

Calculation of Interfacial Tension of Methane + n-Butane Mixture with Gradient Theory Near Critical Conditions

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Abstract

In this work the interfacial tensions (IFT) of methane + n-butane were calculated with gradient theory (GT) of inhomogeneous fluids for planar interface. The inputs of GT are the Helmholtz free energy densities of homogeneous fluids and influence parameters of inhomogeneous interface. The homogeneous fluids properties were computed by applying volume translated Soave-Redlich-Kwong equation of state (SRK EOS). The pure influence parameters were obtained by the correlating the experimental surface tensions of pure fluids, and the influence parameter of the mixtures was determined by using the geometric mixing rule. In this study the gradient theory was applied to the methane + n-butane mixture near the critical conditions where the measured interfacial tensions are above 0.9 mN/m. The predicted interfacial tensions were in excellent agreements with the available measured data to within a few percents. In addition the predicted density profiles in the interface revealed the local enrichment of methane and confirmed the credibility of the gradient theory.

Key words: Interfacial tension; Inhomogeneous; Gradient theory; Equation of state; Influence parameter; Density profiles;

1 Introduction

It is well known that the interfacial tensions of hydrocarbon mixtures are regarded as one of important thermophysical parameters in oil related industrial processes, but there are still a considerable lack of reliable experimental IFT

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data in the open literatures, specially near the critical point. Therefore the theoretical and semiempirical predictions of interfacial tensions are of particular significance.

There are several approaches which have been proposed for the modelling of interfacial tensions. These approaches can be divided into two categories: empirical correlations and statistic thermodynamics-based methods that take into account the density gradient between the bulk phases. For instance, here list a few of techniques. Simple correlations methods: the parachor method [1-2] and corresponding state correlations [3] that are not satisfactory for computing interfacial tension of compounds that exhibit strong hydrogen bonding. Statistic thermodynamics-based methods: the perturbation theory[4], the density function theory[5-7] and the gradient theory[8-9].

In summary the general expression of gradient theory is the integral of the two contributions: the local value of the properties (homogeneous fluid) and the gradient value of the properties[9]. The gradient value of the properties can be derived from the properties of the homogeneous fluids by applying the influence parameters, which are related to the mean square range of the direct correlation functions of the homogeneous fluids[18]. The minimum of this integral with respect to one component density variations corresponds to the free energy of the flat interface, which is equal to surface tension in case of vapor-liquid systems. Hence the inputs of gradient theory are the free energy density of homogeneous fluids and the influence parameters of inhomogeneous fluids[19].

There are lots of efforts that have been done for practical applications of gradient theory to compute the interfacial tensions in different fluids systems. The significant research was firstly started by Carey et al. (1980) [10] that focused on predicting the interfacial tension of polytomic fluids such as nonpolar hydrocarbons and alcohols. Similarly, Sahimi et al. (1985) [11] applied the gradient theory to predict interface composition profiles and interfacial tensions of liquid-liquid, liquid-vapor and liquid-liquid-vapor interface in binary and ternary mixtures of CO_2 with propane and decane. Unlike the previous research work the predictions of interfacial tension was made with Mohanty-Davis equation of state by Perez-Lopez et al. (1992) [12]. After one year Cornelisse et al. (1993) [13] studied the interfacial tension of carbon dioxide + water and benzene + water systems, the results were not satisfactory due to the incapability of the Peng-Robinson as well as the gradient approximation. To save time-consuming density profile computation, Zuo and Stendy et al. [14-16] developed the linear gradient theory for calculating interfacial tension of mixtures that had excellent agreements between the predicted and experimental interfacial tension at high and moderate IFT value. For estimate of interfacial tension of complex mixtures of more than three components, the gradient theory was for the first time applied without any lumping by Miqueu

et al. (2005) [17].

In this study the gradient theory will be utilized to predict the interfacial tensions of methane + n-butane mixture in combination with volume translated Soave-Redlich-Kwong equation of state (SRK EOS). The objective of this survey is to investigate the validity of gradient theory for estimating the interfacial tension of hydrocarbon mixtures near the critical area. First, this paper will begin with the descriptions of gradient theory. Second, the volume translate SRK EOS will be recalled in the section 3. Third, the explanation of influence parameters used in the gradient theory will be found in the section 4. Finally the results of calculated interfacial tensions will be compared with available experimental data, and moreover the estimated density profiles will display the density distribution across the vapor-liquid interface to help us better understanding the interfacial behaviors of methane + n-butane mixture near the critical point.

2 Gradient theory

In this section the theoretical background of gradient theory will be described briefly. Consider there is a planar interface between liquid and vapor bulk phases, the distance normal to this interface is denoted by z which equals to interface thickness. According to gradient theory, in the absence of external potentials, the differential equation that governs the density distribution $\rho(z)$ through the planar interface is of the form:

$$\sum_{j=1}^N \frac{d}{dz} (\kappa_{ij} \frac{d\rho_j}{dz}) - \frac{1}{2} \sum_{j=1}^N \sum_{k=1}^N \frac{\partial c_{jk}}{\partial \rho_i} \frac{d\rho_j}{dz} \frac{d\rho_k}{dz} = \frac{\partial \Phi(\rho)}{\partial \rho_i} \quad (1)$$

where κ denotes the influence parameter of the inhomogeneous fluid at the interface, and $\Phi(\rho)$ is grand thermodynamic potential defined by

$$\Phi(\rho) = f^0(\rho) - \sum_i \rho_i \mu_{iB} \quad (2)$$

$$f^0(\rho) = \rho \mu(\rho) - P(\rho) \quad (3)$$

where $f^0(\rho)$ is the local Helmholtz free energy density of homogeneous fluid at interface grid of density $\rho(z)$, and μ_{iB} is the chemical potential of component i in the bulk phase.

Assuming the influence parameters are independent of density supported by the works of McCoy & Davis et al. (1978) [20] in which density profiles of

simple one-component fluids were shown to be relatively insensitive (10% variation) to the density dependence of the influence parameters. The governing equation (1) for planar interface is reduced to

$$\sum_{j=1}^N \kappa_{ij} \frac{d^2 \rho_j}{dz^2} = \mu_i(\rho) - \mu_{iB} \quad (4)$$

where the $\mu_i(\rho)$ is the chemical potential at the interface grid where the density equals to ρ . Multiplying equation (4) by $d\rho_i/dz$, summing over i and integrating gives

$$\sum_i \sum_j \frac{1}{2} \kappa_{ij} \frac{d\rho_i}{dz} \frac{d\rho_j}{dz} = \Phi(\rho) - \Phi_B \quad (5)$$

where $\Phi_B = -P$, P is the vapor liquid equilibrium pressure. The boundary conditions related with equation (3) are

$$z \longrightarrow +\infty, \rho \longrightarrow \rho^L$$

$$z \longrightarrow -\infty, \rho \longrightarrow \rho^V$$

where the ρ^L and ρ^V are the liquid and vapor phase densities.

The interfacial tension according to gradient theory is calculated as[18]

$$\sigma = \int_{-\infty}^{+\infty} \kappa_{ij} \frac{d\rho_i}{dz} \frac{d\rho_j}{dz} dz \quad (6)$$

To avoid solving a boundary value problem on the infinite interval $[-\infty, +\infty]$, a density variable ρ is defined to eliminate the position coordinate variable z , as z moves from $-\infty$ to $+\infty$, the density variable ρ will increase monotonically from ρ^V to ρ^L . To do this, the following equations will be used

$$\frac{d\rho_i}{dz} = \frac{d\rho_i}{d\rho} \frac{d\rho}{dz} \quad (7)$$

$$\frac{d^2 \rho_i}{dz^2} = \frac{d(\frac{d\rho_i}{d\rho})}{d\rho} \frac{d\rho}{dz} \frac{d\rho}{dz} + \frac{d\rho_i}{d\rho} \frac{d(\frac{d\rho}{dz})}{d\rho} \frac{d\rho}{dz} = \frac{d^2 \rho_i}{d\rho^2} \left(\frac{d\rho}{dz}\right)^2 + \frac{d\rho_i}{d\rho} \frac{d\rho}{dz} \frac{d}{d\rho} \left(\frac{d\rho}{dz}\right) \quad (8)$$

Then dz can be written as by rearranging equation (5)

$$dz = \sqrt{\frac{\sum_i \sum_j \kappa_{ij} \frac{d\rho_i}{d\rho} \frac{d\rho_j}{d\rho}}{2[\Phi(\rho) - \Phi_B]}} d\rho \quad (9)$$

The equation (6) can be rewritten as the following form by using the independent density variable ρ

$$\sigma = \int_{\rho^I}^{\rho^{II}} \sqrt{(2(\Phi(\rho) - \Phi_B) \sum_i \sum_j \kappa_{ij} \frac{d\rho_i}{d\rho} \frac{d\rho_j}{d\rho})} d\rho \quad (10)$$

To calculate the chemical potential μ in each interface grid, the volume translated SRK EOS were utilized. It will be introduced in the next section.

3 Equation of state

In this paper, the volume translated SRK EOS from the work of Lin et al. (2006) [21] is choosed to compute the thermodynamic properties of the bulk phase and interface. The bulk phase density and interface pressure and chemical potential can be estimated with the help of the volume translated SRK EOS. It is defined as

$$p = \frac{RT}{v + c - b} - \frac{a}{(v + c)(v + b + c)} \quad (11)$$

The coefficients a and b are calculated likewise the original SRK EOS by Soave et al. (1972) [22] as

$$a = 0.42748 \frac{R^2 T_c^2}{P_c} \alpha(T) \quad (12)$$

$$b = 0.08664 \frac{RT_c}{P_c} \quad (13)$$

$$\alpha(T) = [1 + m(1 - T_r^{0.5})]^2 \quad (14)$$

$$m = 0.480 + 1.574\omega - 0.176\omega^2 \quad (15)$$

where the T_c and P_c are the critical temperature and critical pressure, the $T_r = T/T_c$ is the reduced temperature and ω is the acentric factor.

The volume translation parameter c can be computed as

$$c = c_c f(T_r) \quad (16)$$

$$c_c = \left(\frac{1}{3} - Z_c\right) \frac{RT_c}{P_c} \quad (17)$$

$$f(T_r) = \begin{cases} \beta + (1 - \beta) \exp[\chi(1 - T_r)], & T_r \leq 1 \\ \beta + (1 - \beta) \exp(0.5\chi), & T_r > 1 \end{cases} \quad (18)$$

$$\beta = -3.7303 \exp[-60.2833(\frac{1}{3} - Z_c)] + 0.2334 \quad (19)$$

$$\chi = -3.4620 = \exp[16.08133 - Z_c] - 4.0957 \quad (20)$$

where the Z_c represents the cirical compressibility factor.

With the help of above volume translated SRK EOS, the thermodynamic properties of homogeneous fluids can be computed, but to obtain the propertis of inhomogeneous fluids in the interface the influence parameters must be applied.

4 Influence parameter

In this part, it will focus on the influence paramters. The theoretical expression for influence paramater is derived by Bongiorno et al. (1976) [23] as

$$\kappa_{ij} = \frac{k_b T}{6} \int_V s^2 C_{ij}^0(s, \rho) ds^3 \quad (21)$$

where k_b is Boltzmann's constant, and C_{ij}^0 is the homogeneous fluid direct correlation function between the component i and j . Due to paucity of the direct correlation function for the majority of the fluids systems, the influence parameters have to be determined based on correlating the avaible experimental surface tension data of pure fluids to the gradient theory as

$$\kappa = \left(\frac{\sigma}{\int_{\rho^I}^{\rho^{II}} \sqrt{2(\Phi(\rho) - \Phi_B)}} \right)^2 = \left(\frac{\sigma}{\int_{\rho^I}^{\rho^{II}} \sqrt{2[\rho(\mu(\rho) - \mu_B)] - (P(\rho) - P_B)}} \right)^2 \quad (22)$$

In this study the influence parameters from Lin et al. (2007) [24] were applied as

$$\ln\left(\frac{\kappa}{ab^{\frac{8}{3}}} N_A^{\frac{8}{3}}\right) = K_0 + K_1 \ln\left(1 - \frac{T}{T_c}\right) + K_2 \left[\ln\left(1 - \frac{T}{T_c}\right)\right]^2 \quad (23)$$

where N_A is avogadro constant($6.0221415 \times 10^{23} mol^{-1}$), and K_0, K_1, K_2 are the correlation coefficients. For pure methane component

$$K_0 = -1.161; K_1 = -0.698; K_2 = -0.098$$

For pure n-butane component

$$K_0 = 1.571; K_1 = -0.840; K_2 = -0.143$$

The geometric mixing rule is used to calculate the cross influence parameter of methane + n-butane mixture. It is computed as

$$\kappa_{ij} = \sqrt{\kappa_{ii}\kappa_{jj}} \quad (24)$$

where κ_{ii} and κ_{jj} are the influence parameters of pure methane and n-butane corresponding to the equation (23).

5 Results and discussion

5.1 Numerical solution

For the binary mixture ($i = 2$), and the governing equation (4) can be restated as

$$\kappa_{11} \frac{d^2 \rho_1}{dz^2} + \kappa_{12} \frac{d^2 \rho_2}{dz^2} = \mu_1(\rho_1, \rho_2) - \mu_{1B} \quad (25)$$

$$\kappa_{21} \frac{d^2 \rho_1}{dz^2} + \kappa_{22} \frac{d^2 \rho_2}{dz^2} = \mu_2(\rho_1, \rho_2) - \mu_{2B} \quad (26)$$

where the cross influence parameters of binary mixture $\kappa_{12} = \kappa_{21} = \sqrt{\kappa_{11}\kappa_{22}}$.

It can be seen that equation (25) $\times \sqrt{\kappa_{22}}$ equals to equation (26) $\times \sqrt{\kappa_{11}}$. At last the object function in the interface can be obtained as

$$F_{obj} = \sqrt{\kappa_{22}}[\mu_1(\rho_1, \rho_2) - \mu_{1B}] = \sqrt{\kappa_{11}}[\mu_2(\rho_1, \rho_2) - \mu_{2B}] = 0 \quad (27)$$

Derivatives to the density of component 1 and component 2 are of form as

$$\left[\sqrt{\kappa_{22}} \frac{\partial \mu_1}{\partial \rho_1} - \sqrt{\kappa_{11}} \frac{\partial \mu_2}{\partial \rho_1} \right] d\rho_1 = 0 \quad (28)$$

$$\left[\sqrt{\kappa_{22}} \frac{\partial \mu_1}{\partial \rho_2} - \sqrt{\kappa_{11}} \frac{\partial \mu_2}{\partial \rho_2} \right] d\rho_2 = 0 \quad (29)$$

where $\partial \mu_1 / \partial \rho_1, \partial \mu_2 / \partial \rho_1, \partial \mu_1 / \partial \rho_2$ and $\partial \mu_2 / \partial \rho_2$ can be derived with the help of volume translated SRK EOS.

The value of $d\rho_1/d\rho_2$ can be obtained by rearranging equation (28) and equation (29)

$$\frac{d\rho_1}{d\rho_2} = \frac{\sqrt{\kappa_{22}} \frac{\partial \mu_1}{\partial \rho_2} - \sqrt{\kappa_{11}} \frac{\partial \mu_2}{\partial \rho_2}}{\sqrt{\kappa_{11}} \frac{\partial \mu_2}{\partial \rho_1} - \sqrt{\kappa_{22}} \frac{\partial \mu_1}{\partial \rho_1}} \quad (30)$$

The matlab code for calculation the thermodynamic properties of methane + n-butane mixture is provided by Tore Haug-Warberg (Norwegian University of Science and Technology). The volume and temperature is assumed to be constant in the volume translated SRK EOS model. The following equations are solved to calculate the value of $d\rho_1/d\rho_2$.

The differential equation for chemical potential is defined as

$$d\mu_i = \left(\frac{\partial \mu_i}{\partial V}\right)_{T,N_1,N_2} dV + \left(\frac{\partial \mu_i}{\partial N_1}\right)_{T,V,N_2} dN_1 + \left(\frac{\partial \mu_i}{\partial N_2}\right)_{T,V,N_1} dN_2 \quad (31)$$

where N_1 and N_2 are mole number of methane and n-butane respectively.

The differential equation for pressure is defined as

$$dP = \left(\frac{\partial P}{\partial V}\right)_{T,N_1,N_2} dV + \left(\frac{\partial P}{\partial N_1}\right)_{T,V,N_2} dN_1 + \left(\frac{\partial P}{\partial N_2}\right)_{T,V,N_1} dN_2 \quad (32)$$

The differential equation for mole number is defined as

$$V d\rho_i + \rho_i dV = dN_i \quad (33)$$

The value of $\partial \mu_i / \partial \rho_1$ was computed by

$$\frac{\partial \mu_i}{\partial \rho_1} = \left[\frac{\left(\frac{\partial \mu_i}{\partial V}\right)_{T,N_1,N_2} dV + \left(\frac{\partial \mu_i}{\partial N_1}\right)_{T,V,N_2} dN_1 + \left(\frac{\partial \mu_i}{\partial N_2}\right)_{T,V,N_1} dN_2}{(dN_1 - \rho_1 dV)/V} \right]_{T,V,\rho_2} \quad (34)$$

The value of $\partial \mu_i / \partial \rho_2$ was calculated by

$$\frac{\partial \mu_i}{\partial \rho_2} = \left[\frac{\left(\frac{\partial \mu_i}{\partial V}\right)_{T,N_1,N_2} dV + \left(\frac{\partial \mu_i}{\partial N_1}\right)_{T,V,N_2} dN_1 + \left(\frac{\partial \mu_i}{\partial N_2}\right)_{T,V,N_1} dN_2}{(dN_2 - \rho_2 dV)/V} \right]_{T,V,\rho_1} \quad (35)$$

All these derivatives had to be computed in each interface grid for deriving the density profiles in the whole interface.

5.2 Calculated density profiles

The prepared methane + n-butane mixture contained 73.6 mole% methane, and before the density profiles in the interface are modelled, the densities of liquid and vapor bulk phases were calculated with an isothermal flash subroutine, the two phase isothermal flash algorithm was presented by Michelsen & Mollerup (2007) [25]. Assuming the density profile of the reference component in the interface as a monotonical function of interface thickness z , according the work of Miqueu et al. (2005) [17] n-butane was taken as the reference fluid to calculate the density variations of methane in the interface. And the interface was divided into 500 grid, to obtain the density of profile of methane across the interface, the densities of methane at each grid were computed. The whole numerical procedure was proceeded as:

(i). Isothermal flash subroutine was applied to calculate bulk phase mole densities (ρ_i^L and ρ_i^V) of methane + n-butane mixtures with volume translated SRK EOS. Methane was numbered as component 1, and n-butane as component 2.

(ii). Initialization: $K = 0$; $\rho_1(0) = \rho_1^V, \rho_2(0) = \rho_2^V$; $\Delta\rho_2 = \frac{(\rho_2^L - \rho_2^V)}{N_{grid}}$.

(iii). $K = K + 1$; initial value of ρ_2 for each grid:

$$\rho_2(K) = \rho_2(K - 1) + \Delta\rho_2 \quad (36)$$

initial guess of ρ_1 for each grid: first Solving equation(30) to compute $d\rho_1/d\rho_2$, then

$$\rho_1(K_{old}) = \rho_1(K - 1) + \frac{d\rho_1}{d\rho_2} \Delta\rho_2 \quad (37)$$

(iv). Calculate $\rho_1(K_{new})$: solving equation (27) by Newton Raphson method

$$\left(\frac{\partial F_{obj}}{\partial \rho_1}\right)(\delta\rho_1) = -F_{obj} \quad (38)$$

until the convergence criteria is satisfied ($\delta\rho_1 < 10^{-8}$). then

$$\rho_1(K_{new}) = \rho_1(K_{old}) + \delta\rho_1 \quad (39)$$

(v). Go back to (iii), terminate when $\rho_2(K) = \rho_2^L$

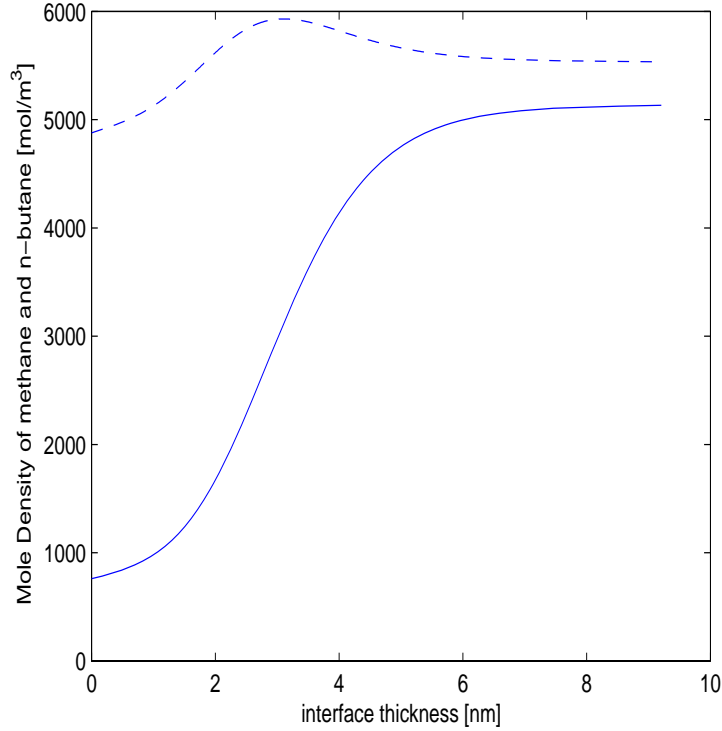


Fig. 1. Density profiles across the interface for methane and n-butane at 310.93K and 106.86Bar: solid line - density of n-butane, dash line - density of methane.

(vi). Determine the density profiles across the z direction according to following equation

$$z = z_0 + \int_{n_2^V}^{n_2^L} \sqrt{\frac{\sum_i \sum_j \kappa_{ij} \frac{d\rho_i}{d\rho} \frac{d\rho_j}{d\rho}}{2(\Phi(\rho) - \Phi_B)}} dn_2 \quad (40)$$

$$z = z_0 + \int_{n_2^V}^{n_2^L} \sqrt{\frac{\sum_i \sum_j \kappa_{ij} \frac{d\rho_i}{d\rho} \frac{d\rho_j}{d\rho}}{2[\sum_i \rho_i (\mu_i(n) - \mu_{iB})] - [P(n) - P_B]}} dn_2 \quad (41)$$

where n_2 is the number density of n-butane that is mole density of n-butane multiplying the Avogadro's number. And z_0 equals to zero at n_2^V . In addition the influence parameter for methane + n-butane mixture can be estimated according geometric mixing rule as

$$\sum_i \sum_j \kappa_{ij} \frac{d\rho_i}{d\rho} \frac{d\rho_j}{d\rho} = \kappa_{11} \left(\frac{d\rho_1}{d\rho_2}\right)^2 + 2\sqrt{\kappa_{11}\kappa_{22}} \frac{d\rho_1}{d\rho_2} + \kappa_{22} \quad (42)$$

In the figure 1 the density profiles of methane and n-butane was plotted at

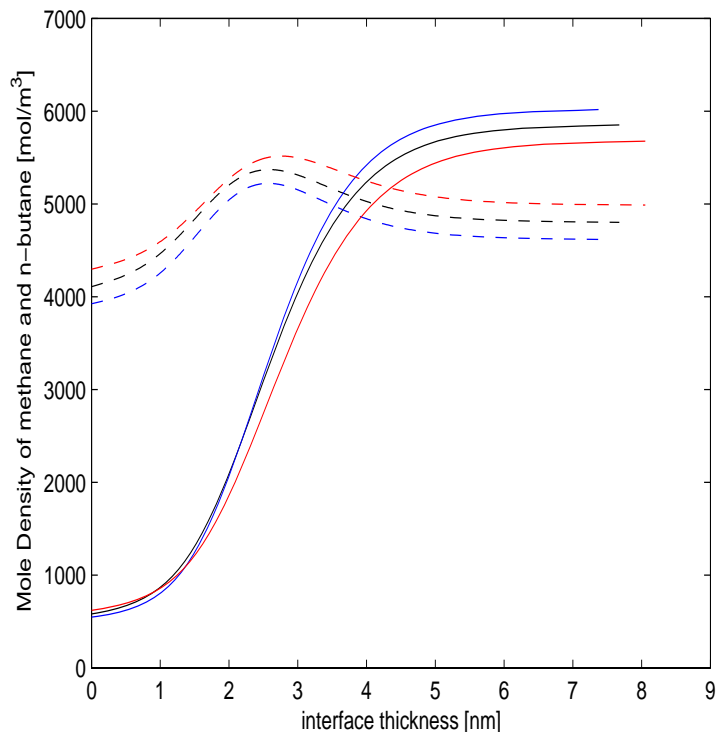


Fig. 2. Density profiles across the interface for methane and n-butane: solid line—density of n-butane, dash line—density of methane, blue color- 89.63Bar, black color - 93.08Bar, red color-96.53Bar.

310.93K and 106.86 Bar. It showed that the densities of n-butane were increasing monotonically across the interface thickness z . In contrast the densities of methane increased to a maximum value that indicated the local enrichment of the methane in the interface. It is known that methane has the lower intrinsic free energy than n-butane. As a result, the Helmholtz energy of the interface was minimized when methane was absorbed in the interface.

Moreover while the pressures increased, the interface thickness increased. It can be seen in the figure 2. In addition the value of maximum density in the interface increased with pressures, but the density differences between liquid and vapor phase decreased while pressure increased. As a fact the maximum density will disappear at critical point. It means that the local accumulation of methane will not exist under critical condition, and the value of interfacial tension will be zero.

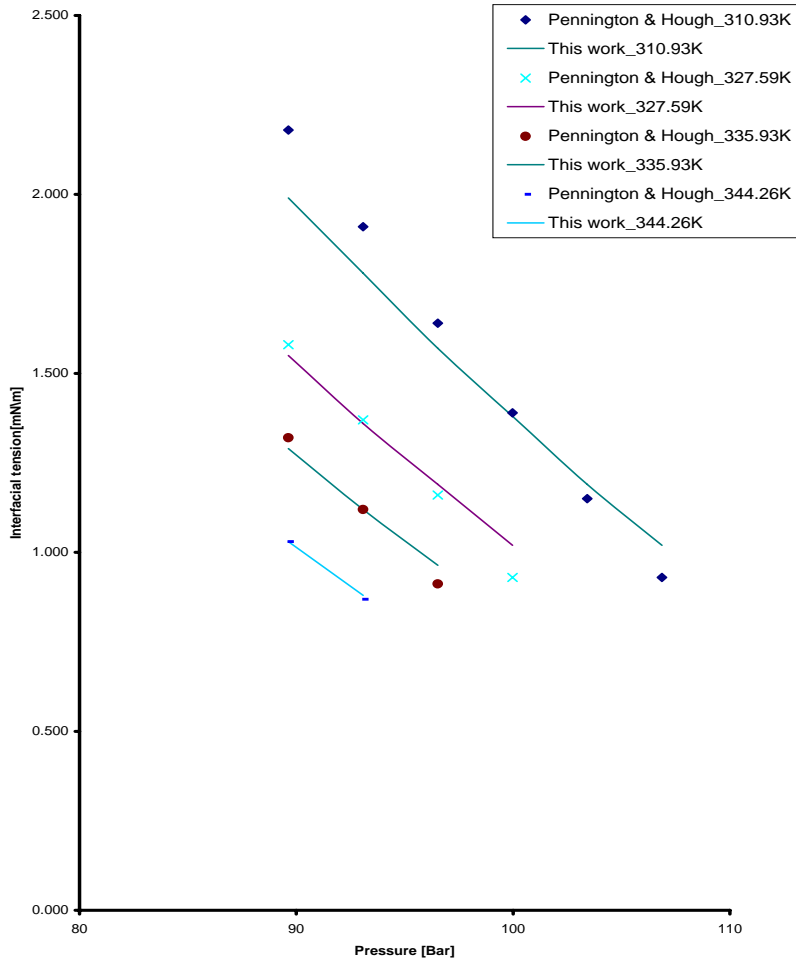


Fig. 3. Interfacial tension of methane + n-butane system data comparison between this work and Pennington et al. (1965) [26]

5.3 Predicted interface tension

Similar numerical procedure was applied to estimate the value of interfacial tension under different temperatures and pressures. The interfacial tensions were computed according to equation (43) after generating the density profiles in the interface.

$$\sigma = \int_{n_2^V}^{n_2^I} \sqrt{\sum_i \sum_j \kappa_{ij} \frac{d\rho_i}{d\rho} \frac{d\rho_j}{d\rho} (2[\sum_i \rho_i (\mu_i(n) - \mu_{iB})] - [P(n) - P_B])} dn_2 \quad (43)$$

The table 1 showed the values of calculated and experimental interfacial tensions. The comparison was plotted in the figure 3. The total average absolute

Table 1

Interfacial tension of methane + n-butane mixtures

Pressure [Bar]	310.93K		327.59K		335.93K		344.26K	
	EXP	CAL	EXP	CAL	EXP	CAL	EXP	CAL
106.97	0.930	1.02						
103.42	1.15	1.19						
99.97	1.39	1.38	0.930	1.02				
96.52	1.64	1.57	1.16	1.19	0.912	0.964		
93.08	1.91	1.78	1.37	1.36	1.12	1.12	0.869	0.880
89.63	2.18	1.99	1.58	1.55	1.32	1.29	1.03	1.03

deviation is 3.85% that is calculated as

$$AAD = (1/N_p) \sum_j |(1 - \sigma_j^{CAL}/\sigma_j^{EXP})| \quad (44)$$

The lowest interfacial tension simulated by gradient theory was 0.869 mN/m in this paper. In addition the average absolute deviation is 6.58 % when the interfacial tensions are lower than 1mN/m. It was due to incapability of both volume translated SRK EOS and gradient theory.

6 Conclusion

By comparing the value of average absolute deviation, it is obviously shown that the average absolute deviation becomes bigger when the IFT is below 1mN/m. But the predicted interfacial tensions were in excellent agreements with the available measured data to within a few percents. When the interfacial tension is bigger than 1mN/m, to predict the ultra low IFT (IFT < 1mN/m), some modification needs to be done to predict the density profiles of lighter hydrocarbon component more accurately. In addition it was shown that the volume translated SRK EOS was not sufficiently enough to compute the liquid bulk near the critical area. In the future work lots of attentions will be focused on establishment of principles for achieving better predictions of ultra low IFT.

Nomenclature

a	energy parameter of volume translated SRK EOS [$J \cdot m^3$]
AAD	average absolute deviation
b	volume parameter of volume translated SRK EOS [m^3]

c	temperature-independent parameter of volume translated SRK EOS
C	direction correction function for influence parameter
f^0	Helmholtz free energy density [$\text{J}\cdot\text{m}^{-3}$]
k_b	Boltzmann constant, $1.38066\times 10^{-23}[\text{J}\cdot\text{K}^{-1}]$
n	number density [m^{-3}]
N_A	Avogadro's number, $6.02205\times 10^{23}[\text{mol}^{-1}]$
P	pressure [Pa]
R	universal gas constant, $8.314471[\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}]$
T	temperature [K]
z	distance normal to the interface [m]
Z	compressibility factor

Greek letters

κ	influence parameter [$\text{J}\cdot\text{m}^5$]
μ	chemical potential [J]
ρ	mole density [$\text{mol}\cdot\text{m}^{-3}$]
σ	interfacial tension [$\text{mN}\cdot\text{m}^{-1}$]
Φ	thermodynamic potential density [$\text{J}\cdot\text{m}^3$]

Superscript

CAL	calculated value
EXP	experimental value
L	liquid phase
V	vapor phase

Subscript

0	homogeneous state
B	bulk phase

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