SIMULTANEOUS CORRELATION OF VAPOR–LIQUID EQUILIBRIUM AND EXCESS ENTHALPIES FOR BINARY MIXTURES OF n-HEXANE AND n-OCTANE WITH HEXANE ISOMERS

J.A. GARCÍA CALZÓN, C. PANDO and J.A.R. RENUNCIO

Faculatad de Química, Universidad de Oviedo, 33007 Oviedo (Spain)

(Received 26 February 1986)

ABSTRACT

Vapor–liquid equilibrium (VLE) data for binary mixtures of n-hexane and n-octane with hexane isomers are accurately predicted from excess enthalpy (h^E) data using the prediction method of Hanks, Gupta and Christensen in conjunction with several well-known models for the excess Gibbs energy. The accuracies of the correlation of data for these nearly ideal mixtures are of similar magnitude to those obtained for the typical non-ideal mixtures previously studied using this method. When the usual approach to correlate h^E and VLE data is attempted, the higher relative errors associated with the evaluation of the small excess Gibbs energies characteristic of the almost ideal systems lead to large errors in the values of the excess enthalpies which are also small. This seems to be a consequence of the error magnification associated with the differentiation process required to obtain h^E data from VLE data.

INTRODUCTION

Excess properties of binary systems containing an n-alkane and a branched hydrocarbon with a similar number of carbon atoms have been given much attention in order to study the effect of chain branching on the excess properties and because of their nearly ideal behavior. Vapor–liquid equilibrium (VLE) data for the binary systems containing n-hexane or n-octane as a first component and a hexane isomer as a second component have been reported by Chen and Zwolinski [1], Ho and Davison [2] and Liu and Davison [3]. These studies included predictions of excess free energies, enthalpies and entropies from the VLE data.

Excess enthalpies (h^E) for systems containing n-hexane were reported by Lam et al. [4] and by Ott et al. [5]. In two recent publications, Ameling et al. [6] and Hamam et al. [7] reported h^E data for systems containing n-octane. The values of h^E calculated from pressure composition data by Ho and Davison [2], Liu and Davison [3] and Ameling et al. [6] were shown to be unrealistically large.

The usual approach to correlate h^E and VLE data is to calculate activity coefficients from total pressure composition (p) or vapor–liquid composition (x–y) data. The excess free energy (g^E) is then computed from the activity coefficients. These g^E data may be directly introduced into the Gibbs–Helmholtz relation

$$h^E = -T^2 \, \partial\left(g^E/T\right) \, \partial T \tag{1}$$

or may be previously fitted to a semiempirical model for g^E (x_j, $A_1 \ldots A_k$) where A_k are adjustable parameters. The equation for g^E is then introduced into eqn. (1). The A_k parameters are usually assumed to be temperature independent. The opposite assumption leads to very complex equations which can be of little practical use.

An extremely accurate description of g^E is always required due to the error magnification inherent in the differentiation process. Excess enthalpies of about 30% inaccuracy can be obtained for typical non-ideal systems. When the systems studied are almost ideal, slight errors in the VLE measurements lead to higher relative errors in the evaluation of the small excess Gibbs energies typical of these systems. These errors are magnified in the differentiation process with the result that inaccuracies of one order of magnitude and higher are obtained. This is the case of the systems studied in this paper. We will show that by reversing the order of the correlation process, the VLE and h^E sets of data can be simultaneously represented using a unique set of parameters of any of several excess free energy models widely used in the literature.

PREDICTION METHOD

The method used in this paper has been proposed by Hanks et al. [8] and provides a simultaneous description of the excess Gibbs energy and excess enthalpy. The A_k parameters of the g^E model are evaluated by curve-fitting experimental binary isothermal h^E data to the algebraic equation $h^E(x_j, A_1, A_2 \ldots A_k)$ derived from the g^E model by application of eqn. (1). These A_k values are then used in the g^E model to calculate the activity coefficients from which the x–y data may be predicted. The Wilson formulation [9] of the Redlich–Kwong equation of state is used to take into account the non-ideality of the vapor. This prediction method (here called the HGC method) has been shown to be successful in the calculation of both isothermal and isobaric VLE data for a variety of binary hydrocarbon mixtures [8,10–13]. It has been also used to correlate data of alcohol–hydrocarbon [14], ether–hydrocarbon and aldehyde–hydrocarbon [15], ketone–hydrocarbon [16], alcohol–alcohol [17], and nitrile–alcohol [18] mixtures. Some multicomponent mixtures have also been studied [12,13]. The mixtures studied show in most cases large or considerable deviations from ideality.

No systematic study on the application of the HGC method to a nearly ideal system has been carried out so far. Therefore, it seems convenient to examine how data for the binary mixtures of n-hexane and n-octane with hexane isomers can be correlated using this method.

MODELS FOR THE EXCESS GIBBS ENERGY

Four widely used models for the excess Gibbs energy: the Wilson model [19], the non-random two liquid (NRTL) model proposed by Renon and Prausnitz [20], the local effective mole fraction (LEMF) model proposed by Marina and Tassios [21] and the universal quasi-chemical (UNIQUAC) model proposed by Abrams and Prausnitz [22] were considered. Their equations for g^E and h^E depend on two or three adjustable parameters and can be found elsewhere. In this paper, we will follow the notation of Gmehling and Onken [23]. Wilson's model has two parameters: $\lambda_{12} - \lambda_{11}$ and $\lambda_{21} - \lambda_{22}$. The NRTL model has three parameters: $g_{12} - g_{22}$, $g_{21} - g_{11}$, and α_{12}. The LEMF model is essentially the NRTL model with $\alpha_{12} = -1$ and has two adjustable parameters: $g_{12} - g_{22}$ and $g_{21} - g_{11}$. The UNIQUAC model also has two adjustable energy interaction parameters: $u_{12} - u_{22}$ and $u_{21} - u_{11}$.

RESULTS AND DISCUSSION

Table 1 lists the six binary systems formed by n-hexane or n-octane and a hexane isomer for which VLE and h^E data exist simultaneously in the literature. Table 1 also lists the source of data. We will refer to the hexane isomers as follows: 2-MP (2-methylpentane), 3-MP (3-methylpentane), 2,2-DMB (2,2-dimethylbutane) and 2,3-DMB (2,3-dimethylbutane). Table 2 shows the temperatures at which h^E data have been measured, the values of the parameters, the standard deviation σ between experimental and calcu-

TABLE 1

Binary systems studied and source of experimental data

System No.	Components	References	
		h^E data	VLE data
I	n-hexane (1) + 2-methylpentane (2)	5	1,2
II	n-hexane (1) + 3-methylpentane (2)	5	1,2
III	n-hexane (1) + 2,2-dimethylbutane (2)	4	1
IV	n-hexane (1) + 2,3-dimethylbutane (2)	5	1
V	n-octane (1) + 2-methylpentane (2)	6,7	3
VI	n-octane (1) + 3-methylpentane (2)	6,7	3

lated values of h^E and the percentage (%) of this standard deviation with respect to the highest value of h^E, for each of the different models used. Best results for the NRTL model were obtained when the parameter α_{12} was set to a constant value of 0.3 as recommended by Renon and Prausnitz [20]. Values for the molar volumes were taken from Timmermans [24]. n-Octane molar volumes at certain temperatures were calculated using the isobaric coefficient of thermal expansion given by Patterson and Bardin [25]. Essentially, the same values are obtained from the molar volume equation for hydrocarbons derived by Meisner [26]. This equation was also used to estimate some molar volumes of the other hydrocarbons. Values of the pure-component molecular-structure constants r and q required in the UNIQUAC equations were taken from Prausnitz et al. [27]. The fits are good in all cases. The highest values for σ/h^E_{max} are obtained when data are scattered (see results for system II at 283.15 and 313.15 K and for system III at 283.15 K in Table 2 and Figs. 2 and 3).

TABLE 2

Calculated values of the parameters (J mol^{-1}), standard deviations, σ, between experimental and calculated h^E data (J mol^{-1}) and ratios of the standard deviation and the maximum value of h^E (%)

System	T (K)	Wilson eqn.		σ	σ/h^E_{max} (%)	NRTL eqn.		σ
		$\lambda_{21}-\lambda_{22}$	$\lambda_{12}-\lambda_{11}$			$g_{12}-g_{22}$	$g_{21}-g_{11}$	
I	283.15	−98.15	124.87	0.08	1.4	−141.99	170.79	0.08
	298.15	−72.15	92.81	0.08	1.7	−103.83	125.70	0.08
	313.15	163.23	−137.96	0.1	3.1	248.49	−220.72	0.1
II	283.15	−26.29	43.97	0.2	4.8	−62.65	80.89	0.2
	298.15	−50.69	61.48	0.06	2.6	−96.25	107.85	0.06
	313.15	182.30	−168.68	0.1	12	237.15	−221.93	0.1
III	298.15	268.31	−213.58	0.02	0.2	394.53	−334.92	0.01
IV	283.15	−252.66	288.96	0.1	10	−344.43	382.60	0.1
	298.15	−223.77	235.79	0.07	2.6	−269.86	277.96	0.07
	313.15	538.38	−465.47	0.2	3.1	660.76	−592.11	0.2
V	283.15	−126.01	303.19	1.2	4.2	−464.79	657.77	1.2
	293.15	−98.20	227.51	0.2	1.2	−440.51	590.36	0.2
	298.15	323.38	−270.92	0.08	0.4	23.80	54.90	0.08
	303.15	−20.48	105.02	0.2	1.2	−361.89	473.16	0.2
	313.15	−165.47	−133.46	0.4	2.7	−217.66	289.00	0.4
VI	283.15	−120.88	288.28	1.0	3.9	−464.53	646.52	1.0
	293.15	212.46	−162.52	0.1	0.8	−146.60	233.55	0.1
	298.15	247.01	−211.93	0.05	0.3	−125.42	197.36	0.05
	303.15	50.48	6.498	0.3	2.2	−307.70	399.48	0.3
	313.15	8.043	47.05	0.2	2.0	−347.30	432.87	0.2

On the other hand, values of σ/h^E_{max} for a certain set of h^E data are very similar for the four g^E models used. Although for the sake of simplicity, the parameters of the g^E models are usually assumed to be temperature independent, they are often weakly dependent on this magnitude and it is interesting to observe the variation of their values when h^E data for a system were taken at several temperatures. h^E data for the n-hexane (1) + 2,2-DMB (2) system were taken at only one temperature. h^E data for the other systems containing n-hexane were taken at 283.15, 298.15 and 313.15 K. When values of the parameters for the four g^E models used are plotted versus temperature, an almost linear variation is observed. As can be seen in Figs. 1–3, these values correspond to endothermic excess enthalpies which decrease with temperature becoming exothermic for n-hexane (1) + 2,3-DMB (2) at 298.15 K. h^E data for the two systems containing n-octane were taken at five different temperatures. Values for the parameters of the LEMF model of these systems show a linear variation with temperature. Values for

| σ/h^E_{max} (%)	LEMF eqn.		σ	σ/h^E_{max} (%)	UNIQUAC eqn.		σ	σ/h^E_{max} (%)
	$g_{12} - g_{22}$	$g_{21} - g_{11}$			$u_{12} - u_{22}$	$u_{21} - u_{11}$		
1.4	−241.66	218.82	0.07	1.3	−81.74	90.74	0.08	1.4
1.7	−218.57	201.62	0.08	1.6	−60.84	67.34	0.08	1.7
3.1	206.54	−227.72	0.1	3.1	127.76	−118.05	0.1	3.1
4.8	−198.22	184.09	0.2	4.7	−37.78	42.85	0.2	4.8
2.6	−154.44	145.38	0.06	2.5	−54.29	57.91	0.06	2.6
12	129.21	−140.07	0.1	12	116.88	−111.09	0.1	12
0.1	275.86	−320.44	0.04	0.5	199.39	−177.95	0.01	0.2
10	−203.27	176.92	0.1	10	−172.01	186.84	0.1	10
2.6	−16.19	6.013	0.07	2.6	−120.83	124.28	0.07	2.6
3.0	154.65	−201.22	0.2	2.8	311.26	−283.01	0.2	3.0
4.6	−627.14	477.63	1.6	6.1	−157.23	196.33	1.2	4.2
1.1	−554.33	435.71	0.3	1.4	−116.85	143.15	0.2	1.2
0.4	−421.95	372.99	0.1	0.5	220.50	−185.92	0.09	0.4
1.2	−494.23	403.05	0.1	0.7	−14.50	30.67	0.2	1.2
2.6	−411.78	355.07	0.3	2.3	134.90	−115.94	0.4	2.7
4.2	−597.72	460.28	1.4	5.4	−161.41	198.95	1.0	3.9
0.8	−453.86	386.59	0.1	0.7	158.39	−131.93	0.1	0.8
0.3	−411.49	357.61	0.07	0.2	166.82	−142.21	0.05	0.3
2.1	−450.10	376.08	0.2	1.6	51.25	−36.31	0.3	2.2
1.9	−423.14	356.39	0.2	1.4	−0.961	12.54	0.2	2.0
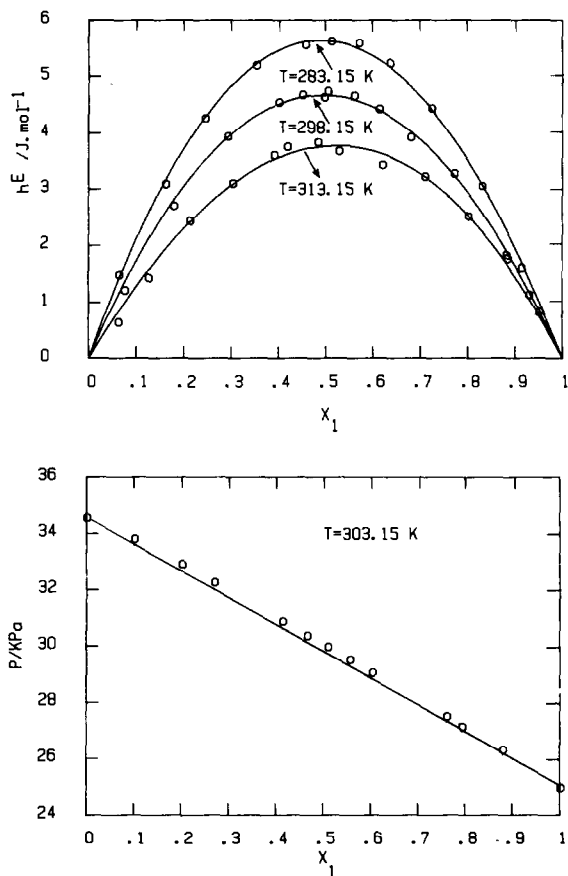
Fig. 1. Comparison of calculated and experimental data for the system n-hexane $(1) + 2$-MP (2): points, experimental values; solid curves are calculated from Wilson's equations; the 303.15 K set of parameters was used to obtain P solid curve.

the parameters of the other models only show a regular variation for the n-octane $(1) + 2$-MP (2) system if the 298.15 K set of parameters is not considered. This is related to the variations of the excess enthalpy with temperature. The 283.15, 293.15, 303.15 and 313.15 K sets of h^E data for systems containing n-octane were measured by Ameling et al. [6], while the 298.15 K sets of data were measured by Hamam et al. [7]. As can be observed in Figs. 4 and 5, these excess enthalpies are always endothermic and decrease with temperature but there are discrepancies between data taken at 293.15, 298.15 and 303.15 K. Values of h^E taken at 298.15 K for the n-octane $(1) + 2$-MP (2) system are too close to those measured at 293.15 K. However, values of h^E taken at 298.15 K for the n-octane $(1) + 3$-MP (2) system are too close to those measured at 303.15 K.

As could be expected, values of the parameters for the n-hexane $(1) + 2$-MP (2) and n-hexane $(1) + 3$-MP (2) systems obtained from h^E data taken
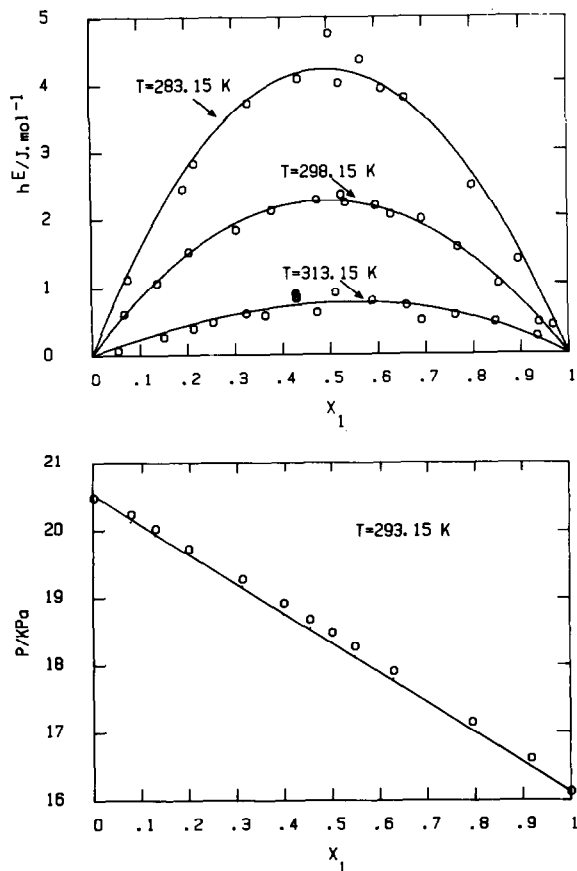
Fig. 2. Comparison of calculated and experimental data for the system n-hexane (1) + 3-MP (2): points, experimental values; solid curves are calculated from NRTL equations; the 298.15 K set of parameters was used to obtain P solid curve.

at the same temperature are always very similar in sign and magnitude for each of the four g^E models studied. The same is true for the LEMF model parameters of the n-octane (1) + 2-MP (2) and n-octane (1) + 3-MP (2) systems. For the remaining g^E models, almost identical sets of parameters are obtained from h^E data taken at 283.15 K while the sets of parameters obtained from h^E data taken at higher temperatures differ sometimes considerably. More h^E data for the systems containing n-octane would be desirable in order to clarify whether these inconsistencies in the values of the parameters are due to errors in experimental data.

Table 3 gives the results of VLE predictions and Figs. 1–5 show some typical examples of results obtained. Application of Wilson's formulation of the Redlich–Kwong equation [9] to take into account the non-ideality of the vapor requires knowledge of the critical constants and acentric factors for pure components. Values for these parameters have been taken from Reid et
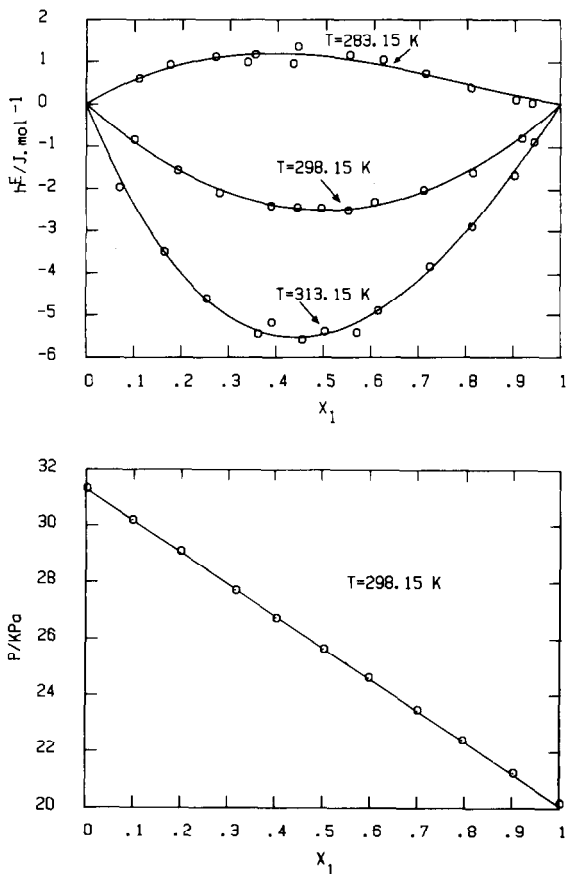
Fig. 3. Comparison of calculated and experimental data for the system n-hexane (1) + 2,3-DMB (2): points, experimental values; solid curves are calculated from LEMF equations; the 313.15 K set of parameters was used to obtain P solid curve.

al. [28]. Values for the pure components vapor pressures were also taken from Reid et al. [28] except for the cases in which these values were reported together with total pressure measurements of the mixtures.

All sets of VLE data are isothermal and were taken at the same or similar temperatures to those of h^E data. The conditions and sources of VLE data are indicated in Table 3. The VLE predictions can be made using the parameters for the g^E model obtained from the h^E data measured at the closest temperature to that of the VLE data. In order to examine how the accuracy of the VLE predictions depends on the parameters used, the set of parameters obtained from h^E data measured at the most distant temperature from that of the VLE data was also used. Finally, in view of the discrepancies observed in data for systems containing n-octane, the 298.15 K set of parameters was also used to predict VLE data for these systems at the four
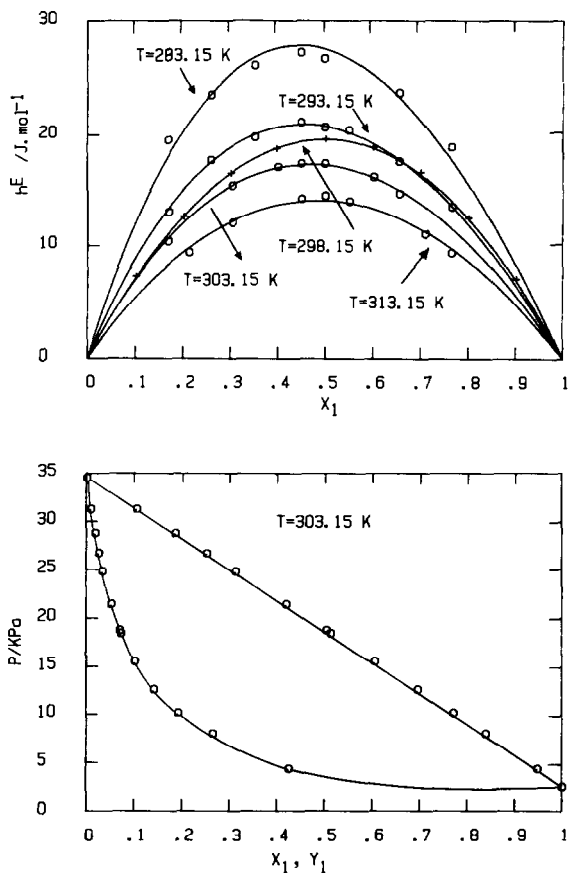
Fig. 4. Comparison of calculated and experimental data for the system n-octane (1) + 2-MP (2): points, experimental values (h^E data: O, Ameling et al. [6]; +, Hamam et al. [7]); solid curves are calculated from UNIQUAC equations; the 283.15 K set of parameters was used to obtain P solid curves.

temperatures studied. The set of parameters used in each prediction is also indicated, in the third column of Table 3.

Since experimental values of y_1 are only available for two of the sets of data studied, the per cent relative standard deviation (%) of the total pressure has been chosen as the criterion to examine the accuracy of the VLE predictions. It may be observed that the agreement between experimental and predicted VLE data is excellent. Relative standard deviation between experimental and calculated total pressures are 1% or less for all sets of data of systems containing n-hexane, and range from 0.2 to 7% for those containing n-octane. Typically, these latter deviations are 1–3% and become higher for the sets of data taken at lower temperatures. Since pressure ranges are different and comparatively low for n-octane-containing mixtures, absolute deviations of the same order of magnitude of those obtained for
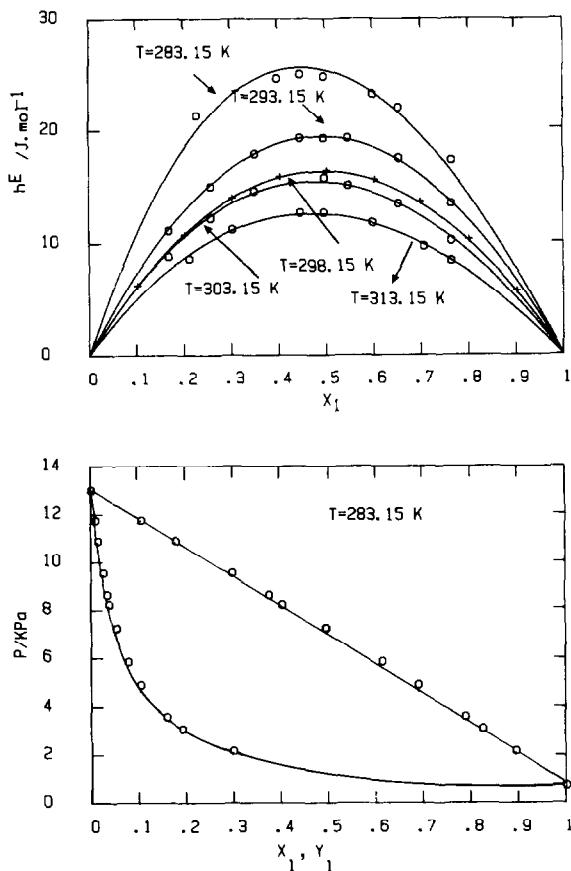
Fig. 5. Comparison of calculated and experimental data for the system n-octane (1) + 3-MP (2): points, experimental values (h^E data: $\bigcirc$, Ameling et al. [6]; +, Hamam et al. [7]); solid curves are calculated from NRTL equations; the 283.15 K set of parameters was used to obtain P solid curves.

systems I–IV lead to higher relative deviations for systems V and VI. On the other hand, predictions of VLE data at certain conditions using different sets of parameters have similar accuracies. The accuracy of the predictions does not seem to depend either on the chosen model for the excess Gibbs energies. Deviations for the four models used are of the same magnitude for each particular set of VLE data.

We may conclude that using the HGC prediction method, a simultaneous and accurate description of the excess enthalpies and VLE data for these nearly ideal systems can be provided. The accuracies of these correlations are of similar magnitude to those obtained for the typical non-ideal systems previously studied using the HGC method [8,10–18]. The VLE and h^E sets of data for systems containing n-hexane or n-octane + a branched hexane are shown to be in agreement, although some discrepancies are observed

TABLE 3

Summary of VLE predictions from h^E data

System	T (K)	Set of parameters (K)	Relative standard deviation in pressure (%)				Ref.
			Wilson's eqn.	NRTL eqn.	LEMF eqn.	UNIQUAC eqn.	
I	283.15	283.15	0.9	0.9	1.1	0.9	2
		313.15	1.0	0.9	1.1	0.9	
	293.15	298.15	0.8	0.8	1.0	0.8	2
		313.15	0.8	0.8	1.0	0.8	
	298.15	298.15	0.8	0.8	1.0	0.8	1
		313.15	0.8	0.8	1.0	0.8	
	303.15	283.15	0.7	0.7	1.0	0.7	2
		298.15	0.8	0.8	1.0	0.8	
	313.15	283.15	0.4	0.4	0.6	0.4	2
		313.15	0.4	0.4	0.6	0.4	
II	283.15	283.15	0.8	0.8	1.0	0.8	2
		313.15	0.9	0.9	1.0	0.9	
	293.15	298.15	0.8	0.8	0.8	0.8	2
		313.15	0.8	0.8	0.9	0.7	
	298.15	298.15	0.6	0.6	0.7	0.6	1
		313.15	0.6	0.6	0.7	0.6	
	303.15	283.15	0.5	0.5	0.6	0.5	2
		298.15	0.6	0.6	0.7	0.6	
	313.15	283.15	0.4	0.4	0.5	0.4	2
		313.15	0.4	0.4	0.5	0.4	
III	298.15	298.15	1.0	1.1	0.6	1.2	1
IV	298.15	298.15	0.2	0.2	0.2	0.2	1
		313.15	0.4	0.4	0.1	0.6	
V	283.15	283.15	5.8	4.5	7.2	5.9	3
		298.15	6.2	5.6	6.6	6.3	
		313.15	6.8	5.9	6.8	7.0	
	293.15	293.15	4.2	3.1	5.0	4.4	3
		298.15	4.1	3.6	4.5	4.2	
		313.15	4.6	3.8	4.6	4.8	
	303.15	283.15	1.8	1.5	3.0	1.9	3
		298.15	2.1	1.6	2.5	2.2	
		303.15	2.5	1.5	2.8	2.8	
	313.15	283.15	0.5	0.9	1.5	0.4	3
		298.15	0.7	0.2	1.0	0.7	
		313.15	1.1	0.4	1.1	1.2	
VI	283.15	283.15	5.0	3.6	6.0	4.9	3
		298.15	5.5	4.7	5.6	5.6	
		313.15	5.9	4.7	5.8	6.2	
	293.15	293.15	3.2	2.4	3.5	3.3	3
		298.15	3.4	2.6	3.5	3.4	
		313.15	3.7	2.6	3.6	4.0	

TABLE 3 (continued)

System	T (K)	Set of parameters (K)	Relative standard deviation in pressure (%)				Ref.
			Wilson's eqn.	NRTL eqn.	LEMF eqn.	UNIQUAC eqn.	
	303.15	283.15	1.5	0.3	2.4	1.4	3
		298.15	2.0	1.2	2.0	2.0	
		303.15	2.2	1.1	2.2	2.3	
	313.15	283.15	0.7	0.7	1.5	0.5	3
		298.15	1.1	0.4	1.1	1.1	
		313.15	1.5	0.4	1.3	1.6	

between the h^E sets of data taken by different authors for the systems containing n-octane. These discrepancies do not prevent the determination from these data of a set of parameters of several widely used g^E models (Wilson, NRTL, LEMF and UNIQUAC) which can be used to predict accurate VLE data within the temperature range of literature data.

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