable	Original Value	Final Value	MMP (MPa)	Error (%)
Tc (K)	703.135	636.027	13.996	5.43
Pc (MPa)	1.986	0.966	14.772	0.19
ω	0.63165	0.42959	14.772	0.19

From Table 12 shows that errors were reduced, especially when the acentric factor or the critical pressure was tuned.

4. CONCLUSIONS

This paper proposes the utilization of an EOS parameter tuning software in order to achieve a satisfactory fit for MMP experimental data set. The results of the proposed formulation were tested for the numerical and the experimental data from the literature. The analysis of the case studies can be divided in three parts. Primarily, the results obtained in all three cases are in a satisfactory range of accuracy, showing the applicability not only of the regression solver software, but also of the method applied.

Cases 1 and 2 are objects of the second part of our analysis. In both cases, the fit of saturation pressure data alone has shown to give results on the same order of accuracy as from those generated by CMG Winprop. This shows the method, as implemented, is already able to give results comparable to a commercial package.

The last part of this investigation concerns the results of case study 3. As observed, the adjustment for both MMP and saturation pressure data generated accurate fit for the regression variables, compared to the fit produced by the MMP data only. This information leads to the conclusion that increasing number of regression parameters does not necessary imply a better adjustment of the PVT data. In fact, using many regression parameters can complicate achieving a good fit.

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