Available online at www.sciencedirect.com

SCIENCE DIRECT®

Thermochimica Acta 411 (2004) 171–176

thermochimica acta

www.elsevier.com/locate/tca

Estimation of interfacial behavior using the global phase diagram approach
I. Carbon dioxide–*n*-alkanes

Andres Mejía[a], Ilya Polishuk[b,*,1], Hugo Segura[a], Jaime Wisniak[b]

[a] *Department of Chemical Engineering, Universidad de Concepción, Concepción, Chile*
[b] *Department of Chemical Engineering, Ben-Gurion University of the Negev, 84105 Beer-Sheva, Israel*

Received 11 June 2003; received in revised form 11 August 2003; accepted 18 August 2003

Abstract

This study looks for the first time at the possibility of predicting the interfacial tension in mixtures without preliminary resource to their experimental data. For this purpose the quantitative global phase diagram (klGPD)-based approach (GPDA), which needs only two or three key experimental points of one homologue for predicting the complete phase behavior in whole homologues series of binary systems, is combined with the gradient theory (GT) methodology. The resulting model is able to predict the data in satisfactory manner, although the increasing asymmetry between the compounds of the mixture probably affects the ability of GPDA to yield accurate predictions of phase equilibria and interface tension simultaneously.

Keywords: Surface tension; Predictive model; Equation of state; Parameter optimization; Carbon dioxide; *n*-Alkanes

---

1. Introduction

A vast body of literature has been devoted to the development of thermodynamic models for the prediction and correlation of vapor–liquid equilibria (VLE), but modeling of other very important thermodynamic properties such as interfacial tension, has not received so far significant attention. Data on interfacial tension are necessary for the description of phenomena that take place at interfacial boundary layers and which define the efficiency of industrial processes such as mass transfer during extraction, heat transfer under boiling conditions, flow in porous catalytic media, enhanced oil recovery, etc. For example, the interfacial tension data of carbon dioxide–hydrocarbon mixtures suggest that CO_2 can be very effective as an oil-displacing agent.

Sahimi and Taylor [1] have demonstrated that the method based on the gradient theory (GT), first developed by van der Waals and lately reformulated by Cahn and Hilliard [2], is more efficient and accurate than the principle of two-scale factor universality (TSFU). Hence, the GT-based approach seems today to be the most promising way to model the interfacial tension in mixtures. The GT approach is based on the mean field approximation that describes a continuous evolution of the density of the Helmholtz energy along the interface and thus it allows description of the interfacial properties such as concentration profile and interfacial tension in mixtures.

The GT-based approach requires the values of the density of the Helmholtz energy of the homogeneous mixture and the influence parameters of the non-homogeneous mixture. The density of the Helmholtz energy can be estimated using an equation of state (EOS) of the homogeneous mixture while the influence parameters, which carry the information on the molecular structure of the interface, are obtained by fitting the interfacial tension data of pure compounds. It should be noticed that the principal advantage of this approach is the fact that common EOS models can be used to calculate the interfacial behavior and the phase equilibrium condition.

Carey [3], Cornelisse [4], Kahl and Enders [5,6] and Poster and Sanchez [7], have discussed in depth the modeling

---

[*] Corresponding author. Tel.: +972-86477930; fax: +972-86472916.
E-mail addresses: amejia@diq.udec.cl (A. Mejía), polishyk@bgumail.bgu.ac.il (I. Polishuk).

[1] Present address: The Department of Chemical Engineering and Biotechnology, The College of Judea and Samaria, Ariel, Israel.

0040-6031/$ – see front matter © 2003 Elsevier B.V. All rights reserved.
doi:10.1016/j.tca.2003.08.006

of interfacial tensions and demonstrated that the experimental data of different kind of mixtures may be accurately described by the GT–EOS approach. However, their calculations were implemented in a correlative rather than in a predictive manner. From these references, it follows that the basic elements to predict interfacial tensions of mixtures are the following.

- An adequate description of the interfacial tension of pures fluids by means of the calculation of pure component influence parameters. According Miqueu et al. [8], generalized techniques have been developed for the purpose. In addition, the availability of interfacial tension data for pure fluids allows to develop generalized correlations of their influence parameter for every EOS model.
- An adequate prediction of the phase equilibrium condition that gives place to coexisting bulk phases. In general, and due to the limited capability of EOS models to predict phase equilibrium in a wide range of conditions, it can be observed that this problem has received minor attention in the field of interfacial tension calculations. Physical coherence is needed between the interfacial tension prediction and the phase equilibrium condition that allows the generation of interfaces. In current practice EOS models are locally fitted to a reduced set of phase equilibrium data and then used to calculate interfacial tensions. The goodness of fit of interfacial tension data is usually expressed in terms of the liquid phase concentration, although rarely discussed in terms of the equilibrium pressure or temperature.
- The availability of a reduced set of experimental data, or theory, from which to infer mixture effects on the interfacial tension. In the GT–EOS approach mixing effects are lumped on the estimation of mixture's influence parameters. Certainly, the development or test of theories, or the direct fit of data, should be based on accurate phase equilibrium predictions.

Modern process design requires models capable of predicting data without preliminary resource to experimental results. At its current state of development, the GT–EOS approach has been shown to be useful for smoothing data. Thus the objective of the present study is to look for the first time at the possibility of "predicting the interface tension of mixtures without fitting data". To validate this possibility, we consider mixtures of carbon dioxide with alkanes and the semi-predictive approach detailed below.

2. Theory

The present development of molecular theory does not allow an adequate evaluation of entirely predictive methods, which could yield reliable predictions of data in asymmetric systems. Therefore, the usual practice is to develop semi-predictive approaches that use some experimental data in order to predict the missing ones. The quality of such approaches is then defined by their accuracy and also by the relation between the amount of data fed to the amount of data predicted.

Recently [9–11] we have proposed the quantitative global phase diagram (klGPD)-based semi-predictive approach (GPDA), that requires no more than two or three experimental critical points to predict the complete phase behavior in whole homologues series of binary systems. This approach is characterized by a very high ratio between the data predicted and the data fed. The successful implementation of GPDA is based on the fact that the configuration of vapor–liquid equilibria phase boundaries at any temperature is defined by the position of the vapor–liquid critical point and by the distance from any particular temperature to the upper critical solution temperature (UCST) of the system at which the homogenous liquid phase splits into two phases. This observation is supported by that fact that the inflections of bubble-point curves always change *continuously* from VLE to liquid–liquid equilibria (LLE). Hence, the accuracy in describing VLE is determined by the exactness with which the model predicts LLE, a fact which is not always evident when dealing with a local fit of data. In other words, different kinds of phase equilibria, such as VLE and LLE, are inter-related not only *qualitatively* but also *quantitatively*.

Thus it appears that an appropriate description of phase equilibria in the system can be achieved by the accurate correlation of only two experimental points that characterize the VLE and LLE in it, namely the upper critical endpoint (UCEP) and the critical pressure maximum (CPM). In addition, it has been demonstrated that the experimental values of these key points in different homologues can be correlated by EOSs using the same values of the binary parameters k_{12} and l_{12} (see Eq. (8)). In other words, each homologue series has its own characteristic balance between VLE and LLE. This observation has allowed us to formulate a novel semi-predictive GPD-based approach (GPDA) involving estimation of the binary interaction parameters for a certain homologue using klGPD, with further implementation for predicting the data of other homologues [9]. Since this approach requires only two to three experimental points of one system in order to predict the complete phase behavior of whole homologue series, it is advantageous over other widely used semi-predictive approaches, which require a large amount of data for evaluating their parameters. Since GPDA considers not just numerous experimental points but VLE, LLE and the critical lines simultaneously, it produces a reasonable distribution of the inevitable deviations from the experimental data over the whole thermodynamic phase space. Hence, this approach can be reliable for prediction of data, which are not available experimentally.

Appreciation of the fact that all parts of the thermodynamic phase space are closely inter-related encourages the development of an equation of state, which would be simultaneously accurate for the largest number of properties and be free of numerical pitfalls. The following EOS that meets these requirements in a satisfactory manner has been recently proposed [10]:

$$P = \frac{RT(\tilde{v} + 0.125b)}{\tilde{v}(\tilde{v} - 0.875b)} - \frac{aT_{\mathrm{r}}^{(m_1 T_{\mathrm{r}}^{m_2})}}{(\tilde{v} + c)(\tilde{v} + d)} \qquad (1)$$

where $\tilde{v}$ is molar volume and m_1 and m_2 are adjustable parameters for the appropriate representation of the vapor pressure curve. Their values for light gases (for which high quality data are available) and for complex polar compounds should be evaluated separately (for example, for CO_2 $m_1 = -0.33595$ and $m_2 = -0.15187$). For other compounds the values of m_1 and m_2 can be generalized. For example, it has been proposed that for *all* hydrocarbons m_2 be taken as 0.25 and for those having a carbon number smaller than 10, be calculated by the following expression:

$$m_1 = \frac{0.00849 - 0.29324\omega + 0.61934\omega^2 - 1.7792\omega^3}{b} \qquad (2)$$

and for the heavier hydrocarbons by

$$m_1 = \frac{-0.4162 + 1.5447\omega - 2.5285\omega^2 + 0.81466\omega^3}{b} \qquad (3)$$

Although b is given in (L/mol), the values of m_1 and m_2 should be considered as dimensionless.

The values of a, b, c, and d are obtained solving the following system of the four equations:

$$\left(\frac{\partial P}{\partial \tilde{v}}\right)_{T_{\mathrm{c}}} = \left(\frac{\partial^2 P}{\partial \tilde{v}^2}\right)_{T_{\mathrm{c}}} = 0 \qquad (4)$$

$$\tilde{v}_{\mathrm{c,EOS}} = \varsigma \tilde{v}_{\mathrm{c,EXPT}} \qquad (5)$$

where ζ is a dimensionless number, having the value $(1 + \tilde{v}_{\text{triple point}})$

$$b = \tfrac{4}{3.5}\tilde{v}_{\text{triple point}} \qquad (6)$$

For light gases and heavy substances having carbon number larger that 10, Eqs. (5) and (6) correspond to the molar volume of the solid phase, and for others: to the liquid one. The pure compound data have been obtained from the DIPPR database [12]. The system of Eqs. (4)–(6) is easily solved.

The parameters of Eq. (1) for mixtures are obtained using the following classical van der Waals mixing rules:

$$z = \sum_{ij} x_i x_j z_{ij} \qquad (7)$$

where $z = a$, b, c, and d.

The cross-interaction parameters are obtained with the following combination rules:

$$\begin{aligned} &a_{21} = a_{12} = (1 - k_{12})\sqrt{a_{11}a_{22}},\\ &b_{12} = b_{21} = (1 - l_{12})(\tfrac{1}{2}b_{11} + b_{22}),\\ &c_{12} = c_{21} = (\tfrac{1}{2}c_{11} + c_{22}), \qquad d_{12} = d_{21} = (\tfrac{1}{2}d_{11} + d_{22}) \end{aligned} \qquad (8)$$

where k_{12} and l_{12} are binary adjustable parameters. The global phase diagram-based semi-predictive approach (GPDA) is centered on the proper evaluation of the values of these parameters. As already pointed out, for members of the same homologue series the intersection between the loci that represent the experimental values of CPM and UCEP on klGPD, necessary for the appropriate and overall description of mixtures [9], usually takes place at similar values of k_{12} and l_{12}. This observation reveals the basis of the GPDA. To predict the complete phase behavior of a whole homologue series it is necessary to know only the experimental value of UCEP (or at least some value of UCST) together with the pressure (and sometimes the temperature of CPM) of one of the homologues. It is helpful to consider as reference systems those homologues that exhibit type II behavior and which have been investigated in detail [11]. In the series under consideration the best candidate is the system CO_2–*n*-decane. Here the binary parameters of the series have already been evaluated using the klGPD of this system [10].

The range of applicability of GPDA can be enlarged substantially if the values of binary interaction parameters vary proportionally to the values of the corresponding pure compound parameters. Such proportionality can be easily established for the case of a linear combination rule for the covolume, as follows:

$$l_{12} = \frac{b_{22} - b_{11}}{b_{22} + b_{11}} L_{12} \qquad (9)$$

where L_{12} is a value characteristic for a given homologues series.

The following proportional relation for the binary interaction parameter k_{12}, including the appropriate temperature dependency, has been developed:

$$k_{12} = \left(K_{11} - l_{12}\frac{T_{\mathrm{c}2}}{T_{\mathrm{c}1}}\right)(1 - t) + K_{22}t \qquad (10)$$

where K_{11} and K_{22} are characteristic values for a given homologues series and t is given by the following dimensionless functionality:

$$t = \tanh\left[\left(\frac{T - T_{\mathrm{c}1}}{T^*_{\mathrm{c}2} - T_{\mathrm{c}1}}\right)^2\right] \qquad (11)$$

For homologues heavier than the reference homologue (CO_2–*n*-decane), $T^*_{\mathrm{c}2} = T_{\mathrm{c}2}$. For lighter homologues $T^*_{\mathrm{c}2}$ is equal to the $T_{\mathrm{c}2}$ of the reference homologue. Therefore, for all lighter homologues $T^*_{\mathrm{c}2}$ will be taken as 617.7 K, the T_{c} of *n*-decane [12]. This will allow keeping the same temperature dependency of k_{12} along the homologues series. For the series CO_2–alkanes $K_{11} = 0.1$, $K_{22} = 0.35$, and $L_{12} = 0.02$.

In what follows, we will describe the procedure of calculation of interface tension from this EOS when the GT is applied to mixtures at a planar interface. The interfacial tension σ for a mixture is given by the following equation [3,4]:

$$\sigma = \int_{\rho_s^{\mathrm{V}}}^{\rho_s^{\mathrm{L}}} \sqrt{2(\Phi + P^0)\sum_{i,j=1}^{n_{\mathrm{c}}} c_{ij}\left(\frac{\mathrm{d}\rho_i}{\mathrm{d}\rho_s}\right)\left(\frac{\mathrm{d}\rho_j}{\mathrm{d}\rho_s}\right)}(\mathrm{d}\rho_s) \qquad (12)$$

where n_c stands for the number of components, c_{ij} the cross-influence parameter ($c_{ij} = c_{ji}$), ρ_i the concentration of component i through the interface. ρ_i the related to the concentration of the mixture ρ_m by $\rho_i = x_i\ \rho_m$, P^0 is the bulk equilibrium pressure, and the superscripts L and V denote the liquid, and vapor bulk equilibrium condition, respectively. The lower script s represents the component (i or j), whose pattern, along the interface region, shows a monotonic behavior. Φ is the *grand thermodynamic potential* defined as

$$\Phi[\rho_i, \rho_m] = a_0[\rho_i, \rho_m] - \sum_{i=1}^{n_c} \rho_i \mu_i^0[T^0, V^0, \rho_i^0] \tag{13}$$

In Eq. (13) a_0 is the density of the Helmholtz energy in the homogeneous system ($a_0 = A/V$), μ_i the chemical potential of component i, V, and T are the volume and temperature, respectively, and the superscript 0 denotes the equilibrium condition (here 0 = V (vapor) or L (liquid)). a_0 and μ_i can be determined directly from the EOS, as follows [13,14]:

$$\frac{\tilde{v} a_0}{RT} = \int_{\tilde{v}}^{\infty} \left(\frac{P}{RT} - \frac{1}{\tilde{v}}\right) \mathrm{d}\tilde{v} - \ln \tilde{v} + \sum_{i=1}^{n_c} x_i \ln x_i \tag{14a}$$

$$\mu_i = \left(\frac{\partial[n\tilde{v}a_0]}{\partial n_i}\right)_{T, n\tilde{v}, n_j} \tag{14b}$$

In Eq. (14) n_i is the number of moles of species i, and n is the total number of moles.

Inspection of Eqs. (12)–(14) reveals that the calculation of σ depends on the EOS model selected and its mixing rules, the c_{ij} and the ρ_i. In this work we have adopted the EOS model given by Eqs. (1)–(11). c_{ij} is calculated using the procedure suggested by Carey [3]. For the case of pure fluids ($i = j$) c_{ii} is calculated at constant temperature from experimental σ values as.

$$c_{ii} = \sigma_{\mathrm{exp}}^2 \left(\int_{\rho_i^{\mathrm{V}}}^{\rho_i^{\mathrm{L}}} \sqrt{2(\Phi + P^0)}\, \mathrm{d}\rho_i\right)^{-2} \tag{15}$$

where σ_{exp} is the experimental values of σ, which can be taken from a data base compilation [15,16]. The pertinent values at the pertinent temperature are listed in Table 1. It should be pointed out that the temperature dependence of c_{ij} may be correlated by a linear function, which will increase the predictive character of the approach.

Table 1
Influence parameter for pure fluids[a]

Fluid	319.3 K	344.3 K	377.6 K
$10^{20} \times c_{ii}^0$ (J m^5 mol^{-2})			
n-Butane	17.34110	18.10632	19.89718
Carbon dioxide	4.93163	5.62942	6.55889
Cyclohexane		37.8986	
n-Decane		106.28063	105.70090
n-Tetradecane		140.54567	

[a] As obtained from Eq. (15).

For the case of mixtures, c_{ij} is obtained by averaging the pure component influence parameters according to the following geometric combining rule:

$$c_{ij} = \sqrt{c_{ii}c_{jj}} \tag{16}$$

The calculation of σ depends not only on the EOS, its mixing rules, and c_{ij}, but also on ρ_i. The variation of ρ_i across to the interface is given by the GT. For the case studied here (planar interface and c_{ij} described by Eq. (16)) this variation is given by the following set of algebraic equations:

$$\begin{gathered}\sqrt{c_{ss}}[\mu_k(\rho) - \mu_k^0] = \sqrt{c_{kk}}[\mu_s(\rho) - \mu_s^0],\\ k = 1, 2, \ldots,\ s-1, s+1, \ldots, n_c\end{gathered} \tag{17}$$

Finally, we can observe from the previous expressions, the present approach needs only pure component data and predicts the interfacial tension in mixtures without resource to experimental results. The predictions yielded by this approach are discussed in the following section.

3. Results

Fig. 1 compares the calculated and experimental isotherm data on the surface tension-pressure projection of the system carbon dioxide–*n*-butane. It can be seen that at 319.3 K GPDA yields an exact prediction of the high-pressure data and slightly overestimates them below 30 bar. In addition, GPDA slightly underestimates the data at 344.3 K; the deviation increases at 377.6 K. However, it should be noticed out that GPDA still predicts the interface tension data more accurately than the EOS of Peng–Robinson with three [1] and

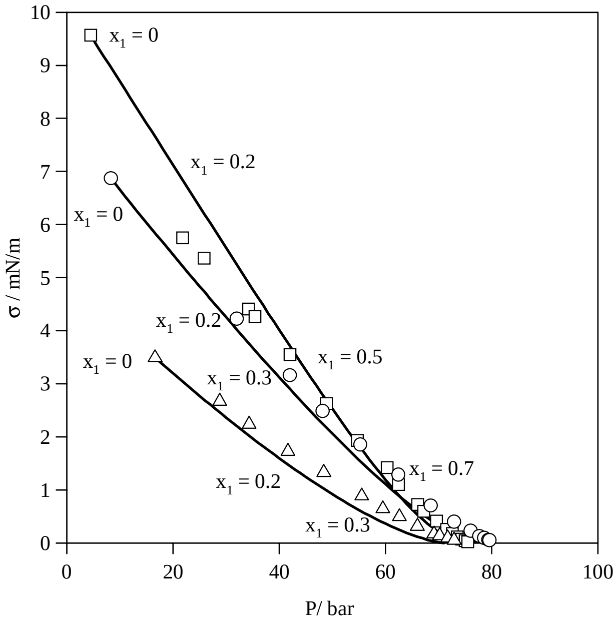

Fig. 1. Interface tension in the system carbon dioxide–*n*-butane: (—) data predicted by GPDA; (□) 319.3 K; (○) 344.3 K; (△) 377.6 K experimental data [17].

one [4] binary parameters adjusted to the VLE data of this particular system. The imperfect results of this EOS combined with the GT approach have been explained [4] so far by two factors: inaccurate description of volumetric properties in pure compounds and inability to describe the scaling behavior around the critical point.

Another very important factor is the accuracy in modeling of VLE data. Comparison between the results of different models is necessary for estimating the influence that these factors exert on the accuracy of modeling of the interface tension data.

It is seen that when the parameters of Peng–Robinson's EOS are locally adjusted to the VLE experimental points of this particular system [1,4]. This EOS correlates the data more accurately than GPDA predicts them. In addition, in these studies the EOS of Peng–Robinson was combined with the GT approach using an additional binary parameter in Eq. (16), omitted by our approach in order to support its predictive character. Therefore, the relative success of GPDA in predicting the interface tension data may be explained by a better accuracy of Eq. (1) in describing the volumetric properties of pure compounds.

In addition, it has also been shown [4] that an improvement of the scaling behavior of the Peng–Robinson EOS significantly improves the accuracy in modeling the interface tension data in the system carbon dioxide–*n*-butane. The results of the EOSs that incorporate the critical scaling terms are superior over the predictions of GPDA. However, these models are rather complex, which hinders their implementation for engineering computations.

Fig. 2 compares the calculated and experimental isotherm data on the surface tension-pressure projection of the system carbon dioxide–*n*-decane. It can be seen that GPDA underestimates the data at both temperatures and this time it is slightly less accurate even in comparison with the results of previous studies [1,4]. Nevertheless, GPDA yields a very accurate prediction of the interface tension data in the system carbon dioxide–cyclohexane (Fig. 3). Presently we do not know the reason for such a difference in results because GPDA predicts the VLE data and the volumetric properties in both systems with the same accuracy. We can only

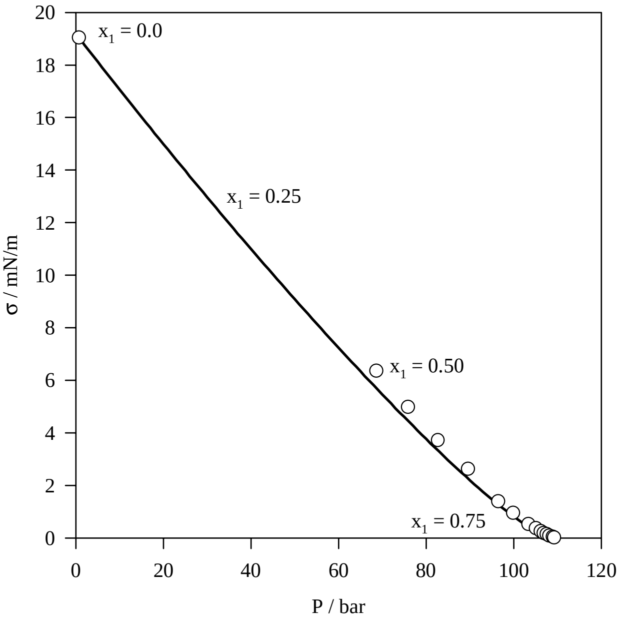

Fig. 3. Interface tension in the system carbon dioxide–*n*-cyclohexane: (—) data predicted by GPDA; (○) 344.3 K experimental data [20].

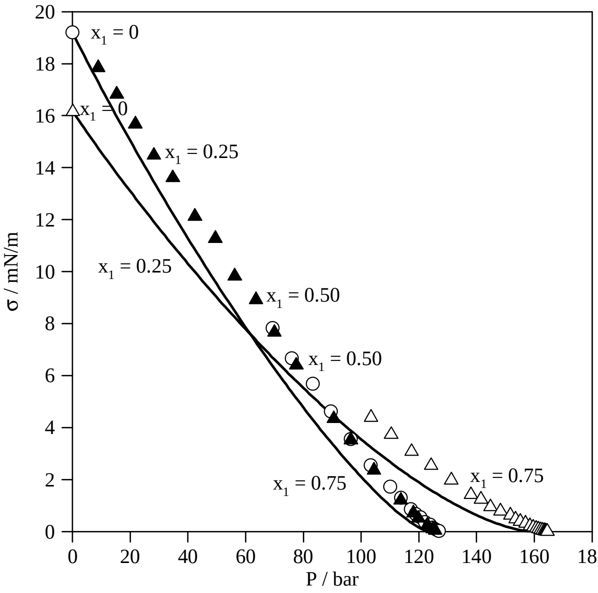

Fig. 2. Interface tension in the system carbon dioxide–*n*-decane: (—) data predicted by GPDA; (○) 344.3 K; (△) 377.6 K experimental data [18]; (▲) 344.3 K experimental data [19].

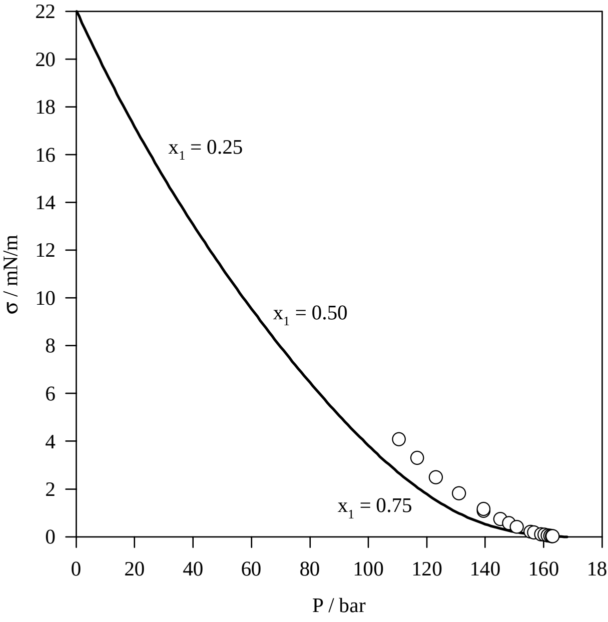

Fig. 4. Interface tension in the system carbon dioxide–*n*-tetradecane: (—) data predicted by GPDA; (○) 344.3 K experimental data [21].

guess that the increasing asymmetry of the system affects the ability of GPDA to yield simultaneous accurate predictions of phase equilibria and interface tension. This observation can be supported by results obtained for the system carbon dioxide–*n*-tetradecane (Fig. 4). However, since the experimental uncertainty of these data may exceed 10% [22], the accuracy of results predicted by GPDA should be considered as satisfactory.

4. Conclusions

This study has looked for the first time at the possibility of predicting the interfacial tension in mixtures without preliminary resource to their experimental data, by combining gradient theory methodology with the klGPD-based approach (GPDA) that needs two or three key experimental points of one homologue for predicting the complete phase behavior in whole homologue series of binary systems. The resulting model was able to predict the data of the systems under consideration in a satisfactory manner. The accuracy with which the GPDA–GT approach predicts the interface tension data is illustrated with isothermal mixtures of carbon dioxide–*n*-alkanes in the high pressure range. According to the results, our predictive approach is comparable to the performance of a locally fitted Peng–Robinson EOS [3]. However, the increasing asymmetry between the compounds of the mixture probably affects the ability of GPDA to yield accurate predictions of phase equilibria, affecting also the prediction of interface tension.

Acknowledgements

This work was financed by the Israel Science Foundation, Grant Number 340/00 and by FONDECYT, Santiago, Chile (Project 2010100).

References

[1] M. Sahimi, B.J. Taylor, J. Chem. Phys. 95 (1991) 6749–6761.
[2] J.W. Cahn, J.E. Hilliard, J. Chem. Phys. 28 (1958) 258–267.
[3] B.S. Carey, The gradient theory of fluid interfaces, Ph.D. thesis, University of Minnesota, 1979.
[4] P.M.W. Cornelisse, The gradient theory applied, simultaneous modelling of interfacial tension and phase behaviour, Ph.D. thesis, Delft University, 1997.
[5] H. Kahl, S. Enders, Fluid Phase Equilib. 172 (2000) 27–42.
[6] H. Kahl, S. Enders, Phys. Chem. Chem. Phys. 4 (2002) 931–936.
[7] C. Poster, I. Sanchez, Macromolecules 14 (1981) 361–370.
[8] C. Miqueu, B. Mendiboure, A. Gracia, J. Lachaise, Fluid Phase Equilib. 207 (2003) 225–246.
[9] I. Polishuk, J. Wisniak, H. Segura, Chem. Eng. Sci. 56 (2001) 6485–6510.
[10] I. Polishuk, J. Wisniak, H. Segura, Chem. Eng. Sci., 2003, in press.
[11] I. Polishuk, J. Wisniak, H. Segura, J. Phys. Chem. B 107 (2003) 1864–1874.
[12] T.E. Daubert, R.P. Danner, H.M. Sibul, C.C. Stebbins, Physical and Thermodynamic Properties of Pure Chemicals. Data Compilations, Taylor & Francis, Bristol, 1989–2002.
[13] J. Wisniak, A. Apelblat, H. Segura, Chem. Eng. Sci. 53 (1998) 743–751.
[14] H. Van Ness, M. Abbott, Classical Thermodynamics of Nonelectrolyte Solutions, McGraw-Hill, New York, 1982.
[15] J.J. Jasper, J. Phys. Chem. Ref. Data 1 (1972) 841–1009.
[16] Ch. Wohlfarth, B. Wohlfarth, in: Landolt-Börnstein, New Series Group IV Physical Chemistry, vol. 16, seventh ed., Springer-Verlag, Berlin, 1997, pp. 7–284.
[17] J.C. Hsu, N. Nagarajan, R.L. Robinson Jr., J. Chem. Eng. Data 30 (1985) 485–491.
[18] N. Nagarajan, R.L. Robinson Jr., J. Chem. Eng. Data 31 (1986) 168–171.
[19] R.D. Shaver, R.L. Robinson Jr., K.A.M. Gasem, Fluid Phase Equilib. 179 (2000) 43–66.
[20] N. Nagarajan, R.L. Robinson Jr., J. Chem. Eng. Data 32 (1987) 369–371.
[21] K.A.M. Gasem, K.B. Dickson, P.B. Dulcamara, N. Nagarajan, R.L. Robinson Jr., J. Chem. Eng. Data 34 (1989) 191–195.
[22] A. Danesh, A.C. Todd, J. Somerville, A. Dandekar, Trans. I: Chem. E 68 (1990) 325–331.