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Prediction of vapor-liquid equilibrium in highly asymmetric paraffinic systems with new modified EOS-G^E model

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ABSTRACT

A new modified EOS-G^E model is developed for the highly asymmetric paraffinic systems, where the volume translated Peng-Robinson EOS is adopted coupled with the LCVM mixing rule. In the new modified EOS-G^E model, the original UNIFAC is replaced by a newly established UNIFAC where the nonlinear calculation of the segment fractions of molecules in γ^C (the combinatorial activity coefficient) is introduced to modify the traditional assumption that “all groups are isotropic in solution”. A total of 956 vapor-liquid experimental bubble points in highly asymmetric paraffinic systems including binary systems, ternary systems, quaternary systems and multiple systems are used to test the new developed EOS-G^E model. Results show that the original UNIFAC and the improved UNIFAC both perform well if the molefractions of light components (CH_4 or C_2H_6) are low; however, with the increase of the light components, the improved UNIFAC is remarkably superior to the original UNIFAC.

1. Introduction

In petroleum production, the vapor-liquid equilibrium plays an extremely important role in the process of exploitation, gathering and transportation and rectification. Therefore, the accurate prediction of vapor-liquid equilibrium is critical for the petroleum industry. In the modeling of vapor-liquid equilibrium, the vapor phase is usually described by cubic Equation of State (Redlich and Kwong, 1949; Soave, 1972; Stryjek and Vera, 2010; Patel and Teja, 1982); while the liquid phase can be modeled in two different ways: Equation of State (EOS) (Redlich and Kwong, 1949; Soave, 1972; Stryjek and Vera, 2010; Patel and Teja, 1982) or activity coefficient method (G^E) (Hildebrand, 1929; Flory, 1942; Huggins, 1942; Wilson, 1964; Renon and Prausnitz, 1968; Abrams and Prausnitz, 1975; Fredenslund et al., 1975). The objective with the use of EoS/G^E models is to combine the “advantages” of cubic EOS and of the local composition activity coefficient models incorporated (Kontogeorgis and Coutsikos, 2012). The EOS can deal with the influence of large pressure variation, but it is not suitable for the systems with high polarity and high asymmetry. On the contrary, the activity coefficient method (G^E) can describe the non-ideality of polar and asymmetric systems well without the capability to reflect the effects of pressure variation. Therefore, it is necessary to build a bridge between EOS and G^E.

To introduce G^E into EOS, the traditional linear mixing rule is modified. Huron and Vidal (1979) assumed that fluid systems were in a state of liquid or nearly liquid at the infinite pressure and established the HV mixing rule which predicts well for some complicated fluid systems. Mollerup (1981), Heidemann and Kolal (Heidemann and Kokal, 1990) proved the possibility that G^E and EOS could be integrated at zero or low pressure. Later, Michelsen et al (Michelsen, 1990a, 1990b; Dahl and Michelsen, 1990). developed the mixing rule at zero pressure (MHV1) and amplified the application range of EOS-G^E. Boukouvalas et al. (1994). found that as the size difference of tested systems increases, the HV mixing rule led to underprediction and the MHV1 mixing rule led to overprediction. Therefore, Boukouvalas et al. (1994). proposed the LCVM mixing rule (Linear Combination of the Vidal and Michelsen mixing rules) to make up for the weakness of the HV mixing rule and the MHV1 mixing rule. These EOS/G^E mixing rules realized two progresses (Kontogeorgis and Coutsikos, 2012). First of all, the cubic EOS is successfully applied to the mixtures of compounds of wide complexity and

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Table 1
Parameters of Eq. (11).

Constants	Values
A	
k_0	−4.1034
k_1	31.723
k_2	0.0531
k_3	188.68
k_4	0.0057
k_5	20,196
k_6	0.0003
B	
k_0	−0.3489
k_1	−28.547
k_2	0.0687
k_3	−817.73
k_4	0.0007
k_5	−65.067
k_6	0.0076

asymmetry in size and energies. Secondly, the incorporated activity coefficient models established at low pressure can be extrapolated to the higher pressure conditions.

For the high prediction accuracy of the vapor-liquid equilibrium, the calculation method for G^E should be improved. UNIFAC is an approximation method where the properties of the practical systems are predicted by the properties of the composed chemical groups. The original UNIFAC is not suitable for systems with large size difference due to the assumption that "all groups are isotropic in solution" (Deiters, 1989). Deiters et al. (Deiters, 1989) proposed a nonlinear calculation for the volume fractions of non-spherical molecules. Li et al. (1998). employed the concept of effective R_k^* and Q_k^* to describe the local characteristic of groups. Sayegh and Vera (1980) pointed out that the Staverman-Guggenheim correction may give unrealistic large corrections to the combinatorial excess entropy. Consequently, Larsen et al. (1987). and Kikic et al. (1980), dropped the Staverman-Guggenheim correction in the UNIFAC model:

$$\ln\gamma_i^C = \ln\left(\frac{\phi_i}{x_i}\right) + 1 - \frac{\phi_i}{x_i} \tag{1}$$

$$\phi_i = \frac{x_i r_i^{2/3}}{\sum_j x_j r_j^{2/3}} \tag{2}$$

In 1993, Gmehling et al (Weidlich and Gmehling, 1987). developed another way to improve the calculation method for the combinatorial part:

$$\ln\gamma_i^C = 1 - \phi_i' + \ln\phi_i' - 5q_i\left(1 - \frac{\phi_i}{\theta_i} + \ln\frac{\phi_i}{\theta_i}\right) \tag{3}$$

$$\phi_i' = \frac{r_i^{3/4}}{\sum_j r_j^{3/4} x_j} \tag{4}$$

Similarly, to improve the phase equilibria prediction of the highly asymmetric paraffinic systems, this work develops a new modified EOS-G^E model where the volume translated PR-EOS with the LCVM mixing rule is adopted. And G^E is calculated by the newly improved UNIFAC with the nonlinear calculation of the molecule's segment fractions to consider the anisotropy of groups in solution.

2. The equation of state

The PR-EOS with the consideration of the volume translation effects (Mathias et al., 1989) is used:

$$P = \frac{RT}{V + t - b} - \frac{a}{(V + t)(V + t + b) + b(V + t - b)} \tag{5}$$

where P is the pressure of the system; T is the temperature of the system; R is the gas universal constant; V is the volume of gas or liquid; t is the translation volume. For pure component, parameter *a* is calculated by (Stryjek and Vera, 2010):

$$a = 0.45724\frac{R^2T_c^2}{p_c}\cdot\alpha(T) \tag{6}$$

$$\alpha(T) = \left[1 + k\left(1 - T_r^{0.5}\right)\right]^2 \tag{7}$$

$$k = 0.37464 + 1.54226\omega - 0.26992\omega^2 \tag{8}$$

Table 2
The tested pressure range and the composition of the systems.

Tested system	light component content range	Pressure range (MPa)	Temperature range(K)	Number of points	Reference
Binary system					
C1+C10	0.1–0.55	1–32	243.15–313.15	61	(Rijkers et al., 1992a)
C1+C12	0.1–0.6	1–23	255–320	38	(Rijkers et al., 1992b)
C1+C16	0.1–0.6	2–26	285–360	84	(Glaser et al., 1985)
C1+C17	0.2–0.6	4–27	293–373	29	(Pauly et al., 2007)
C1+C20	0.025–0.65	0–32	303–370	83	(Van der Kooi et al., 1995)
C1+C24	0.1–0.7	1–30	315–450	127	(Flöter et al., 1997)
C1+C32	0.1–0.325	1.5–7	343.15	10	(Cordeiro et al., 1973)
C2+C10	0.017–0.995	0.1–11	277.6–510.9	107	(Reamer and Sage, 1962)
C2+C16	0.2–0.875	0.5–16	260–450	148	(De Goede et al., 1989)
C2+C20	0.07–0.47	0.5–4	373.75–572.85	11	(Huang et al., 1988)
C2+C22	0.05–0.9	0.1–9.5	290–370	110	(Peters et al., 1988)
C2+C28	0.1–0.5	0.5–5.5	348–423	24	(Gasem et al., 1989)
C2+C36	0.087–0.531	0.3–5	373–423	13	(Gasem et al., 1989)
C2+C44	0.1–0.52	0.3–3.5	373–423	15	(Gasem et al., 1989)
Ternary system					
C1+C10 + C32	0.025–0.4	0.1–10	330–340	28	(Cordeiro et al., 1973)
Quaternary system					
C1+C16 + C17 + C18	0.2–0.6	3–30	293–373	14	(Pauly et al., 2010)
Multiple system					
C1+C10+ Multiple-paraffin	C1:0.436–0.440 C10:0.458–0.462	12–16	293–423	54	(Daridon et al., 1996)
Total number of points				956	

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