Table 1 Activity Coefficient Equations for Binary Systems

Type of equation	Adjustable parameters	$\ln \gamma_1 =$ $\ln \gamma_2 =$	
Margules [15]	A_{12}	$[A_{12} + 2(A_{21} - A_{12})\, x_1]\, x_2^2$	(28a)
	A_{21}	$[A_{21} + 2(A_{12} - A_{21})\, x_2]\, x_1^2$	(28b)
van Laar [24]	A_{12}	$A_{12} \left(\frac{A_{21} x_2}{A_{12} x_1 + A_{21} x_2}\right)^2$	(29a)
	A_{21}	$A_{21} \left(\frac{A_{12} x_1}{A_{12} x_1 + A_{21} x_2}\right)^2$	(29b)
Wilson [27]	$\lambda_{12} - \lambda_{11}$ [1]	$\ln (x_1 + \Lambda_{12} x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right)$	(30a)
	$\lambda_{21} - \lambda_{22}$	$-\ln (x_2 + \Lambda_{21} x_1) - x_1 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{\Lambda_{21} x_1 + x_2}\right)$	(30b)
NRTL [22]	$g_{12} - g_{22}$ [2]	$x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}}\right)^2 + \left(\frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2}\right)\right]$	(31a)
	$g_{21} - g_{11}$ α_{12}	$x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}}\right)^2 + \left(\frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2}\right)\right]$	(31b)
(continued)			

Table 1 Activity Coefficient Equations for Binary Systems (continued)

Type of equation	Adjustable parameters	$\ln \gamma_1 =$ $\ln \gamma_2 =$	
UNIQUAC [1]	$u_{12} - u_{22}$ [3]	$\ln \gamma_1^C + \ln \gamma_1^R$ [3]	(32a)
	$u_{21} - u_{11}$	$\ln \gamma_2^C + \ln \gamma_2^R$	(32b)

1) $\Lambda_{12} = \frac{V_2^L}{V_1^L} \exp - \frac{\lambda_{12} - \lambda_{11}}{RT}$ $\qquad \Lambda_{21} = \frac{V_1^L}{V_2^L} \exp - \frac{\lambda_{21} - \lambda_{22}}{RT}$

V_i^L molar volume of pure liquid component i. For values of V_i^L see Appendix A.

λ_{ij} interaction energy between components i and j $\lambda_{ij} = \lambda_{ji}$

2) $\tau_{12} = \frac{g_{12} - g_{22}}{RT}$ $\qquad \tau_{21} = \frac{g_{21} - g_{11}}{RT}$

$G_{12} = \exp(-\alpha_{12}\tau_{12})$ $\qquad G_{21} = \exp(-\alpha_{21}\tau_{21})$

g_{ij} parameter for interaction between components i and j; $g_{ij} = g_{ji}$

α_{ij} nonrandomness parameter; $\alpha_{ij} = \alpha_{ji}$

3) for detailed equations see table 2

Table 2 UNIQUAC Activity Coefficient Equations [1] for Binary Systems

$$\ln \gamma_1 = \ln \gamma_1^C + \ln \gamma_1^R \tag{32a}$$

$$\ln \gamma_1^C = \ln \frac{\varphi_1}{x_1} + \frac{z}{2} q_1 \ln \frac{\vartheta_1}{\varphi_1} + \varphi_2 \left(l_1 - \frac{r_1}{r_2} l_2 \right) \tag{33a}$$

$$\ln \gamma_1^R = -q_1 \ln (\vartheta_1 + \vartheta_2 \tau_{21}) + \vartheta_2 q_1 \left(\frac{\tau_{21}}{\vartheta_1 + \vartheta_2 \tau_{21}} - \frac{\tau_{12}}{\vartheta_1 \tau_{12} + \vartheta_2} \right) \tag{34a}$$

$$\ln \gamma_2 = \ln \gamma_2^C + \ln \gamma_2^R \tag{32b}$$

$$\ln \gamma_2^C = \ln \frac{\varphi_2}{x_2} + \frac{z}{2} q_2 \ln \frac{\vartheta_2}{\varphi_2} + \varphi_1 \left(l_2 - \frac{r_2}{r_1} l_1 \right) \tag{33b}$$

$$\ln \gamma_2^R = -q_2 \ln (\vartheta_1 \tau_{12} + \vartheta_2) + \vartheta_1 q_2 \left(\frac{\tau_{12}}{\vartheta_1 \tau_{12} + \vartheta_2} - \frac{\tau_{21}}{\vartheta_1 + \vartheta_2 \tau_{21}} \right) \tag{34b}$$

$$l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1) \qquad z = 10 \tag{35}$$

Symbols

l_i see equation (35)

q_i area parameter of component i *)

r_i volume parameter of component i *)

u_{ij} Parameter of interaction between components i and j; $u_{ij} = u_{ji}$

z coordination number

γ_i^C combinatorial part of activity coefficient of component i

γ_i^R residual part of activity coefficient of component i

$\vartheta_i = \dfrac{q_i x_i}{\sum_j q_j x_j}$ area fraction of component i

$\varphi_i = \dfrac{r_i x_i}{\sum_j r_j x_j}$ volume fraction of component i

τ_{ij} see Table 4

*) For values of r_i and q_i see Appendix A

Table 4 Activity Coefficient equations for Multicomponent Systems

Type of equation	Parameters	$\ln \gamma_i =$
Wilson [27] *)	$\Lambda_{ij} = \frac{V_j^L}{V_i^L} \exp - \left[\frac{(\lambda_{ij} - \lambda_{ii})}{RT}\right]$ 1) $\Lambda_{ii} = \Lambda_{jj} = 1$	$-\ln\left(\sum_{j=1}^{m} x_j \Lambda_{ij}\right) + 1 - \sum_{k=1}^{m} \frac{x_k \Lambda_{ki}}{\sum_{j=1}^{m} x_j \Lambda_{kj}}$ 1) (36)
NRTL [22]	$\tau_{ji} = \frac{(g_{ji} - g_{ii})}{RT}$ 2) $G_{ji} = \exp(-\alpha_{ji}\tau_{ji})$ $\tau_{ii} = \tau_{jj} = 0$ $G_{ii} = G_{jj} = 1$	$\frac{\sum_{j=1}^{m} \tau_{ji} G_{ji} x_j}{\sum_{l=1}^{m} G_{li} x_l} + \sum_{j=1}^{m} \frac{x_j G_{ij}}{\sum_{l=1}^{m} G_{lj} x_l} \left(\tau_{ij} - \frac{\sum_{n=1}^{m} x_n \tau_{nj} G_{nj}}{\sum_{l=1}^{m} G_{lj} x_l}\right)$ (37)
UNIQUAC [1] (continued)	$\tau_{ji} = \exp - \left(\frac{u_{ji} - u_{ii}}{RT}\right)$ 3)	$\ln \gamma_i^C + \ln \gamma_i^R$ 3) (38)

Table 4 Activity Coefficient Equations for Multicomponent Systems (cont.)

		$\ln \gamma_i^C = \ln \frac{\varphi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\vartheta_i}{\varphi_i} + l_i - \frac{\varphi_i}{x_i} \sum_j x_j l_j$	(39)
	$\tau_{ii} = \tau_{jj} = 1$	$\ln \gamma_i^R = q_i \left[1 - \ln\left(\sum_{j=1}^{m} \vartheta_j \tau_{ji} \right) - \sum_{j=1}^{m} \frac{\vartheta_j \tau_{ij}}{\sum_{k=1}^{m} \vartheta_k \tau_{kj}} \right]$	(40)
		$l_i = \frac{z}{2} (r_i - q_i) - (r_i - 1) \qquad z = 10$	(35)

1) explanation of symbols see footnote 1 of table 1
2) explanation of symbols see footnote 2 of table 1
3) explanation of symbols see table 2

*) For values of V_i^L, r_i and q_i see Appendix A