PREDICTION OF VAPOR-LIQUID EQUILIBRIA BY USING EQUATIONS OF STATE WITH ZERO-PRESSURE EXCESS GIBBS ENERGY MIXING RULES. THE RKU2 MODEL FOR MODERATE TEMPERATURES

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A zero-pressure mixing rule for the energy parameter in cubic equations of state has been developed. The composition dependence of the mixture volume $u = v/b$ at zero pressure is approximated by a two-parameter Redlich-Kister expansion (RKU2). The RKU2 coefficients are determined from pure component parameters of a cubic equation of state and activity coefficients at infinite dilutions.

The RKU2 mixing rule combined with the SRK equation of state has been tested for seven isothermal and nine isobaric binary systems. At moderate temperatures the model performs comparably to the treatment requiring an additional iterative procedure (Heidemann and Kokal, 1990). Extensions to ternary systems and the importance of correct temperature dependence of the activity coefficient models used in the mixing rules are discussed.

Introduction

Chemical engineering practice deals with a large number of systems which can not be successfully described by equations of state with conventional mixing rules. Following the procedure of Huron and Vidal[10], more flexible mixing rules can be obtained by combining equations of state with excess Gibbs energy (g^E) models.

An advantage of the equation of state approach is the possibility of predicting phase equilibria in a wide range of conditions from a known g^E correlation.

In the original suggestion[10], the excess Gibbs energy expression from an equation of state is equated with a g^E model at infinite pressure. Predictive capabilities of the models are limited because the g^E parameters at infinite pressure are too remote from real conditions and are not directly determinable.

Independent low-pressure activity coefficients have been incorporated in the g^E mixing rules only very recently[8, 13]. Correct employment of the zero-pressure standard state requires, however, an additional iterative procedure for mixture standard-state volume.

Michelsen[14] simplified the treatment with approximations yielding zero-pressure mixing rules with one or two coefficients optimized for two parameter cubic equations of state (the MHV models).

The objective of this work is to investigate another approach for avoiding the iterative procedure in the zero-pressure g^E mixing rules. Conceptually, at moderate temperatures the equation of state should closely follow the underlying excess Gibbs energy model with no need of adjustment of parameters.

1. Zero-pressure g^E Mixing Rules

The excess Gibbs energy g^E is defined as a deviation of the mixture Gibbs energy from the ideal solution:

$$g^E = g - g^{IS} = g - \Sigma x_i g_i - RT\Sigma x_i ln x_i \qquad (1)$$

The mixture molar Gibbs energy g can be expressed from equations of state by means of the following thermodynamic relation:

$$g = \int_v^\infty [P - RT/v] \, dv - RTln (P_0 v/RT) + {} + Pv + RT\Sigma x_i ln x_i + RT\Sigma x_i g_i^* \qquad (2)$$

where the superscript * refers to the ideal gas state at temperature T and pressure P_0. When $x_i = 1$ and $v = v_i$, Eq. (2) gives a relation for the molar Gibbs energy of a pure component, g_i.

Combining Eq. (1) and Eq. (2) results in the general expression for the excess Gibbs energy from equations of state:

$$g^E = \int_v^\infty [P - RT/v] \, dv - \Sigma x_i \int_v^\infty [P - RT/v_i] \, dv_i - {} - RT\Sigma x_i ln (v/v_i) + PV - \Sigma x_i Pv_i \qquad (3)$$

The equation of state considered in this work is that of Soave-Redlich-Kwong (SRK)[18]:

$$P(v, T) = RT/(v-b) - a(T)/[v(v+b)] \qquad (4)$$

where a and b are the equation of state energy and size parameters, respectively.

At zero pressure, Eq. (4) can be written in an equivalent form:

$$z(u, \alpha) = Pb/RT = 1/(u-1) - \alpha/[u(u+1)] = 0 \quad (5)$$

which gives a relation between the dimensionless energy

Table 1. VLE calculations of isothermal systems by zero-pressure g^E mixing rules

model			RKU2			Heidemann[8]			MHV2[14]			MHV1[14]			
system	T K	N_d	$\Delta P/P$	Δy (× 100)	$\Delta\gamma/\gamma$	$\Delta P/P$	Δy (× 100)	$\Delta\gamma/\gamma$	$\Delta P/P$	Δy (× 100)	$\Delta\gamma/\gamma$	$\Delta P/P$	Δy (× 100)	$\Delta\gamma/\gamma$	Ref.
Ethanol(1) -Water(2)	313	13	2.2	0.6	0.0	2.2	0.6	0.0	2.6	0.9	1.0	2.8	1.3	4.3	4
	343	13	1.0	0.4	0.0	1.0	0.4	0.0	0.9	0.4	0.2	1.0	0.9	2.9	4
	423	17	2.1	1.5	0.0	2.1	1.5	0.0	1.9	1.2	0.8	2.0	1.5	0.9	2
Acetone(1) -Water(2)	333	9	1.9	0.9	0.1	1.9	0.9	0.0	2.3	1.0	0.7	5.4	1.8	6.7	4
Methanol(1) -Benzene(2)	328	9	1.3	0.6	0.0	1.3	0.6	0.0	1.6	0.7	0.7	1.2	0.7	0.3	4
Methanol(1)- n Hexane(2)	333	28	1.8	1.1	0.2	1.8	1.0	0.0	2.1	1.0	0.7	0.9	0.9	2.1	4
Chloroform(1) -Acetone(2)	323	15	0.3	0.1	0.0	0.3	0.1	0.0	0.4	0.2	0.2	0.2	0.1	0.2	5
Methanol(1)- Chloroform(2)	323	25	0.1	0.1	0.0	0.1	0.1	0.0	0.4	0.2	0.4	0.2	0.2	0.3	5
Methanol(1)- Acetone(2)	323	20	0.1	0.2	0.0	0.1	0.2	0.0	0.1	0.2	0.2	0.1	0.2	0.4	5
Methanol(1) Chloroform(2) Acetone(3)	323	42	0.2	0.4	0.0	0.2	0.4	0.0	0.3	0.4	0.3	0.2	0.4	0.3	5

$$\Delta P/P = (1/N_d) \Sigma_{j=1}^{N_d} \left| (P_j^{cal} - P_j^{exp}) / P_j^{exp} \right|$$

parameter $\alpha = a/RTb$ and the zero-pressure volume reduced by the equation of state size parameter, $u = v_0/b$.

For cubic equations of state at the zero pressure standard state, the general expression for the excess Gibbs energy of Eq. (3) can be conveniently written in the form:

$$g_0^E/RT + \Sigma x_i ln\,(b/b_i) = Q - \Sigma x_i Q_i \qquad (6)$$

where Q is the dimensionless zero-pressure fugacity,

$$Q = ln\,(f_0 b/RT) = \int_u^\infty (z - 1/u)\,du - ln\,(u) - 1 \qquad (7)$$

and Q_i is the same quantity evaluated for a pure component i.

For the SRK equation of state at zero pressure, Eq. (7) becomes

$$Q\,[u, \alpha] = -ln\,(u - 1) - \alpha ln\,[\,(u + 1)/u] - 1 \qquad (8)$$

At low pressures, the change in excess Gibbs energy with pressure is very small. This allows the use of the approximation g_0^E (zero pressure) $= g^E$ (low pressure). Eqs. (5), (6) and (8) can hence be combined with a g^E model with independently determined parameters and solved iteratively for the mixture parameter $u^{8,\,13)}$. Back-substitution to Eq.(5) then gives the required mixture energy parameter α.

2. Development of RKU2 Model

The idea followed in this work is to avoid the iterative procedure in the g^E mixing rules by direct expliciting the composition dependence of the mixture parameter u.

$$\Delta \gamma/\gamma = (1/2N_d) \cdot \Sigma_{j=1}^{N_d} \Sigma_{i=1}^{2} \left| (\gamma_{i,j}^{cal} - \gamma_{i,j}^{mod}) / \gamma_{i,j}^{mod} \right|$$

Figure 1 shows typical examples of the composition dependence of the deviation parameter Δu,

$$u = x_1 u_1 + x_2 u_2 + \Delta u \qquad (9)$$

for isothermal binary systems at about normal boiling points as calculated by the iterative method of Heidemann[8] with the SRK equation of state. This procedure was taken as a standard since at low pressures the model usually follows activity coefficient correlations with no loss in accuracy (cf. **Table 1**).

From Fig. 1 it can be seen that the Δu composition dependencies exhibit rather regular behaviour. This observation can be viewed as a consequence of the common use of the linear mixing rule for the size parameter b in the g^E mixing rules, i.e. $b = x_1 b_1 + x_2 b_2$. As reported elsewhere, the equation of state is unable to describe strong variations in mixture liquid volume if the binary interaction parameter in the covolume mixing rule has a zero value[7].

It therefore appears that the Δu composition dependence could be sufficiently approximated by the Redlich-Kister expansion[16] with two coefficients (RKU2):

$$\Delta u = x_1 x_2 [\,(c + d)\,x_1 + (c - d)\,x_2] \qquad (10)$$

The RKU2 coefficients c and d can be conveniently determined from pure-component parameters a_i, b_i and activity coefficients by applying the conditions for infinite dilutions in binary systems. (Details of the derivation and the expression for fugacity coefficients can be found in the **Appendix**.)
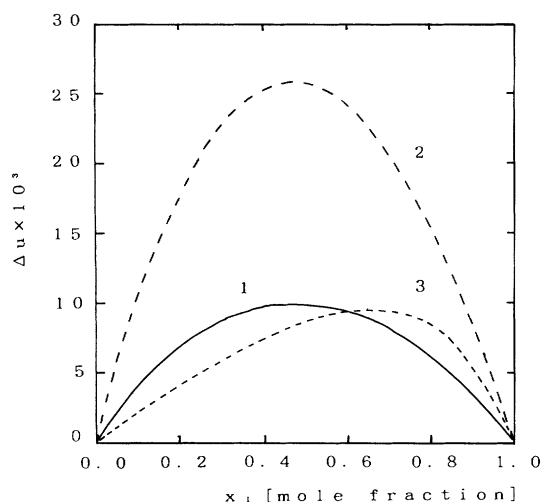
Fig. 1 Composition dependence of mixture parameter Δu. 1 - ethanol(1)-water(2) at 343 K, 2 - methanol(1)-benzene(2) at 328 K, 3 - acetone(1)-water(2) at 333 K.

Fig. 2 Composition dependence of deviations in predicted mixture α from the iterative method[8] for MHV2 and RKU2 mixing rules. $\Delta\alpha = \alpha - \alpha^{cal}$.
1 - ethanol(1)-water(2) at 343 K, 2 - methanol(1)-benzene(2) at 328 K, 3 - acetone(1)-water(2) at 333 K.

The RKU2 coefficients c and d are obtained by solving the following linear equations:

$$c - d = (1/h_2)\, [\,(Q_1 - Q_2) + \ln\gamma_1^\infty - \ln(b_1/b_2) + $$
$$+\, b_2/b_1 - 1\,] - (u_1 - u_2) \tag{11}$$

$$c + d = (1/h_1)\, [Q_2 - Q_1 + \ln\gamma_2^\infty - \ln(b_2/b_1) + $$
$$+\, b_2/b_1 - 1\,] + (u_1 - u_2) \tag{12}$$

where Q_i for the SRK equation of state is defined by Eq. (8) and

$$h_i = -[\,(u_i^2 - 2u_i - 1)/(u_i - 1)^2\,]\ln[\,(u_i + 1)/u_i] \tag{13}$$

The resulting mixing rule for the energy parameter a of the SRK equation of state has the form:

$$\alpha = \{-1/\ln[\,(u + 1)/u]\,\} \cdot [\ln(u - 1)$$

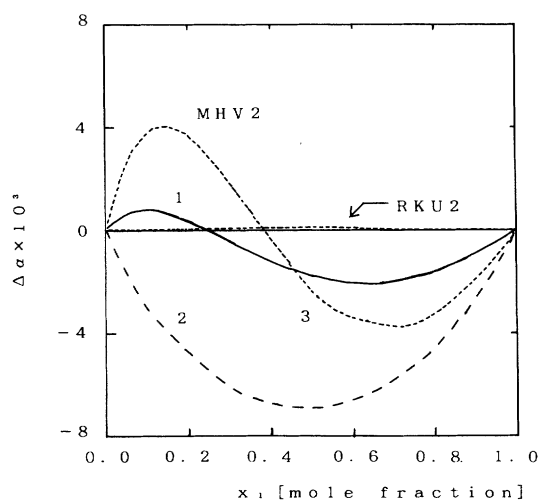$$+x_1\,(Q_1 - \ln b_1\,) - x_2\,(Q_2 - \ln b_2\,) + g_0^E/RT + \ln b + 1\,](14)$$

with u given now explicitly by Eqs. (9) and (10).

3. Calculated Results and Discussion

3.1 Binary systems

The RKU2 model combined with the SRK equation of state was applied to a variety of binary systems at conditions of about normal boiling points. Pure-component critical parameters used in the calculations with the equation of state were taken from Reid et al.[17]. The acentric factor in the Graboski-Daubert modification[6] of the Soave expression[18] was adjusted so to give correct values of saturated vapor pressures for pure components.

In selecting the input data an attempt was made to include only complete data sets which would successfully pass the Overall Thermodynamic Consistency Test[11]. Calculations with the g^E mixing rules were based on the Wilson equation[20] with parameters evaluated in the Dechema Series[4]. In case of systems containing chloroform or showing liquid immiscibility (2-butanone-water) the Redlich-Kister equation[16] was used instead.

Parameters of the equation were taken from the literature[5, 15].

In Table 1, the RKU2 results for isothermal systems are compared with the iterative method of Heidemann[8] and the MHV models[14]. The activity coefficient deviations $\Delta\gamma/\gamma$ listed in Table 1 are defined as relative differences of the activity coefficients calculated by an equation of state and those given by the Wilson or Redlich-Kister equation at the experimental points. The activity coefficients of the RKU2 model and a g^E correlation are nearly identical, with deviations usually well below 0.1%. The MHV models produce the deviations of about one order higher.

Figure 2 shows details of the comparison reflected in deviation of the calculated mixture energy parameter α from the iterative method[8].

Calculations by the RKU2 mixing rule were extended to isobaric systems (**Table 2**). **Figure 3** presents an example of the performance of the g^E mixing rules for a system with a limited liquid miscibility[15].

In the case of isobaric systems the only expense for the RKU2 model is to reevaluate the activity coefficients at infinite dilution when the temperature changes. The computational excess is only moderate since local composition g^E models provide simple expressions for the activity coefficients at infinite dilutions in binary systems.

3.2 Ternary systems

Because of the observed regularity of Δu composition dependencies in constituent binary systems, Δu for ternary systems was approximated by the following expression:

$$\Delta u_{123} = \Delta u_{12} + \Delta u_{23} + \Delta u_{31} \tag{15}$$

Table 1 shows results of isothermal calculations of the system acetone-methanol-chloroform exhibiting a saddle-type ternary azeotrope[5]. It can be seen that the

Table 2. .VLE calculations of isobaric binary systems at 101.3kPa

system	T K	N_d	RKU2 $\Delta T/T$	Δy (×100)	$\Delta\gamma/\gamma$	Heidemann[8] $\Delta T/T$	Δy (×100)	$\Delta\gamma/\gamma$	MHV2[14] $\Delta T/T$	Δy (×100)	$\Delta\gamma/\gamma$	MHV1[14] $\Delta T/T$	Δy (×100)	$\Delta\gamma/\gamma$	Ref.
Ethanol(1)-Water(2)	351 373	15	0.2	0.8	0.0	0.2	0.8	0.0	0.2	0.8	0.4	0.4	0.9	2.4	4
Acetone(1)-Water(2)	329 373	19	1.0	1.1	0.1	1.0	1.1	0.0	0.9	1.1	0.5	0.9	0.8	4.9	4
2-Butanone(1)-Water(2)	347 373	33	0.3	0.6	0.0	0.3	0.6	0.0	0.1	0.7	0.7	1.8	3.0	6.8	15
Methanol(2)-Water(2)	338 373	13	0.2	0.8	0.0	0.2	0.8	0.0	0.2	0.9	0.2	0.8	1.3	2.4	4
Acetone(1)-Methanol(2)	329 338	23	0.4	0.3	0.0	0.4	0.3	0.0	0.4	0.3	0.3	0.4	0.3	0.2	4
Cyclohexane(1)-1-Propanol(2)	348 370	21	0.09	1.1	0.1	0.09	1.2	0.0	0.12	1.1	0.4	0.18	1.4	0.5	4
Benzene(1)-1-Propanol(2)	350 370	23	0.4	0.6	0.0	0.4	0.6	0.0	0.5	0.6	0.3	0.3	0.7	0.4	4
Benzene(1)-Cyclohexane(2)	348 350	29	0.05	0.1	0.0	0.05	0.1	0.0	0.06	0.1	0.1	0.04	0.1	0.3	1
Methanol(1)-Benzene(2)	338 350	18	0.3	0.4	0.0	0.3	0.4	0.0	0.4	0.5	0.5	0.3	0.4	0.4	4

$$\Delta T/T = (1/N_d) \, \Sigma_{j=1}^{N_d} \left| (T_j^{cal} - T_j^{exp}) / (T_j^{exp} - 273.15) \right|$$

$$\Delta y/y = (1/N_d) \cdot \Sigma_{j=1}^{N_d} \left| y_{1,j}^{cal} - y_{1,j}^{exp} \right|$$

simple RKU2 model extends favourably to even this complex multicomponent case.

Partial difficulties may, however, arise when the model is extended to isobaric multicomponent systems with varying temperature described by not fully adequate local composition g^E models.

An example of such a situation is presented in **Figs. 4a, b**, which show the temperature dependence of the activity coefficients at infinite dilution prescribed by Dechema Wilson parameters for the ternary system acetone-methanol-water at 101.3 kPa[4]. It appears that the ternary Wilson parameters were rather overcorrelated, causing incorrect temperature dependence of the activity coefficients at infinite dilution (**Table 3**).

3.3 g^E temperature dependence

The importance of inserting proper temperature dependence in an activity coefficient expression is quite general for all kinds of g^E mixing rules. It is particularly significant in an extrapolation outside the range of conditions where the parameters were evaluated.

Figure 5 gives an example of the temperature dependence of the activity coefficients at infinite dilution in the system ethanol-water, showing the maximum between 70-100°C. **Figure 6** presents calculations of the azeotropic line in this system. Apparently, any extrapolation with temperature-independent Wilson parameters determined at atmospheric pressure can yield incorrect results. Alternatively, the Wilson parameters with quadratic temperature dependence evaluated between 30-

150°C may in extrapolation beyond the critical point of ethanol lead to highly erroneous results.

Conclusion

A model based on an approximation of composition dependence of mixture zero pressure reduced volume u by a two-parameter Redlich-Kister expansion (RKU2) has been tested. The RKU2 mixing rule is suited for moderate temperatures and may be useful for predicting phase equilibria at elevated pressures.

Appendix

RKU2 parameters c and d at infinite dilutions

For the SRK equation of state at zero pressure the following formula can be derived from Eq.(8):

$$h = dQ/du = (\partial Q/\partial\alpha) \, d\alpha/du \qquad (A1)$$

where

$$(\partial Q/\partial\alpha) = -\ln[(u+1)/u] \qquad (A2)$$

$$d\alpha/du = (u^2 - 2u - 1)/(u-1)^2 \qquad (A3)$$

The composition derivative of function Q follows from Eq. (6),

$$\tilde{Q}_i = (\partial Q/\partial x_i) = (\partial g_0^E/\partial x_i) - \ln b_i +$$
$$+ (\partial b/\partial x_i) \cdot (1/b) - Q_i \qquad (A4)$$

Typically, the linear mixing rule is assumed for the equation of state size parameter b, i.e.
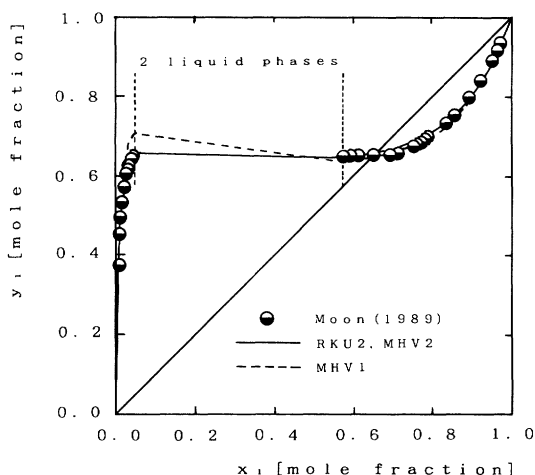
Fig. 3 Experimental and calculated x-y diagram for 2-butanone(1)-water(2) at 101.3 kPa.

$$b = \Sigma x_i b_i, \quad (\partial b / \partial x_i) = b_i.$$

For binary systems, the deviation function Δu of Eq. (9) is approximated in this work by the Redlich-Kister expansion with two coefficients, Eq. (10). The RKU2 coefficients c and d can be determined by applying the following relations valid at infinite dilutions in binary systems:

$$(\Delta u / x_1 x_2)_{x_1 = 0} = (d\Delta u / dx_1)_{x_1 = 0} = c - d \quad (A5)$$

$$(\Delta u / x_1 x_2)_{x_2 = 0} = (d\Delta u / dx_2)_{x_2 = 0} = c + d \quad (A6)$$

with

$$(d\Delta u / dx_1)_{x_1 = 0} = (du / dx_1)_{x_1 = 0} - (u_1 - u_2) \quad (A7)$$

$$(d\Delta u / dx_2)_{x_2 = 0} = (du / dx_2)_{x_2 = 0} + (u_1 - u_2) \quad (A8)$$

The composition derivatives at the terminal points $(du/dx_i)_{x_i = 0}$ can be found by differentiating Eq. (A9), which defines a relation between the excess Gibbs energy and an equation of state at zero pressure in binary systems:

$$g_0^E / RT + \ln b = Q - x_1 (Q_1 - \ln b_1) - x_2 (Q_2 - \ln b_2) \quad (A9)$$

In Eqs. (A10), (A11) these derivatives are expressed by means of the differential quantities defined by Eqs. (A1), (A4):

$$(du / dx_1)_{x_1 = 0} = (1/h_2) (\tilde{Q}_1 - \tilde{Q}_2)_{x_1 = 0}$$
$$= (1/h_2) [Q_1 - Q_2 + \ln \gamma_1^\infty - \ln (b_1/b_2) + b_1/b_2 - 1] \quad (A10)$$

$$(du / dx_2)_{x_2 = 0} = (1/h_1) (\tilde{Q}_2 - \tilde{Q}_1)_{x_2 = 0}$$
$$= (1/h_1) [Q_2 - Q_1 + \ln \gamma_2^\infty - \ln (b_2/b_1) + b_2/b_1 - 1] \quad (A11)$$

where $h_i = dQ_i / du_i$.

Expression for Fugacity Coefficients

Fugacity coefficients are calculated from the SRK equation of state and zero pressure g^E mixing rules by the following relation:
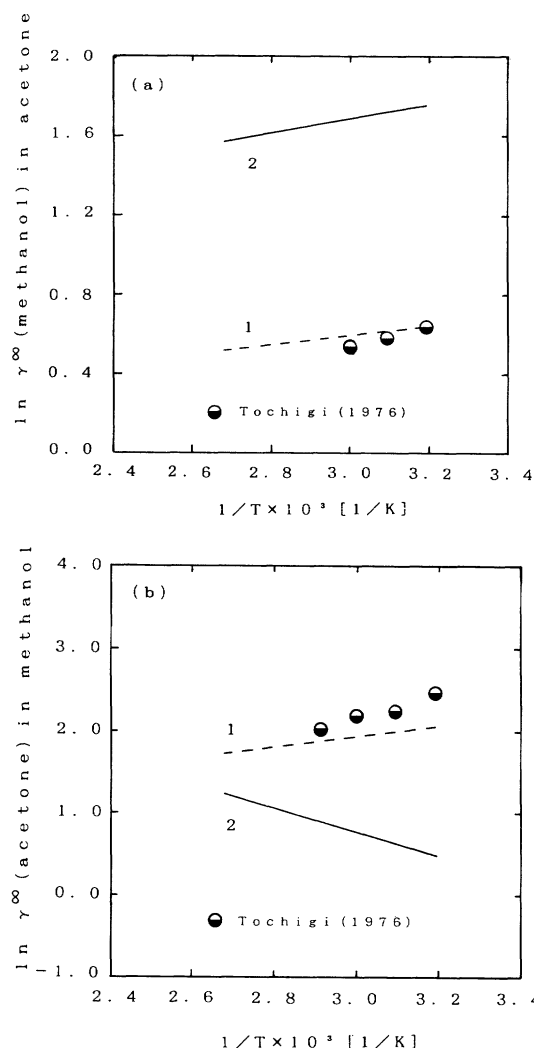

Fig. 4 Temperature dependence of activity coefficients at infinite dilution.
a) Methanol in acetone
b) Acetone in methanol
1 - prediction by Wilson parameters for methanol-acetone at 101.3 kPa[4], 2-prediction by Wilson parameters for methanol-acetone-water at 101.3 kPa[4]. Experimental data by Tochigi et al. (1976)[19] for methanol-acetone at 101.3 kPa.

$$\ln (f / x_i P) = (b_i / b) (Pv / RT + 1) - \ln [P(v - b) / RT]$$
$$- [\partial (n\alpha) / \partial n_i] \ln [(v + b) / v] \quad (A12)$$

The composition derivative of the combined mixture parameter α in the RKU2 mixing rule can be again found by using Eq. (A4):

$$\partial (n\alpha) / \partial n_i = \alpha + 1/(\partial Q / \partial \alpha) \cdot [\tilde{Q}_i - \Sigma x_k \tilde{Q}_k] \quad (A13)$$

with $(\partial Q / \partial \alpha)$ defined by Eq. (A2).

Nomenclature

|			
a	=	equation of state energy parameter	$[Pa(m^3/mol)^2]$
b	=	equation of state size parameter	$[m^3/mol]$
b_i	=	pure component value of b	$[m^3/mol]$
c, d	=	parameters of RKU2 model	$[-]$
f	=	fugacity	$[Pa]$
g	=	molar Gibbs energy	$[J/mol]$

Table 3. VLE calculations of isobaric binary systems at 101.3kPa

model					RKU2			Heidemann[8]			MHV2[14]			MHV1[14]			
system	T K	N_d	$\Delta T/T$	Δy ($\times 100$)	$\Delta\gamma/\gamma$	$\Delta T/T$	Δy ($\times 100$)	$\Delta\gamma/\gamma$	$\Delta T/T$	Δy ($\times 100$)	$\Delta\gamma/\gamma$	$\Delta T/T$	Δy ($\times 100$)	$\Delta\gamma/\gamma$		Ref.
Acetone(1) Methanol(2) Water(3)	329 373	36	0.9	1.3	1.1	0.9	1.4	0.0	0.8	1.3	0.4	1.1	1.2	3.0		4
Benzene(1) Cyclohexane(2) 1-Propanol(3)	347 354	56	0.01	0.4	0.2	0.01	0.4	0.0	0.01	0.4	0.4	0.03	0.4	0.3		4,9
Benzene(1) Cyclohexane(2) 1-Propanol(3)	347 371	69	0.5	1.4	0.5	0.6	1.3	0.0	0.5	1.3	0.4	0.6	1.3	0.3		1

$$\Delta y = (1/2 \ N_d) \cdot \Sigma_{j=1}^{N_d} \Sigma_{i=1}^{2} \left| y_{i,j}^{cal} - y_{i,j}^{exp} \right|$$

$$\Delta \gamma/\gamma = (1/3N_d) \cdot \Sigma_{j=1}^{Nd} \Sigma_{j=1}^{3} \left| (\gamma_{i,j}^{cal} - \gamma_{i,j}^{mod}) / \gamma_{i,j}^{mod} \right|$$
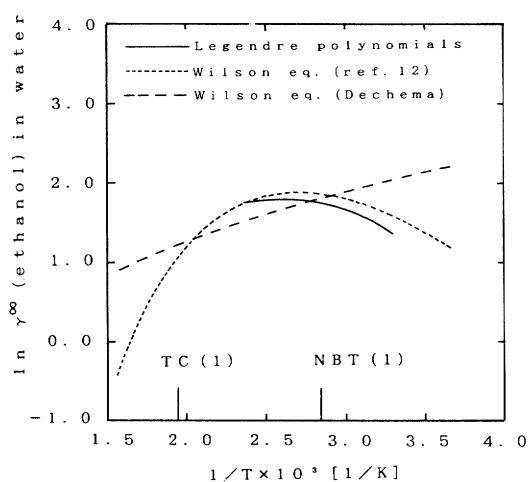
Fig. 5 Temperature dependence of the infinite dilution activity coefficient of ethanol(1) in water(2).
NBT(1)-normal boiling temperature of ethanol (351 K), TC(1)-critical temperature of ethanol (516 K).

Fig. 6 SRK calculations of the azeotropic line for ethanol(1)-water(2) based on different g^E models.

g_i	=	pure component value of g [J/mol]
g^E	=	molar excess Gibbs energy [J/mol]
h	=	function defined by Eq. (A1) [–]
h_i	=	pure component value of h [–]
N_d	=	number of data points [–]
n	=	mole number [mol]
P	=	pressure [Pa]
Q	=	dimensionless zero-pressure fugacity, Eq. (7) [–]
Q_i	=	pure component value of Q [–]
$\tilde{Q}_i$	=	derivative of Q with mole fraction [–]
R	=	gas constant [J/(mol K)]
T	=	temperature [K]
u	=	reduced molar volume v_0/b at zero pressure [–]
u_i	=	pure component value of u [–]
v	=	molar volume [m^3/mol]
v_i	=	pure component value of v [m^3/mol]
x_i	=	mole fraction of component i [–]
z	=	Pb/RT, Eq. (5) [–]
α	=	combined parameter of equation of state, $\alpha = a/RTb$ [–]
α_i	=	pure component value of α [–]
γ_i	=	activity coefficient of component i [–]
Δu	=	deviation function of u, Eq. (10) [–]

<Subscripts>
1,2,i,k	=	component index
0	=	standard state

<Superscripts>
*	=	ideal gas property
∞	=	at infinite dilution
cal	=	calculated by equation of state
exp	=	experimental value
IS	=	ideal solution
mod	=	model value, from a g^E correlation of experimental data

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