REFERENCES

Abrams, D. S., and Prausnitz, J. M. A new expression for the excess gibbs free energy of partly or completely miscible systems. AICHE Journal 21 (1975): 116-128.

Assael, M. J., Trusler, J. P. M., and Tsolakis, T. F. An introduction to their prediction thermophysical properties of fluids. London: Imperial College Press, 1996.

Comelli, F., and Francesconi, R. Thermodynamic properties of binary mixtures containing 1,2-epoxybutane + four alkanols at 298.15 K. J. Chem. Eng. Data 41 (1996): 1392-1396.

Garriga, R., Sanchez, F., Perez, P., and Gracia, M. Excess gibbs free energies at eight temperatures and excess enthalpies and volumes at T=298.15 K for butanemitrile + 2-butanol. J. Chem. Eng. Data 42 (1997): 78-83.

Hala, E., Pick, J., Fried, V., and Vilim, O. Vapor-liquid equilibrium. 2nd English ed. translated by Standart, G. Oxford: Pergamon, 1967.

Hsu, K.Y., and Clever, H.L. The excess enthalpies of the 15 binary mixtures formed from cyclohexane, benzene, toluene, 1,4-dimethylbenzene, 1,2,4-trimethylbenzene, and 1,3,5-trimethylbenzene at 298.15 K. J. Chem. Thermodynamics 19 (1975): 435-442.

Kurihara, K., Uchiyama, M. and Kojima, K. Isothermal vapor-liquid equilibria for benzene + cyclohexane + 1-propanol and for three constituent binary systems. J. Chem. Eng. Data 42 (1997): 149-154.

Kuus, M., Kirss, H., Siimer, E. and Kudryavtseva, L. Excess enthalpies for the systems 1,3-butanediol + cyclohexanol + decane and 1,2-propanediol + 1,3-butanediol + cyclohexanol and for constituent binaries at 318.15 K. J. Chem. Eng. Data 41 (1996): 1206-1209.

Meyer, R. J., Giusti, G., Vincent, E. J., and Meyer, M. The thermodynamic properties of actals + heptane mixtures at 298.15 K Thermochimica Acta 19 (1977): 153-160.

Ohta, T. and Nagata, I. Thermodynamic properties of four ester-hydrocarbon mixtures. J. Chem. Eng. Data 25 (1980): 283-286.

Paul, H I., Krug, J., Gutsche, B.,and Knapp, H. Measurements of VLE, h^E, and v^E for binary mixtures of dibutyl ether with 1-chlorohexane, 1,2-dichloro-elthane, and 1,1,1- Trichloroethane. J. Chem. Eng. Data 31 (1986): 448-456.

Paul, H. I., Krug, J., and Knapp, H. Measurements of VLE, v^E, and h^E for binary mixtures of 1-chlorohexane with three n-alkylbenzenes: toluene, ethylbenzene, n-propylbenzene. J. Chem. Eng. Data 33 (1988): 453-460.

Prausnitz, J. M., Eckert, C. A., Orye, R. V., and O'Connell, J. P. Computer calculations of multicomponent vapor-liquid equilibria. New Jersey: Prentice Hall, 1967.

Renon, H. and Prausnitz, J. M. Local compositions in thermodynamic excess functions for liquid mixtures. AICHE Journal 14 (1968): 135-144.

Stokes, R. H., Marsh, K. N., Tomlins, R. P. An isothermal displacement calorimeter for endothermic enthalpies of mixing. J. Chem. Thermodynamics. 1 (1969): 211-221.

Van Ness, H. C., and Abbott, M. M. Classical thermodynamics of nonelectrolyte solutions: with applications to phase equilibria. New York: McGraw-Hill, 1982.

Walas, S. M. Phase equilibria in chemical engineering. Boston: Butterworth, 1985.

Wilson, G. M. Vapor-liquid-equilibrium. xi. a new expression for the excess gibbs free energy of mixing. J. Amer. Chem. Soc. 86 (1964): 127-130.

APPENDICES

APPENDIX A

PHYSICAL PROPERTIES

Table A.1 Vapor pressure P^{o} and molar volumes v^{o} of the pure compounds used in this work.

Compound	T/K	v^*/cm^3mol^{-1}	P*/kPa	compound	T/K	v^*/cm^3mol^{-1}	P*/kPa
Benzene	323.15	92.26	36.2078	cyclohexane	323.15	116.20	36.2457
	333.15	98.02	52.2703		333.15	117.92	51.8959
Butanenitrile	278.15	86.25	0.8250	1,2-dichloroethane	330.00	82.58	406.8000
	288.15	86.88	1.5270		350.00	84.78	820.3000
	293.15	87.36	2.0350		370.00	87.18	1515.3000
	298.15	87.87	2.6890	di-n-butyl ether	313.15	173.26	20.3000
	303.15	88.42	3.4930		323.15	175.30	33.8000
	308.15	88.96	4.4860		330.00	176.74	47.9000
	313.15	89.57	5.7160		343.15	179.62	86.3000
	323.15	90.66	9.0130		350.00	181.19	114.5000
2-butanol	278.15	90.47	0.5080		370.00	186.04	248.8000
	288.15	91.38	1.1150	1,2-epoxybutane	298.15	87.44	23.3948
	293.15	91.86	1.6320	ethanol	298.15	58.67	7.8463
	298.15	92.35	2.3060	ethylbenzene	323.15	125.89	4.6500
	303.15	92.84	3.2370		343.15	128.67	11.2600
	308.15	93.34	4.4400	ethyl formate	323.15	83.87	85.7067
	313.15	93.86	6.0460	methanol	298.15	40.74	16.9082
	323.15	94.92	10.7200	2-propanol	298.15	76.96	5.7434
1-chlorohexane	323.15	141.82	4.6800	n-propylbenzene	363.15	149.76	11.3200
	343.15	144.82	11.4000	toluene	323.15	109.56	12.2800
	363.15	147.81	24.6500		343.15	112.17	27.1600
1-chloropentane	313.15	123.51	84.6000	1,1,1-trichloroethane	323.15	103.52	451.2000
	323.15	124.96	131.9000		343.15	106.38	893.1000

Table A.2 Pure components properties r = relative van der Waals volume, q = relative van der Waals surface area (q' = q).

Compound	formula	r	q
Benzene	C_6H_6	3.1878	2.4000
Butanenitrile	C_4H_7N	3.2189	2.804
2-butanol	$C_4H_{10}O$	3.4535	3.0480
1-chlorohexane	$C_6H_{13}Cl$	5.0641	4.2720
1-chloropentane	$C_5H_{11}Cl$	4.3897	3.7320
Cyclohexane	C_6H_{12}	4.0464	3.2400
1,2-dichloroethane	$C_2H_4C_{l2}$	2.9308	2.5280
di-n-butyl ether	$C_8H_{18}O$	6.0925	5.1760
1,2-epoxybutane	C_4H_8O	2.9407	2.3960
Ethanol	C_2H_6O	2.1055	1.9720
Ethylbenzene	C_8H_{10}	4.5972	3.508
ethyl formate	$C_3H_6O_2$	2.8175	2.5760
Methanol	CH_4O	1.4311	1.4320
2-propanol	C_3H_8O	2.7791	2.5080
n-propylbenzene	C_9H_{12}	5.2716	4.0480
Toluene	C_7H_8	3.9228	2.9680
1,1,1-trichloroethane	$C_2H_3Cl_3$	3.5412	3.0320

Table A.3 The Ewell classification of molecules based on potential for forming hydrogen bonds (Hala et al., 1967).

Class	Description	Example
I	Molecules capable of forming three-dimensional networks of strong H-bonds	Water, glycols, glycerol, amino alcohols, hydroxylamines, hydroxyacids, polyphenols, and amides
II	Other molecules containing both active hydrogen atoms and donor atoms (O, N, and F)	Alcohols, acids, phenols, primary and secondary amines, oximes, nitro and nitrile compounds with α-hydrogen atoms, ammonia, hydrazine, hydrogen fluoride, and hydrogen cyanide
III	Molecules containing donor atoms but no active hydrogen atoms	Ethers, ketones, aldehydes, esters, tertiary amines (including pyridine type), and nitro and nitrile compounds without with α-hydrogen atoms
IV	Molecules containing active hydrogen atoms but no donor atoms that have two or three chlorine atoms on the same carbon atom as a hydrogen or one chlorine on the carbon atom and one or more chlorine atoms on adjacent carbon atoms	$CHCl_3$, CH_2Cl_2, CH_3CHCl_2, CH_2ClCH_2Cl, $CH_2ClCHClCH_2Cl$, and $CH_2ClCHCl_2$
V	All other molecules having neither active hydrogen atoms nor donor atoms	Hydrocarbons, carbon disulfide, sulfides, mercaptans, and halohydrocarbons not in class IV

APPENDIX B

CORRELATIONS OF EXCESS ENTHALPY

In order to represent excess enthalpy as a function of activity coefficients, the following expression and derivatives are required.

$$H^E = -RT^2 \sum_i x_i \left(\frac{\partial \ln \gamma_i}{\partial T} \right)_{P,x} \qquad \text{(B.1)}$$

B.1 Derivatives of the activity coefficients with respect to temperature.

For binary system, the activity coefficients of the Wilson equation are rewritten

$$\ln \gamma_1 = -\ln(x_1 + x_2 \Lambda_{12}) + x_2 \beta$$
$$\ln \gamma_2 = -\ln(x_2 + x_1 \Lambda_{21}) - x_1 \beta$$

where $\beta = \frac{\Lambda_{12}}{x_1 + x_2 \Lambda_{12}} - \frac{\Lambda_{21}}{x_2 + x_1 \Lambda_{21}}$ and $\Lambda_{ij} = \frac{v_j}{v_i} \exp\left(-\frac{\lambda_{ij}}{RT} \right)$

The derivatives are

$$\frac{\partial \ln \gamma_1}{\partial T} = -\frac{x_2 \frac{\partial \Lambda_{12}}{\partial T}}{x_1 + x_2 \Lambda_{12}} + x_2 \frac{\partial \beta}{\partial T} \qquad \text{(B.2)}$$

$$\frac{\partial \ln \gamma_2}{\partial T} = -\frac{x_1 \frac{\partial \Lambda_{21}}{\partial T}}{x_2 + x_1 \Lambda_{21}} - x_1 \frac{\partial \beta}{\partial T} \qquad \text{(B.3)}$$

Substitutes equations B.2 -3 into equation B.1, gives

$$H^E = -RT^2 \left(x_1 \frac{\partial \ln \gamma_1}{\partial T} + x_2 \frac{\partial \ln \gamma_2}{\partial T} \right)$$
$$= RT^2 x_1 x_2 \left(\frac{\partial \Lambda_{12}/\partial T}{x_1 + x_2 \Lambda_{12}} + \frac{\partial \Lambda_{12}/\partial T}{x_2 + x_1 \Lambda_{21}} \right) \qquad \text{(B.4)}$$

Assumes that the λ_{ij} are constant, so that

$$\frac{\partial \Lambda_{ij}}{\partial T} = \Lambda_{ij} \frac{\partial\left(-\lambda_{ij}/RT\right)}{\partial T} \qquad \text{and} \qquad \frac{\partial\left(-\lambda_{ij}/RT\right)}{\partial T} = \frac{\lambda_{ij}}{RT^2}$$

therefore,

$$\frac{\partial \Lambda_{ij}}{\partial T} = \frac{\Lambda_{ij}\lambda_{ij}}{RT^2} \tag{B.5}$$

Substitutes Eq. B.5 into Eq. B.4 gives

$$H^E = x_1 x_2 \left(\frac{\lambda_{12}\Lambda_{12}}{x_1 + x_2\Lambda_{12}} + \frac{\lambda_{21}\Lambda_{21}}{x_2 + x_1\Lambda_{21}} \right) \tag{B.6}$$

In term of the UNIQUAC equation, it would be convenient to find the relations of the excess enthalpy to interaction parameters by differentiate the gibbs energy with respect to temperature. The following expressions for a binary mixture are required.

$$H^E = -RT^2 \left[\frac{\partial\left(G^E/RT\right)}{\partial T} \right]_{P,x_i} \tag{B.7}$$

and the gibbs energy of the UNIQUAC model are rewritten

$$G^E/RT = \left(G^E_{con}/RT\right) + \left(G^E_{res}/RT\right) \tag{B.8}$$

where

$$\left.\begin{aligned} G^E_{con}/RT &= x_1\left[\ln\left(\frac{\phi_1}{x_1}\right) + \frac{1}{2}q_1 z \ln\left(\frac{\theta_1}{\phi_1}\right)\right] + x_2\left[\ln\left(\frac{\phi_2}{x_2}\right) + \frac{1}{2}q_2 z \ln\left(\frac{\theta_2}{\phi_2}\right)\right] \\ G^E_{res}/RT &= -x_1 q_1' \ln\left(\theta_1' + \theta_2'\tau_{21}\right) - x_2 q_2' \ln\left(\theta_1'\tau_{12} + \theta_2'\right) \end{aligned}\right\} \tag{B.9}$$

$z = 10$, $\phi_i = \dfrac{x_i r_i}{x_1 r_1 + x_2 r_2}$, $\theta_i = \dfrac{x_i q_i}{x_1 q_1 + x_2 q_2}$, $\theta_i' = \theta_i$, and $\tau_{ij} = \exp\left(-\dfrac{u_{ij}}{RT}\right) = \exp\left(-\dfrac{a_{ij}}{T}\right)$

The derivatives are

$$\frac{\partial\left(G_{con}^{E}/RT\right)}{\partial T}=0 \tag{B.10}$$

$$\frac{\partial\left(G_{res}^{E}/RT\right)}{\partial T}=-\frac{x_1 q_1^{'}\theta_2^{'}}{\theta_1^{'}+\theta_2^{'}\tau_{21}}\frac{\partial\tau_{21}}{\partial T}-\frac{x_2 q_2^{'}\theta_1^{'}}{\theta_2^{'}+\theta_1^{'}\tau_{12}}\frac{\partial\tau_{12}}{\partial T} \tag{B.11}$$

Assumes that the a_{ij} are constant, therefore

$$\frac{\partial\tau_{ij}}{\partial T}=\frac{\tau_{ij}a_{ij}}{T^2} \tag{B.12}$$

Substitutes Eq. B.10 - B.12 into Eq. B.7 gives

$$\begin{aligned}H^{E}&=-RT^2\left[\frac{\partial\left(G_{con}^{E}/RT\right)}{\partial T}+\frac{\partial\left(G_{res}^{E}/RT\right)}{\partial T}\right]_{P,x_i}\\&=-RT^2\left(0-\frac{x_1 q_1^{'}\theta_2^{'}}{\theta_1^{'}+\theta_2^{'}\tau_{21}}\frac{\partial\tau_{21}}{\partial T}-\frac{x_2 q_2^{'}\theta_1^{'}}{\theta_2^{'}+\theta_1^{'}\tau_{12}}\frac{\partial\tau_{12}}{\partial T}\right)\\&=R\left[\frac{q_1^{'}x_1}{\theta_1^{'}+\theta_2^{'}\tau_{21}}\left(\theta_2^{'}\tau_{21}a_{21}\right)+\frac{q_2^{'}x_2}{\theta_1^{'}\tau_{12}+\theta_2^{'}}\left(\theta_1^{'}\tau_{12}a_{12}\right)\right]\end{aligned} \tag{B.13}$$

Moreover, the complex expressions for excess enthalpy are reported in Table B.1 when assumes the parameters are dependent on temperature.

Table B.1. Excess enthalpy with the activity coefficient models

Equation	Expression

Wilson: $$H^E = RT^2 \sum_{i=1}^{m} x_i \left(\frac{\sum_{j=1}^{m} x_j \frac{d\Lambda_{ij}}{dT}}{\sum_{j}^{m} x_j \Lambda_{ij}} + \sum_{k=1}^{m} x_k \left[\frac{\frac{d\Lambda_{ki}}{dT} \sum_{j=1}^{m} x_j \Lambda_{kj} - \Lambda_{ki} \sum_{j=1}^{m} x_j \frac{d\Lambda_{kj}}{dT}}{\left(\sum_{j=1}^{m} x_j \Lambda_{kj} \right)^2} \right] \right) \quad (2.43)$$

where $$\Lambda_{ji} = \exp\left(-\frac{\lambda_{ji}^0 + \lambda_{ji}^1 / T}{RT} \right) \text{ and } \frac{d\Lambda_{ji}}{dT} = \frac{\Lambda_{ji} \left(\lambda_{ji}^0 + 2\lambda_{ji}^1 / T \right)}{RT^2}$$

NRTL: $$H^E = \sum_{i=1}^{m} \frac{x_i}{\sum_{k=1}^{m} x_k G_{ki}} \sum_{j=1}^{m} x_j G_{ji} g_{ji}^0 \left(1 - \alpha_{ij} \left(\tau_{ji} - \frac{\sum_{k=1}^{m} \tau_{ki} G_{ki} x_k}{\sum_{k=1}^{m} G_{ki} x_k} \right) \right) \quad (2.44)$$

where $$\tau_{ji} = \exp\left(-\frac{g_{ji}^0 + g_{ji}^1 T}{RT} \right)$$

UNIQUAC: $$H^E = R \sum_{i=1}^{m} \left[\frac{q_i' x_i}{\sum_{j=1}^{m} \theta_i' \tau_{ji}} \left(\sum_{j=1}^{m} \theta_j' \tau_{ji} \left(a_{ji}^0 + 2a_{ji}^1 / T \right) \right) \right] \quad (2.45)$$

where $$\tau_{ji} = \exp\left(-\frac{a_{ji}^0 + a_{ji}^1 / T}{T} \right)$$

APPENDIX C

LINEARIZATION OF THE OBJECTIVE FUNCTION

Because the objective function is not linear in the parameters, $\{\theta_j\}$, an iterative Newton Raphson solution of linearized equations is required to determine the best values of the $\{\theta_j\}$ which used the Taylor series expansion through first order.

$\{\theta_j\}$ is the difference of parameter from the true value of the parameter. The objective function, S, can be expressed explicitly as a function of the parameter change, $\{\delta\theta_j\}$.

$$S = \sum_{i=1}^{n}\left[f_i^r + \sum_{j=1}^{m}\left[\frac{\partial f_i^r}{\partial \theta_j}\delta\theta_j\right]\right]^2 \qquad \text{(C.1)}$$

Necessary conditions for the objective function S to be a minimum require that the derivatives of S with respect to the parameter changes are zero.

$$\frac{\partial S}{\partial(\delta\theta_k)} = \sum_{i=1}^{n}\left[f_i^r + \sum_{j=1}^{m}\left[\frac{\partial f_i^r}{\partial \theta_j}\delta\theta_j\right]\frac{\partial f_i^r}{\partial \theta_k}\right] = 0 \qquad \text{(C.2)}$$

This yields a set of m simultaneous equations with the following matrix form.

$$AA^r \Delta\Theta^r = BB^r \qquad \text{(C.3)}$$

where

$$AA^r = \begin{pmatrix} \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_1}\right)\left(\frac{\partial f_i^r}{\partial \theta_1}\right) & \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_1}\right)\left(\frac{\partial f_i^r}{\partial \theta_2}\right) & \cdots & \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_1}\right)\left(\frac{\partial f_i^r}{\partial \theta_m}\right) \\ \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_2}\right)\left(\frac{\partial f_i^r}{\partial \theta 1}\right) & \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_2}\right)\left(\frac{\partial f_i^r}{\partial \theta_2}\right) & \cdots & \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_2}\right)\left(\frac{\partial f_i^r}{\partial \theta_m}\right) \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_m}\right)\left(\frac{\partial f_i^r}{\partial \theta_1}\right) & \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_m}\right)\left(\frac{\partial f_i^r}{\partial \theta_2}\right) & \cdots & \sum_{i=1}^{n}\left(\frac{\partial f_i^r}{\partial \theta_m}\right)\left(\frac{\partial f_i^r}{\partial \theta_m}\right) \end{pmatrix}$$

$$\Delta\left(\Theta^r\right)^T = \left(\delta\theta_1^r \quad \delta\theta_2^r \quad \cdots \quad \delta\theta_m^r\right)$$

and

$$BB^r = -\begin{pmatrix} \sum_{i=1}^{n} f_i^r \left[\frac{\partial f_i^r}{\partial \theta_1}\right] \\ \vdots \\ \sum_{i=1}^{n} f_i^r \left[\frac{\partial f_i^r}{\partial \theta_m}\right] \end{pmatrix}$$

$\delta\Theta$ was calculated until all of $\Delta\theta_j^{r+1}/\theta_j^r$ is less than the certain criteria, ε.

C.1 Derivatives of the excess properties with respect to the Wilson parameters

The binary parameters of the Wilson model can be solved by means of Newton-Raphson method that the partial derivatives of the excess properties with respect to the unknown parameters are required.

C.1.1 The excess Gibbs free energy property

The Wilson parameters for the binary systems are found by using the excess Gibbs energy (G^E) relation:

$$\frac{G^E}{RT} = \left(x_1 \ln\gamma_1 + x_2 \ln\gamma_2\right) \qquad \text{(C.4)}$$

The Wilson equations are written in the forms,

$$F_k = \left(x_1 \ln\gamma_1 + x_2 \ln\gamma_2\right)_k - \left(-x_1 \ln\left(x_1 + \Lambda_{12}x_2\right) - x_2 \ln\left(x_2 + \Lambda_{21}x_1\right)\right)_k \qquad \text{(C.5)}$$

The derivatives of F_k are

$$F1_k = \frac{\partial F_k}{\partial \Lambda_{12}} = \left(\frac{x_1 x_2}{x_1 + \Lambda_{12}x_2}\frac{\partial \Lambda_{12}}{\partial \Lambda_{12}} - \frac{x_1 x_2}{x_2 + \Lambda_{21}x_1}\frac{\partial \Lambda_{21}}{\partial \Lambda_{12}}\right)_k \qquad \text{(C.6)}$$

$$F1_k = \frac{\partial F_k}{\partial \Lambda_{12}} = \left(\frac{x_1 x_2}{x_1 + \Lambda_{12} x_2} \right)_k \tag{C.7}$$

$$F2_k = \frac{\partial F_k}{\partial \Lambda_{21}} = \left(\frac{x_1 x_2}{x_1 + \Lambda_{12} x_2} \frac{\partial \Lambda_{12}}{\partial \Lambda_{21}} - \frac{x_1 x_2}{x_2 + \Lambda_{21} x_1} \frac{\partial \Lambda_{21}}{\partial \Lambda_{21}} \right)_k \tag{C.8}$$

$$F2_k = \frac{\partial F_k}{\partial \Lambda_{21}} = \left(\frac{x_1 x_2}{x_2 + \Lambda_{21} x_1} \right)_k \tag{C.9}$$

C.1.2 The excess enthalpy property

Relation of excess enthalpy to the Wilson parameters is rewritten

$$F_k = \left(H^E_{exp} - x_1 x_2 \left[\frac{\lambda_{12} \Lambda_{12}}{x_1 + \Lambda_{12} x_2} + \frac{\lambda_{21} \Lambda_{21}}{x_2 + \Lambda_{21} x_1} \right] \right)_k \tag{C.10}$$

The derivatives are

$$F1_k = \frac{\partial F_k}{\partial \lambda_{12}} = \left(-x_1 x_2 \left[\frac{\partial}{\partial \lambda_{12}} \left(\frac{\lambda_{12} \Lambda_{12}}{x_1 + \Lambda_{12} x_2} \right) + \frac{\partial}{\partial \lambda_{12}} \left(\frac{\lambda_{21} \Lambda_{21}}{x_2 + \Lambda_{21} x_1} \right) \right] \right)_k \tag{C.11}$$

$$F2_k = \frac{\partial F_k}{\partial \lambda_{21}} = \left(-x_1 x_2 \left[\frac{\partial}{\partial \lambda_{21}} \left(\frac{\lambda_{12} \Lambda_{12}}{x_1 + \Lambda_{12} x_2} \right) + \frac{\partial}{\partial \lambda_{21}} \left(\frac{\lambda_{21} \Lambda_{21}}{x_2 + \Lambda_{21} x_1} \right) \right] \right)_k \tag{C.12}$$

and the need expressions are required

$$\begin{aligned}
\frac{\partial}{\partial \lambda_{ij}} \left(\frac{\lambda_{ij} \Lambda_{ij}}{x_i + \Lambda_{ij} x_j} \right) &= \frac{\left(x_i + \Lambda_{ij} x_j \right) \frac{\partial \left(\lambda_{ij} \Lambda_{ij} \right)}{\partial \lambda_{ij}} - \lambda_{ij} \Lambda_{ij} \frac{\partial \left(x_i + \Lambda_{ij} x_j \right)}{\partial \lambda_{ij}}}{\left(x_i + \Lambda_{ij} x_j \right)^2} \\
&= \frac{1}{\left(x_i + \Lambda_{ij} x_j \right)} \left[\left(\lambda_{ij} \frac{\partial \Lambda_{ij}}{\partial \lambda_{ij}} + \Lambda_{ij} \frac{\partial \lambda_{ij}}{\partial \lambda_{ij}} \right) - \frac{\lambda_{ij} \Lambda_{ij}}{\left(x_i + \Lambda_{ij} x_j \right)} \left(\frac{x_j \partial \Lambda_{ij}}{\partial \lambda_{ij}} \right) \right] \\
&= \frac{1}{\left(x_i + \Lambda_{ij} x_j \right)} \left[\Lambda_{ij} + \frac{\partial \Lambda_{ij}}{\partial \lambda_{ij}} \left(\lambda_{ij} - \frac{\lambda_{ij} \Lambda_{ij} x_j}{\left(x_i + \Lambda_{ij} x_j \right)} \right) \right] \\
&= \frac{1}{\left(x_i + \Lambda_{ij} x_j \right)} \left[\Lambda_{ij} - \frac{\Lambda_{ij}}{RT} \left(\frac{\lambda_{ij} x_i}{\left(x_i + \Lambda_{ij} x_j \right)} \right) \right] \\
&= \frac{\Lambda_{ij}}{\left(x_i + \Lambda_{ij} x_j \right)} \left[1 - \frac{1}{RT} \left(\frac{\lambda_{ij} x_i}{\left(x_i + \Lambda_{ij} x_j \right)} \right) \right]
\end{aligned} \tag{C.13}$$

$$\frac{\partial}{\partial \lambda_{ji}} \left(\frac{\lambda_{ij} \Lambda_{ij}}{x_i + \Lambda_{ij} x_j} \right) = 0 \tag{C.14}$$

Therefore, Eqs C.12 - C.13 are rewritten

$$F1_k = \frac{\partial F_k}{\partial \lambda_{12}} = \left(\frac{x_1 x_2 \Lambda_{12}}{x_1 + \Lambda_{12} x_2} \left[1 - \frac{\lambda_{12} x_1}{RT(x_1 + \Lambda_{12} x_2)} \right] \right)_k \quad \text{(C.15)}$$

$$F2_k = \frac{\partial F_k}{\partial \lambda_{21}} = \left(\frac{x_1 x_2 \Lambda_{21}}{x_2 + \Lambda_{21} x_1} \left[1 - \frac{\lambda_{21} x_2}{RT(x_2 + \Lambda_{21} x_1)} \right] \right)_k \quad \text{(C.16)}$$

C.2 Derivatives of the excess properties with respect to the UNIQUAC parameters

Similarly, the UNIQUAC parameters are determined by differentiated the excess properties respect to the binary parameters as shown below.

C.2.1 The excess Gibbs free energy property

For a binary system, the UNIQUAC model gives the excess Gibbs free energy as

$$F_k = \left((x_1 \ln \gamma_1 + x_2 \ln \gamma_2) - \frac{1}{RT} \left(G^E_{con} + G^E_{res} \right) \right)_k \quad \text{(C.17)}$$

where

$$\left(\frac{G^E_{con}}{RT} \right)_k = \left(x_1 \ln \left(\frac{\phi_1}{x_1} \right) + x_2 \ln \left(\frac{\phi_2}{x_2} \right) + 5 \left(q_1 x_1 \ln \left(\frac{\phi_1}{x_1} \right) + q_2 x_2 \ln \left(\frac{\phi_2}{x_2} \right) \right) \right)_k \quad \text{(C.18)}$$

$$\left(\frac{G^E_{res}}{RT} \right)_k = \left(- q_1 x_1 \ln(\theta_1 + \theta_2 \tau_{21}) - q_2 x_2 \ln(\theta_2 + \theta_1 \tau_{12}) \right)_k \quad \text{(C.19)}$$

Differentiates Eqs. C.18 - C.19 with respect to binary parameters, yields

$$\frac{\partial \left(G^E_{con} / RT \right)_k}{\partial \tau_{ij}} = 0 \quad \text{(C.20)}$$

$$\frac{\partial \left(G^E_{res} / RT \right)_k}{\partial \tau_{ij}} = \left(- \frac{q_1 x_1 \theta_2}{(\theta_1 + \theta_2 \tau_{21})} \frac{\partial \tau_{21}}{\partial \tau_{ij}} - \frac{q_2 x_2 \theta_1}{(\theta_2 + \theta_1 \tau_{12})} \frac{\partial \tau_{12}}{\partial \tau_{ij}} \right)_k \quad \text{(C.21)}$$

Therefore, derivatives of F_k are

$$F1_k = \frac{\partial F_k}{\partial \tau_{12}} = \left(\frac{q_2 x_2 \theta_1}{(\theta_2 + \theta_1 \tau_{12})} \right)_k \quad \text{(C.22)}$$

$$F2_k = \frac{\partial F_k}{\partial a_{21}} = \left(\frac{q_1 x_1 \theta_2 \tau_{21}}{(\theta_1 + \theta_2 \tau_{21})} \right)_k \quad \text{(C.23)}$$

C.2.2 The excess enthalpy property

Relation of excess enthalpy to the UNIQUAC parameters is rewritten

$$F_k = \left(H^E_{exp} - R\left[\frac{q_1 x_1}{\theta_1 + \theta_2 \tau_{21}} (\theta_2 \tau_{21} a_{21}) + \frac{q_2 x_2}{\theta_2 + \theta_1 \tau_{12}} (\theta_1 \tau_{12} a_{12}) \right] \right)_k \quad \text{(C.24)}$$

The derivatives are

$$F1_k = \frac{\partial F_k}{\partial a_{12}} = \left(-R \frac{\partial}{\partial a_{12}} \left[\frac{q_1 x_1}{\theta_1 + \theta_2 \tau_{21}} (\theta_2 \tau_{21} a_{21}) + \frac{q_2 x_2}{\theta_2 + \theta_1 \tau_{12}} (\theta_1 \tau_{12} a_{12}) \right] \right)_k \quad \text{(C.25)}$$

$$F2_k = \frac{\partial F_k}{\partial a_{21}} = \left(-R \frac{\partial}{\partial a_{21}} \left[\frac{q_1 x_1}{\theta_1 + \theta_2 \tau_{21}} (\theta_2 \tau_{21} a_{21}) + \frac{q_2 x_2}{\theta_2 + \theta_1 \tau_{12}} (\theta_1 \tau_{12} a_{12}) \right] \right)_k \quad \text{(C.26)}$$

and

$$\begin{aligned}
&\frac{\partial}{\partial a_{ij}} \left[\frac{q_i x_i}{\theta_i + \theta_j \tau_{ji}} (\theta_j \tau_{ji} a_{ji}) + \frac{q_j x_j}{\theta_j + \theta_i \tau_{ij}} (\theta_i \tau_{ij} a_{ij}) \right] \\
&= 0 + q_j x_j \left[\frac{(\theta_j + \theta_i \tau_{ij}) \theta_i \frac{\partial (\tau_{ij} a_{ij})}{\partial a_{ij}} - (\theta_i \tau_{ij} a_{ij}) \frac{\partial (\theta_j + \theta_i \tau_{ij})}{\partial a_{ij}}}{(\theta_j + \theta_i \tau_{ij})^2} \right] \\
&= \frac{q_j x_j}{(\theta_j + \theta_i \tau_{ij})^2} \left[(\theta_j + \theta_i \tau_{ij}) \theta_i \left(\tau_{ij} + a_{ij} \frac{\partial \tau_{ij}}{\partial a_{ij}} \right) - \theta_i^2 \tau_{ij} a_{ij} \frac{\partial \tau_{ij}}{\partial a_{ij}} \right] \\
&= \frac{q_j x_j \theta_i \tau_{ij}}{(\theta_j + \theta_i \tau_{ij})^2} \left[\theta_j - \frac{\theta_j a_{ij}}{T} + \theta_i \tau_{ij} \right]
\end{aligned} \quad \text{(C.27)}$$

where $\frac{\partial \tau_{ij}}{\partial a_{ij}} = -\frac{\tau_{ij}}{T}$ and $\frac{\partial \tau_{ij}}{\partial a_{ji}} = 0$ (C.28)

So that

$$F1_k = \frac{\partial F_k}{\partial a_{12}} = \left(-R\left[\frac{q_2 x_2 \theta_1 \tau_{12}}{(\theta_2 + \theta_1 \tau_{12})^2} \left(\theta_1 \tau_{12} + \theta_2 - \frac{\theta_2 a_{12}}{T} \right) \right] \right)_k \qquad \text{(C.29)}$$

$$F2_k = \frac{\partial F_k}{\partial a_{21}} = \left(-R\left[\frac{q_1 x_1 \theta_2 \tau_{21}}{(\theta_1 + \theta_2 \tau_{21})^2} \left(\theta_2 \tau_{21} + \theta_1 - \frac{\theta_1 a_{21}}{T} \right) \right] \right)_k \qquad \text{(C.30)}$$

APPENDIX D

SUBROUTINES

The following discussion of the subroutines is not intended to direct the approach that the user must take, but is merely to give him an idea of what is to be calculated at each stage of the overall solution to the specific problem.

D.1 Func WilsonG

Func WilsonG determines the Wilson parameters from vapor-liquid equilibrium data. The calculation procedure may be briefly outlined as follows:

1. For given pressures, composition, and activity coefficient values, and the assumed values of parameters calculate excess gibbs energy by means of Equations (2.13) and (2.14) which expressed in terms of the Wilson parameters.
2. Calculate derivatives of equation (2.13) with respect to parameters.
3. Substitute values obtained from step 1 and 2 into Newton Raphson 's equation and solve simultaneously for another set of roots of parameters.
4. Substitute new parameters from step 3 into Equation (2.13) and calculate new excess gibbs energy and compare it with the experimental data

An iteration loop in Newton method is thus built up until the change of value of parameters is less than the specified tolerance. A schematic diagram outlining the evaluation is represented in Figure D.1 (see p.114).

D.2 Func UNIQG

Func UNIQG calculates the UNIQUAC parameters from VLE data. The calculation procedure is similar to Func WilsonG.

For UNIQUAC equation, substitute Equation (2.21) into Equation (2.13) and repeat the steps 1-4 finding the new values of UNIQUAC parameters. A schematic block diagram of subroutine Func UNIQP is represented in Figure D.2 (see p.115).

D.3 Other subroutines using VLE data

Func DGW, Func Gcal, Func Sumf and Func AADP could be employed to determine the parameters of the Wilson equation. For UNIQUAC model, substitute Func DGU into Func DGW to determine the parameters. Figures D.3 through D.7 illustrate the block diagram of these subroutines, respectively (see p.116 - p.120).

D.4 Func Wilson

Func Wilson determines the Wilson parameters from heat of mixing data. The calculation procedure may be briefly outlined as follows:

1. For a given value of excess enthalpy, and the assumed values of parameters calculate excess enthalpy by means of Equation (2.33) which expressed in terms of the Wilson parameters.
2. Calculate derivatives of equation (2.33) with respect to parameters.
3. Substitute values obtained from step 1 and 2 into Newton Raphson 's equation and solve simultaneously for another set of roots of parameters.
4. Substitute new parameters from step 3 into Equation (2.33) and calculate new excess enthalpy and compare it with the experimental data

An iteration loop in Newton method is thus built up until the change of value of parameters is less than the specified tolerance. A schematic diagram outlining the evaluation is given in Figure D.8 (see p.121).

D.4 Func UNIQ

Func UNIQ calculates the UNIQUAC parameters from heat of mixing data. The calculation procedure is similar to Func Wilson.

For UNIQUAC equation, substitute Equation (2.34) into Equation (2.33) and repeat the steps 1-4 finding the new values of UNIQUAC parameters. A schematic block diagram of subroutine Func UNIQ is given in Figure D.9 (see p.122).

D.3 Other subroutines using H^E data

Func DHW or Func DHU, with Func Heatcal, Func Sumf (see p.118) and Func AAD could be employed to determine the parameters of given excess enthalpy in binary mixture. Figures D.10 through D.13 illustrate the block diagram of these subroutines, respectively (see p.123 - p.126).

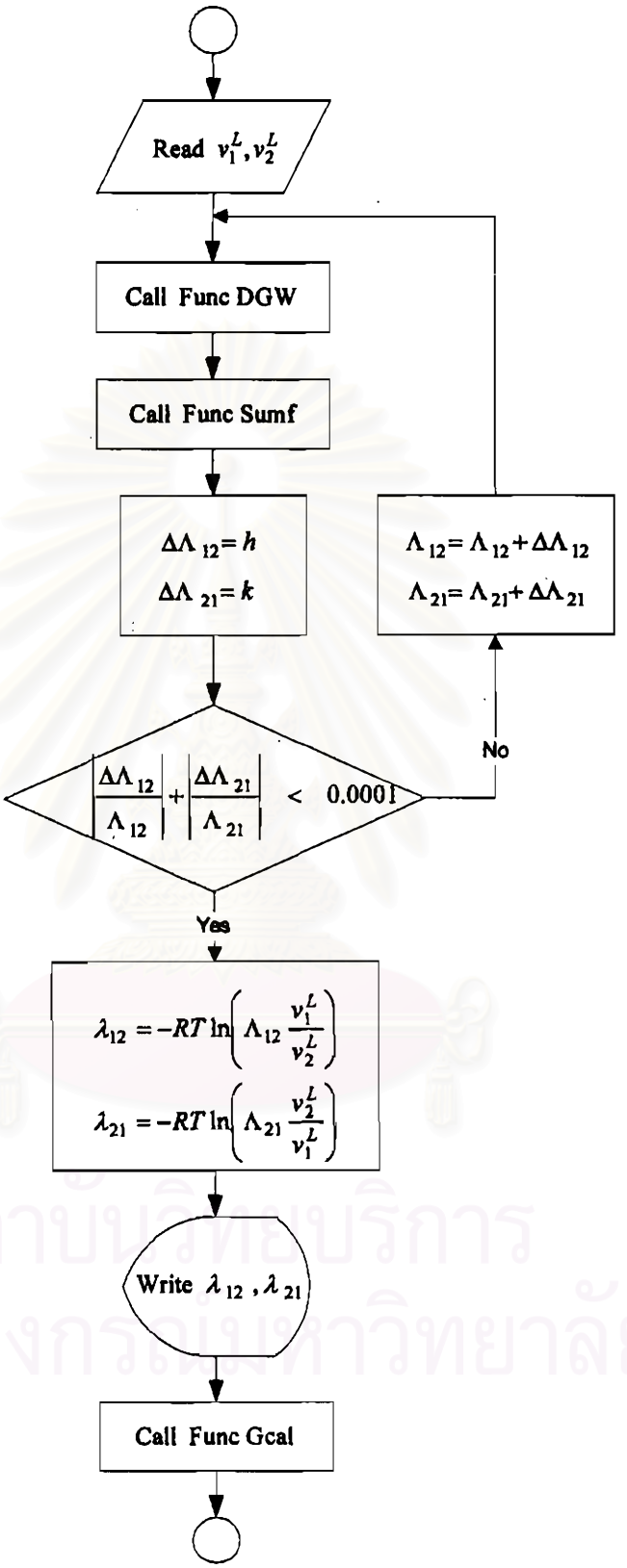

Figure D.1 A schematic diagram of subroutine Func WilsonG.

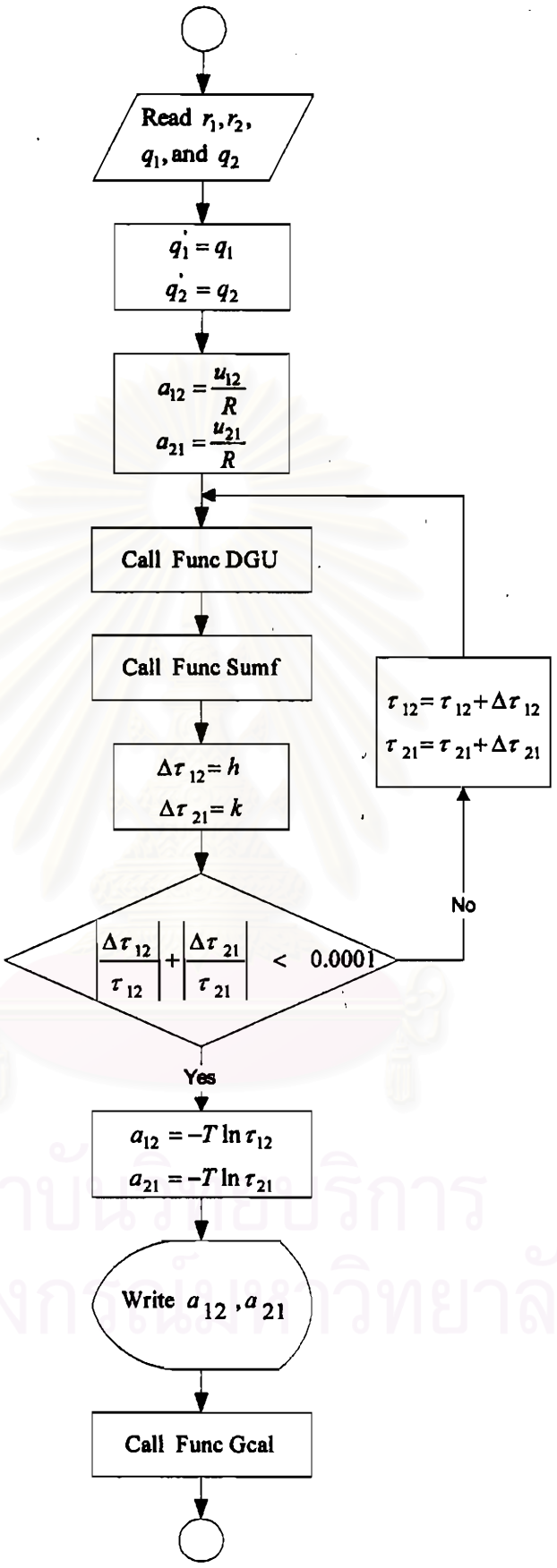

Figure D.2 A schematic diagram of subroutine Func UNIQG.

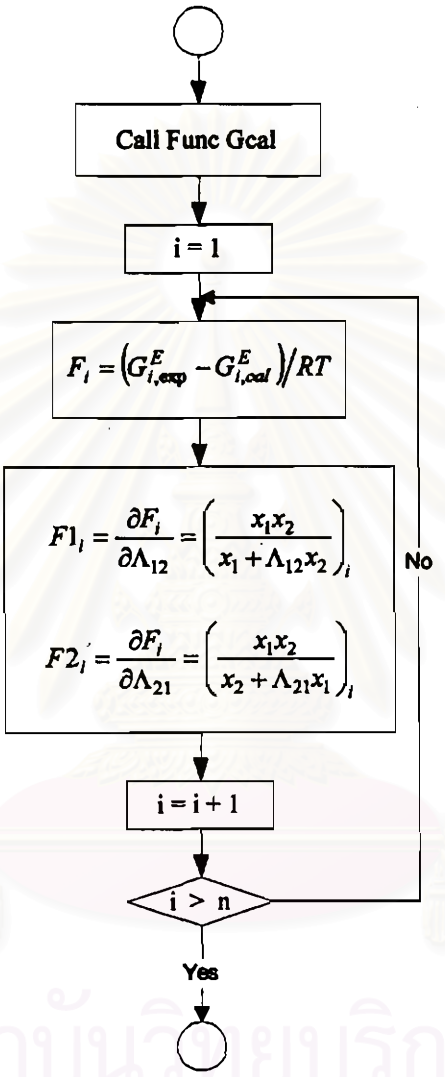

Figure D.3 A schematic diagram of subroutine Func DGW.

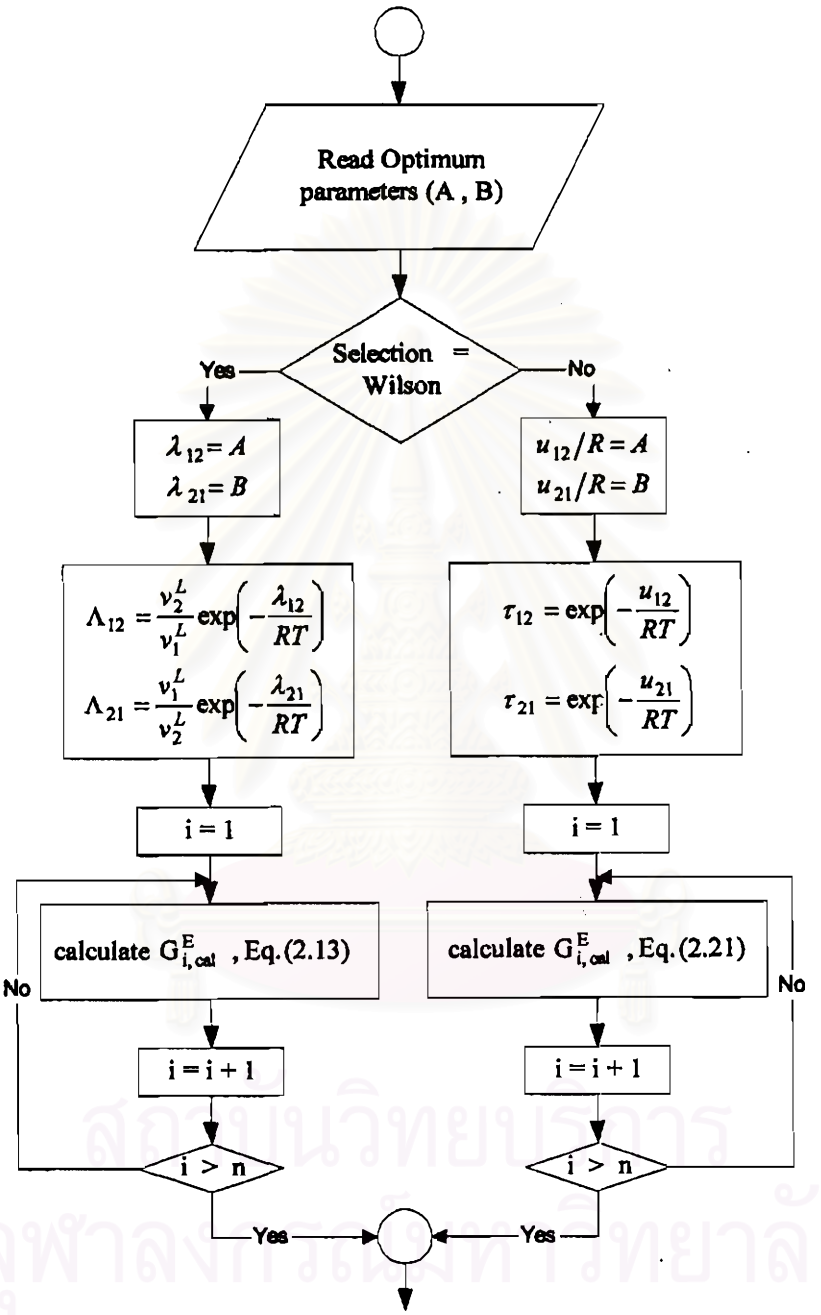

Figure D.4 A schematic diagram of subroutine Func Gcal.

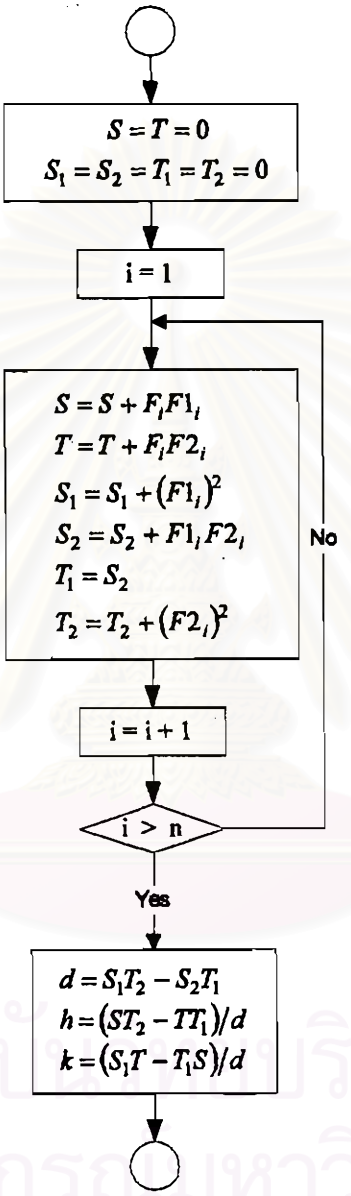

Figure D.5 A schematic diagram of subroutine Func Sumf.

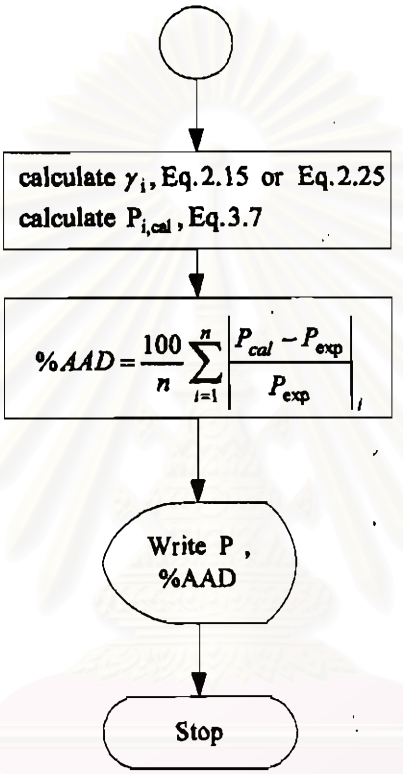

Figure D.6 A schematic diagram of subroutine Func AADP.

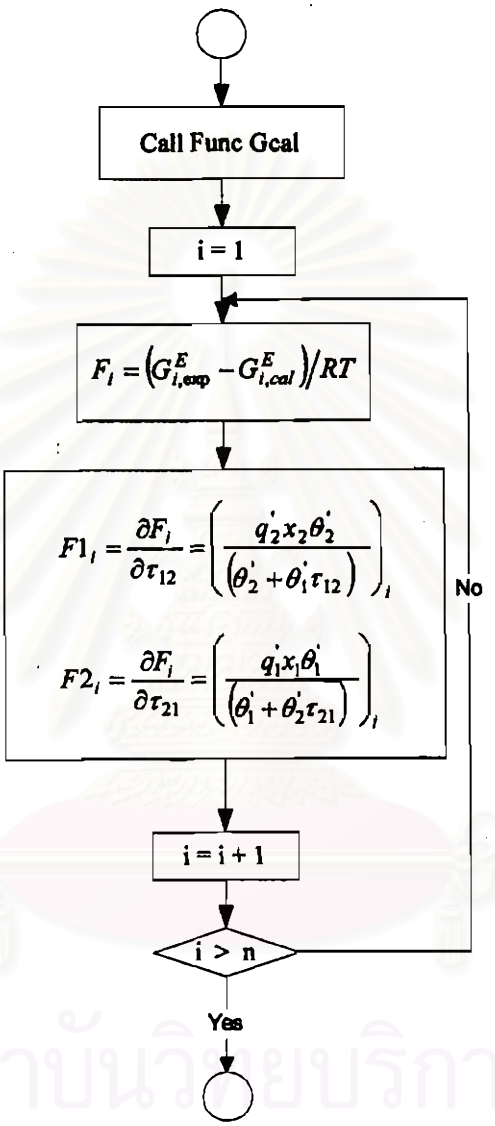

Figure D.7 A schematic diagram of subroutine Func DGU.

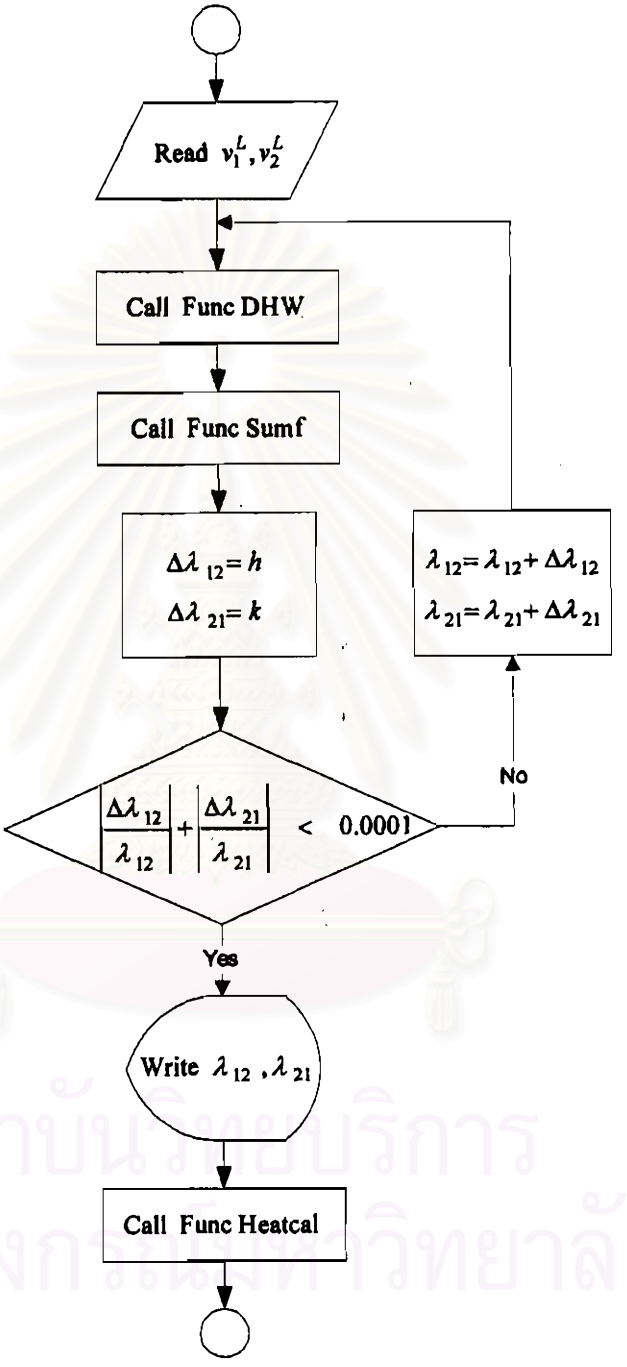

Figure D.8 A schematic diagram of subroutine Func Wilson.

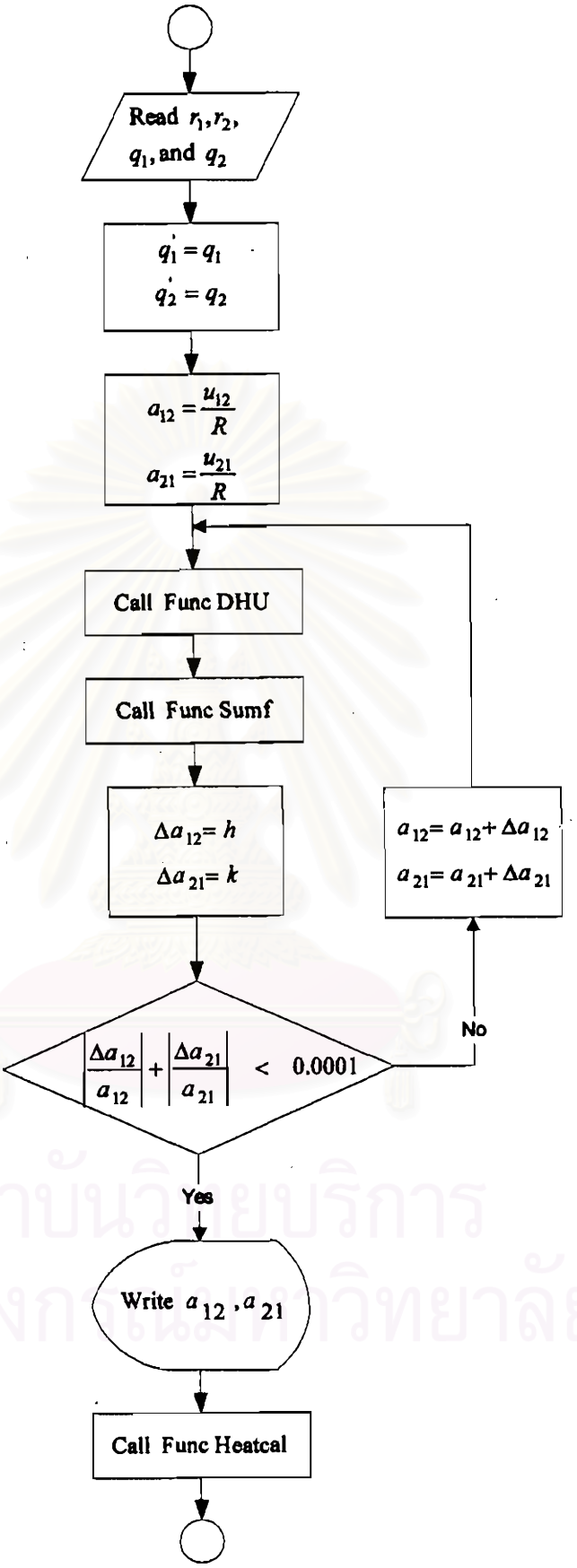

Figure D.9 A schematic diagram of subroutine Func UNIQ.

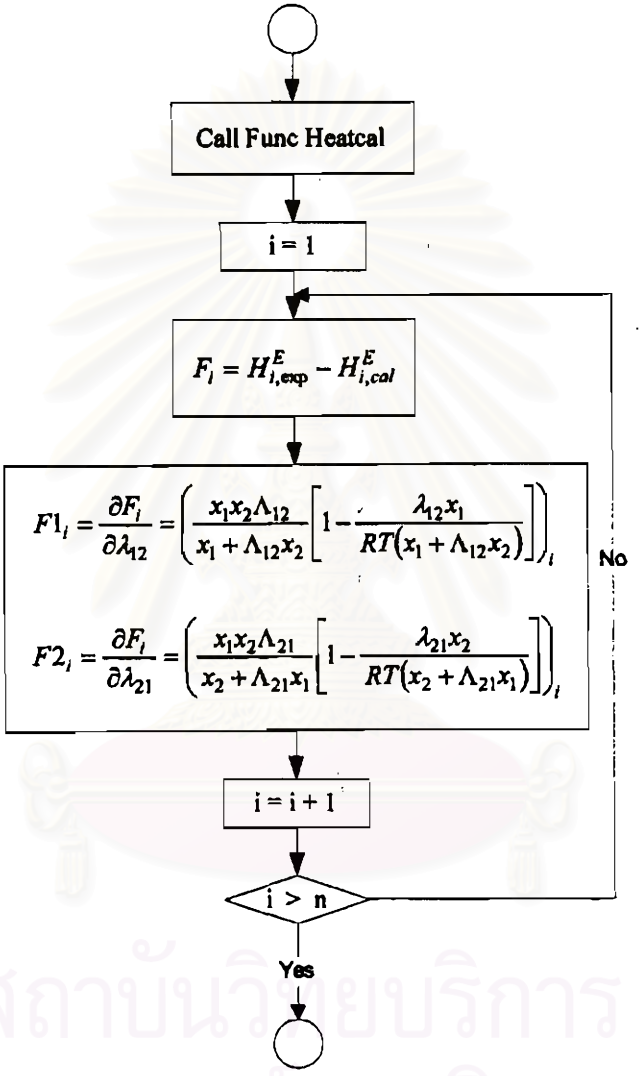

Figure D.10 A schematic diagram of subroutine Func DHW.

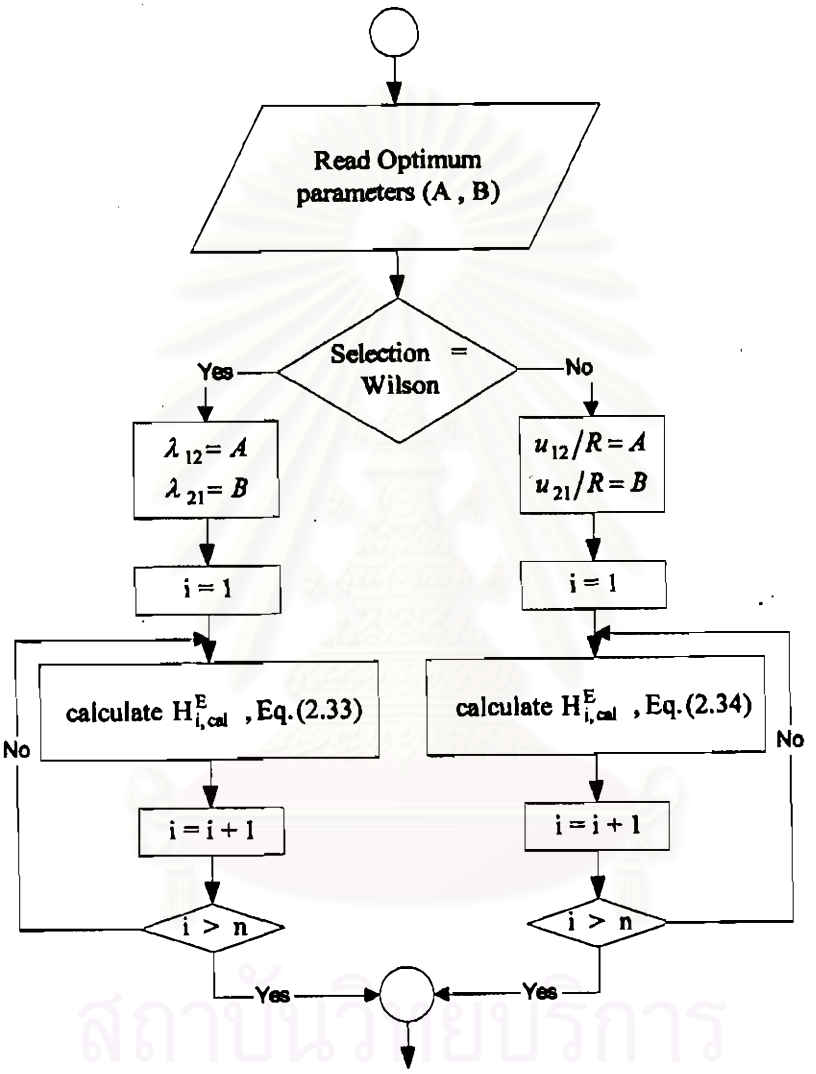

Figure D.11 A schematic diagram of subroutine Func Heatcal.

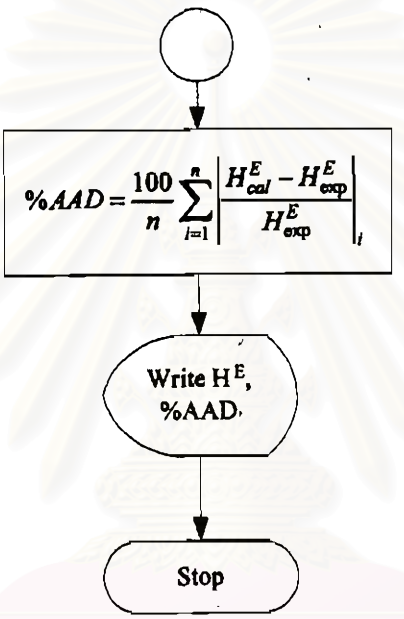

Figure D.12 A schematic diagram of subroutine Func AAD.

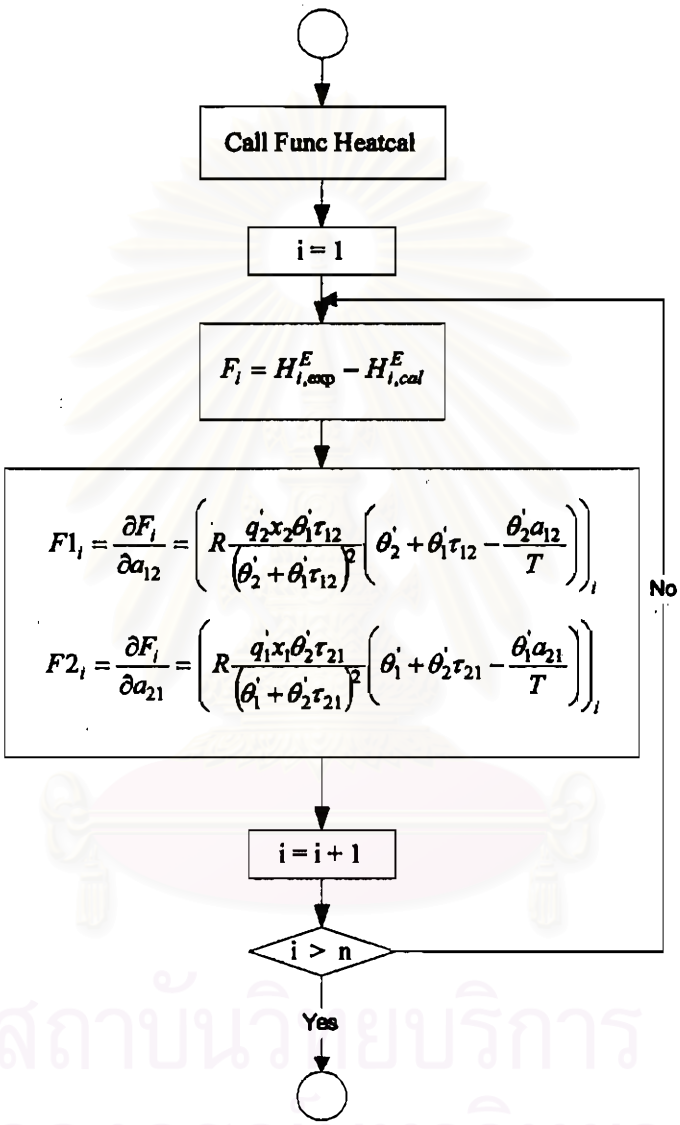

Figure D.13 A schematic diagram of subroutine Func DHU.

APPENDIX E

CALCULATED DATA

E.1 VLE data

Table E.1.1 P (kPa) of benzene (1) and cyclohexane (2) system (Kurihara et al., 1997).

	T = 323.15 K				T = 333.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0340	36.8800	36.8326	36.8308	0.0700	53.5600	53.4470	53.4439
0.0740	37.4800	37.4485	37.4468	0.0760	53.6800	53.5660	53.5618
0.1070	37.9400	37.9008	37.8977	0.1020	54.1000	54.0510	54.0475
0.1380	38.3100	38.2824	38.2797	0.1260	54.4800	54.4645	54.4609
0.1470	38.4200	38.3858	38.3832	0.1780	55.4800	55.2618	55.2488
0.2010	39.0500	38.9402	38.9383	0.2020	55.6100	55.5683	55.5657
0.2390	39.3600	39.2665	39.2653	0.2340	56.1900	55.9471	55.9450
0.2740	39.5700	39.5236	39.5230	0.2700	56.2800	56.3172	56.3159
0.2870	39.6700	39.6090	39.6086	0.3360	56.9300	56.8519	56.8517
0.3350	39.9900	39.8788	39.8792	0.3510	57.0200	56.9488	56.9488
0.3470	40.0300	39.9355	39.9360	0.3740	57.0300	57.0803	57.0806
0.3480	39.9800	39.9400	39.9405	0.4400	57.4400	57.3468	57.3477
0.3650	40.0900	40.0126	40.0133	0.4500	57.4600	57.3731	57.3741
0.4040	40.2100	40.1480	40.1491	0.4610	57.4900	57.3979	57.3989
0.4220	40.2700	40.1962	40.1974	0.4710	57.5200	57.4166	57.4176
0.4340	40.2700	40.2233	40.2247	0.4780	57.5600	57.4275	57.4286
0.4480	40.3100	40.2501	40.2515	0.4880	57.5900	57.4401	57.4412
0.4630	40.4000	40.2728	40.2743	0.4990	57.6000	57.4497	57.4509
0.4770	40.3200	40.2886	40.2901	0.5090	57.6100	57.4547	57.4558
0.4930	40.3300	40.3001	40.3017	0.5180	57.6200	57.4561	57.4572
0.4970	40.3300	40.3019	40.3035	0.5280	57.6200	57.4541	57.4553
0.5090	40.3500	40.3048	40.3064	0.5330	57.6100	57.4518	57.4530
0.5240	40.3500	40.3029	40.3045	0.5380	57.6000	57.4486	57.4498
0.5310	40.3300	40.2999	40.3015	0.5470	57.5900	57.4405	57.4416
0.5600	40.3100	40.2734	40.2749	0.5580	57.5700	57.4294	57.4306
0.5910	40.2700	40.2193	40.2207	0.6020	57.4300	57.3261	57.3269
0.6570	40.0700	40.0125	40.0133	0.6730	57.1300	57.0071	57.0073
0.6900	39.9500	39.8596	39.8600	0.7090	56.8900	56.7669	56.7666
0.7550	39.5500	39.4524	39.4517	0.7640	56.4200	56.2887	56.2875
0.7950	39.2200	39.1246	39.1232	0.7880	56.1300	56.0348	56.0330
0.8120	39.0200	38.9657	38.9639	0.8260	55.6900	55.5448	55.5424
0.8440	38.6800	38.6322	38.6297	0.8700	54.9600	54.9328	54.9298
0.8970	38.0500	37.9705	37.9675	0.8950	54.4300	54.5166	54.5134
0.9140	37.8100	37.7263	37.7232	0.9030	54.3000	54.3746	54.3714
0.9340	37.4700	37.4171	37.4142	0.9170	54.1000	54.1155	54.1124
				0.9440	53.5800	53.5757	53.5729

Table E.1.2 P (kPa) of 1-chloropentane (1) and di-n-butyl ether (2) system (Paul et al., 1986).

	T = 313.15 K				T = 323.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0774	25.5000	25.5607	25.5611	0.0831	40.7000	40.6286	40.6208
0.1209	28.5000	28.4564	28.4707	0.1416	48.6000	48.6153	48.6096
0.2242	35.3000	35.2554	35.2686	0.2652	60.9000	60.9495	60.9553
0.2877	39.2000	39.3694	39.3841	0.3509	69.3000	69.3704	69.3814
0.3549	43.5000	43.6877	43.6996	0.4291	76.8000	76.9856	76.9972
0.3978	46.4000	46.4299	46.4380	0.5480	88.0000	88.2841	88.2899
0.5515	56.1000	56.1949	56.1822	0.5890	93.3000	93.3838	93.3856
0.5678	56.9000	57.2271	57.2121	0.6220	95.4000	95.5940	95.5940
0.6810	64.2000	64.3878	64.3619	0.6552	98.7000	98.7619	98.7795
0.6964	65.2000	65.3616	65.3350	0.6952	102.7000	102.6203	102.6152
0.7793	70.4000	70.6049	70.5790	0.7789	110.7000	110.6483	110.6403
0.8225	73.1000	73.3392	73.3168	0.8443	117.0000	116.9235	116.9160
0.8985	78.1000	78.1548	78.1417	0.9042	122.7000	122.6773	122.6722
0.9307	80.1000	80.1976	80.1892	0.9474	126.6000	126.6325	126.6299
				0.9860	130.6000	130.5503	130.5497

Table E.1.3 P (kPa) of 1,2-dichloroethane (1) and di-n-butyl ether (2) system (Paul et al., 1986).

	T = 330.00 K				T = 350.00 K				T = 370.00 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0374	64.8000	64.8107	64.7534	0.0163	129.1000	129.0004	128.9849	0.0097	264.1000	263.5242	263.5185
0.0695	79.2000	79.2053	79.1192	0.0340	144.7000	144.6537	144.6261	0.0502	326.6000	324.6187	324.3012
0.1046	95.2000	94.8056	94.7075	0.0578	166.5000	165.5458	165.5091	0.0842	380.0000	375.4060	375.3917
0.1272	103.5000	104.7665	104.6702	0.1382	232.9000	234.7279	234.7092	0.1490	473.3000	470.8272	470.8420
0.2073	138.3000	139.4772	139.4360	0.3871	418.5000	418.2751	418.4443	0.2902	680.6000	671.6876	671.7941
0.3339	191.5000	192.0840	192.2129	0.5089	520.6000	519.2415	519.3936	0.3475	758.1000	750.0931	750.2176
0.4304	218.6000	229.9103	230.1539	0.5908	577.6000	575.5067	575.5593	0.3999	828.5000	820.0727	820.1921
0.4817	248.0000	249.0845	249.3580	0.7080	653.9000	648.9263	648.7752	0.4571	902.3000	894.4942	894.5794
0.5424	267.4000	270.8498	271.1171	0.7754	693.1000	688.8438	688.5972	0.5032	957.8000	952.9288	952.9634
0.6096	288.6000	293.7056	293.9058	0.8334	725.3000	722.3084	722.0345	0.5690	1040.3000	1033.9011	1033.8312
0.7350	329.2000	332.7541	332.6920	0.8843	754.2000	751.4488	751.2109	0.6388	1119.2000	1114.1283	1113.9256
0.8277	355.6000	358.8957	358.6529	0.9197	773.8000	771.8799	771.7083	0.7851	1282.8000	1280.9405	1280.5139
0.9060	375.6000	380.0033	379.7716	0.9337	783.0000	780.0602	779.9175	0.8555	1357.5000	1356.9000	1356.5087
0.9700	396.9000	397.7626	397.7102	0.9692	803.0000	801.2233	801.1650	0.9259	1432.5000	1432.7332	1432.5081
				0.9788	808.1000	807.0839	807.0469	0.9899	1505.2000	1503.7258	1503.7031
				0.9896	815.7000	813.7657	813.7497				

Table E.1.4 P (kPa) of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system (Paul et al., 1986).

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0517	53.6000	54.6609	54.0279	0.0380	114.4000	112.5842	112.6062
0.1152	78.8000	77.9002	78.6389	0.0955	155.2000	153.4628	153.5144
0.1575	95.3000	93.3453	94.9776	0.1557	203.2000	197.6994	197.7815
0.3082	156.7000	151.6024	153.6224	0.2194	252.8000	246.1081	246.2198
0.3613	178.4000	173.4240	174.6882	0.2889	306.7000	300.7666	300.9056
0.4270	206.7000	201.1658	201.1935	0.3638	359.4000	353.4671	353.6226
0.4821	228.8000	224.9213	223.8582	0.4870	468.9000	466.0155	466.1482
0.5367	253.2000	248.7741	246.7371	0.5616	533.4000	530.9635	531.0234
0.5861	272.8000	270.5316	267.6110	0.5664	535.3000	535.1710	535.2242
0.6558	303.7000	301.3699	298.1247	0.6444	602.0000	603.7004	603.6014
0.7085	328.0000	323.8130	320.5550	0.7002	650.8000	652.4887	652.2312
0.7656	352.1000	349.8980	347.0107	0.7246	673.1000	673.6161	673.2788
0.8271	377.9000	376.8732	374.7325	0.7979	739.1000	735.7392	735.1675
0.8707	397.4000	395.6517	394.3717	0.8533	792.7000	780.7766	780.0823
0.9492	432.6000	429.6390	429.2781	0.8665	800.4000	791.2126	790.5146
0.9544	434.5000	431.8576	431.5533	0.8795	822.3000	801.3762	800.6873
0.9771	442.6000	441.5123	441.4077	0.9223	851.4000	834.1064	833.5583
				0.9508	870.7000	855.3342	854.9808
				0.9631	875.5000	864.7087	864.4597
				0.9776	884.1000	875.6764	875.5488
				0.9904	889.6000	885.5322	885.4935

Table E.1.5 P (kPa) of toluene (1) and 1-chlorohexane (2) system (Paul et al., 1988).

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.2877	6.6800	6.7080	6.7037	0.0389	11.9400	11.9459	11.9508
0.3200	6.9300	6.9494	6.9423	0.1029	12.8400	12.8610	12.8696
0.3891	7.3100	7.3202	7.3095	0.1647	13.7400	13.7646	13.7725
0.4230	7.6900	7.7320	7.7187	0.2308	14.7300	14.7488	14.7528
0.4578	8.0000	8.0002	7.9863	0.3046	15.8700	15.8785	15.8759
0.5248	8.5100	8.5207	8.5085	0.3707	16.8900	16.9079	16.8993
0.6070	9.1700	9.1652	9.1600	0.4388	17.9700	17.9866	17.9733
0.6979	9.9000	9.8832	9.8698	0.4783	18.5800	18.6197	18.6050
0.7969	10.6900	10.6686	10.6664	0.5129	19.1300	19.1763	19.1634
0.8698	11.4000	11.4065	11.4242	0.5900	20.4000	20.4341	20.4226
0.9600	11.9700	11.9633	11.9708	0.6739	21.7900	21.8128	21.8106
				0.7464	22.9900	23.0085	23.0170
				0.8017	23.9000	23.9199	23.9356
				0.8666	24.9800	24.9858	25.0050
				0.9288	26.0300	26.0019	26.0162
				0.9731	26.7600	26.7228	26.7286

Table E.1.6 P (kPa) of 1-chlorohexane (1) and ethylbenzene (2) system (Paul et al., 1988).

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0331	4.6400	4.6426	4.6426	0.0351	11.2500	11.2577	11.2601
0.0883	4.6300	4.6353	4.6353	0.1054	11.2500	11.2622	11.2658
0.1376	4.6200	4.6225	4.6225	0.1768	11.2400	11.2465	11.2489
0.2182	4.6100	4.6104	4.6104	0.2394	11.2400	11.2423	11.2432
0.3132	4.6000	4.5998	4.5998	0.3187	11.2400	11.2391	11.2383
0.3942	4.6000	4.5941	4.5941	0.3397	11.2400	11.2387	11.2377
0.4482	4.5900	4.5919	4.5919	0.3762	11.2400	11.2386	11.2373
0.4825	4.5900	4.5911	4.5911	0.3859	11.2400	11.2388	11.2373
0.4903	4.5900	4.5910	4.5910	0.4399	11.2400	11.2404	11.2390
0.5537	4.5900	4.5912	4.5913	0.4468	11.2400	11.2407	11.2394
0.5554	4.6000	4.5913	4.5913	0.4860	11.2400	11.2433	11.2423
0.6356	4.5900	4.5941	4.5942	0.4973	11.2400	11.2442	11.2433
0.7358	4.6000	4.6015	4.6015	0.5119	11.2500	11.2455	11.2449
0.8389	4.6100	4.6133	4.6134	0.6803	11.2500	11.2537	11.2542
0.9377	4.6300	4.6285	4.6286	0.7059	11.2800	11.2777	11.2806
0.9915	4.6400	4.6384	4.6384	0.8037	11.3100	11.3046	11.3085
				0.9029	11.3400	11.3392	11.3424
				0.9909	11.3700	11.3759	11.3763

Table E.1. 7 P (kPa) of 1-chlorhexane (1) and n-propylbenzen (2) system at 363.15 K (Paul et al., 1988).

	T = 363.15 K		
x_1	Exp	Wilson	UNIQUAC
0.0416	11.8700	11.9033	11.9063
0.1809	13.7100	13.7966	13.7969
0.2503	14.6500	14.7210	14.7187
0.3289	15.6700	15.7610	15.7575
0.4125	16.7800	16.8639	16.8611
0.4528	17.3200	17.3953	17.3935
0.4699	17.5100	17.6209	17.6195
0.5375	18.4800	18.5130	18.5136
0.6230	19.5800	19.6432	19.6462
0.7063	20.6900	20.7466	20.7512
0.7899	21.8300	21.8561	21.8606
0.8803	23.0400	23.0577	23.0610
0.9560	24.0600	24.0846	24.0860

Table E.1.8 P (kPa) of butanenitrile (1) and 2-butanol (2) system (Garriga et al., 1997).

	T = 278.15 K				T = 288.15 K				T = 293.15 K				T = 298.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.9411	0.9090	0.8958	0.8895	0.9411	1.6570	1.6544	1.6468	0.9411	2.2300	2.2100	2.2018	0.9411	2.9140	2.9205	2.9115
0.9158	0.9270	0.9170	0.9104	0.9158	1.7130	1.6956	1.6874	0.9158	2.2880	2.2678	2.2591	0.9158	3.0250	2.9988	2.9891
0.8745	0.9250	0.9432	0.9374	0.8745	1.7450	1.7495	1.7421	0.8745	2.3490	2.3448	2.3370	0.8745	3.0980	3.1047	3.0960
0.7794	0.9710	0.9766	0.9740	0.7794	1.8270	1.8270	1.8239	0.7794	2.4660	2.4600	2.4571	0.7794	3.2930	3.2691	3.2661
0.7500	0.9670	0.9819	0.9800	0.7500	1.8350	1.8414	1.8395	0.7500	2.4760	2.4826	2.4811	0.7500	3.2960	3.3028	3.3015
0.6382	0.9880	0.9889	0.9889	0.6382	1.8610	1.8691	1.8703	0.6382	2.5330	2.5307	2.5327	0.6382	3.3930	3.3798	3.3827
0.6056	0.9970	0.9882	0.9886	0.6056	1.8720	1.8711	1.8728	0.6056	2.5490	2.5361	2.5386	0.6056	3.4060	3.3903	3.3938
0.5541	0.9840	0.9854	0.9866	0.5541	1.8530	1.8701	1.8726	0.5541	2.5460	2.5385	2.5418	0.5541	3.3920	3.3983	3.4026
0.5315	1.0000	0.9836	0.9851	0.5315	1.8790	1.8683	1.8711	0.5315	2.5340	2.5375	2.5410	0.5315	3.3880	3.3988	3.4034
0.4304	0.9840	0.9714	0.9757	0.4304	1.8570	1.8502	1.8555	0.4304	2.4960	2.5184	2.5239	0.4304	3.3640	3.3809	3.3871
0.4298	0.9810	0.9713	0.9756	0.4298	1.8670	1.8501	1.8554	0.4298	2.5040	2.5182	2.5238	0.4298	3.3920	3.3807	3.3869
0.3716	0.9610	0.9606	0.9674	0.3716	1.8240	1.8321	1.8395	0.3716	2.4810	2.4961	2.5032	0.3716	3.3570	3.3548	3.3624
0.3037	0.9240	0.9439	0.9530	0.3036	1.7920	1.8019	1.8116	0.3036	2.4520	2.4570	2.4657	0.3036	3.2900	3.3071	3.3160
0.2892	0.9430	0.9393	0.9489	0.2892	1.7970	1.7938	1.8038	0.2892	2.4140	2.4464	2.4552	0.2892	3.3280	3.2939	3.3029
0.2197	0.8910	0.9106	0.9203	0.2197	1.7210	1.7426	1.7523	0.2197	2.3650	2.3788	2.3886	0.2196	3.1730	3.2093	3.2170
0.2072	0.9090	0.9038	0.9131	0.2071	1.7650	1.7304	1.7396	0.2071	2.3620	2.3628	2.3699	0.2071	3.2010	3.1895	3.1964
0.1785	0.8760	0.8852	0.8928	0.1785	1.6810	1.6981	1.7053	0.1784	2.3080	2.3205	2.3255	0.1784	3.1140	3.1367	3.1413
0.1503	0.8680	0.8621	0.8668	0.1502	1.6560	1.6582	1.6622	0.1502	2.2840	2.2691	2.2710	0.1502	3.0620	3.0728	3.0742
0.0962	0.8040	0.7960	0.7922	0.0962	1.5710	1.5488	1.5437	0.0962	2.1660	2.1316	2.1254	0.0962	2.9260	2.9034	2.8966
0.0689	0.7560	0.7454	0.7368	0.0688	1.4630	1.4675	1.4577	0.0688	2.0350	2.0330	2.0229	0.0688	2.8220	2.7833	2.7727

Table E.1.8 (continued)

	T = 303.15 K				T = 308.15 K				T = 313.15 K				T = 323.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.9412	3.8450	3.8064	3.7967	0.9413	4.9410	4.9058	4.8943	0.9413	6.3140	6.2661	6.2540	0.9414	9.9370	9.9146	9.9009
0.9158	3.9200	3.9149	3.9044	0.9158	5.0680	5.0531	5.0409	0.9160	6.4710	6.4598	6.4468	0.9161	10.2390	10.2398	10.2253
0.8747	4.1200	4.0622	4.0530	0.8748	5.2810	5.2537	5.2430	0.8749	6.7590	6.7284	6.7172	0.8754	10.7870	10.6948	10.6825
0.7795	4.2980	4.2995	4.2971	0.7796	5.6100	5.5837	5.5811	0.7796	7.1980	7.1779	7.1759	0.7798	11.5390	11.4974	11.4961
0.7500	4.3420	4.3502	4.3497	0.7500	5.6320	5.6561	5.6559	0.7502	7.2930	7.2783	7.2788	0.7505	11.7240	11.6834	11.6854
0.6383	4.4720	4.4726	4.4768	0.6383	5.8530	5.8371	5.8426	0.6384	7.5430	7.5405	7.5471	0.6387	12.2260	12.2020	12.2113
0.6056	4.5130	4.4919	4.4968	0.6056	5.8890	5.8682	5.8744	0.6058	7.6140	7.5884	7.5957	0.6060	12.3760	12.3070	12.3170
0.5541	4.5290	4.5105	4.5160	0.5542	5.9280	5.9011	5.9078	0.5542	7.6430	7.6431	7.6509	0.5544	12.4630	12.4377	12.4479
0.5315	4.5020	4.5144	4.5201	0.5315	5.9090	5.9099	5.9169	0.5316	7.6770	7.6597	7.6676	0.5318	12.5000	12.4827	12.4927
0.4304	4.5050	4.5040	4.5108	0.4304	5.9050	5.9116	5.9191	0.4304	7.6890	7.6839	7.6917	0.4305	12.5950	12.6016	12.6100
0.4298	4.4900	4.5038	4.5106	0.4298	5.9090	5.9114	5.9189	0.4298	7.6530	7.6838	7.6916	0.4299	12.6350	12.6019	12.6103
0.3716	4.4530	4.4767	4.4843	0.3716	5.8520	5.8841	5.8922	0.3717	7.6570	7.6608	7.6686	0.3717	12.5790	12.6106	12.6177
0.3035	4.4120	4.4217	4.4299	0.3035	5.8020	5.8218	5.8301	0.3038	7.5980	7.5954	7.6025	0.3038	12.5300	12.5613	12.5665
0.2893	4.3980	4.4063	4.4146	0.2893	5.7900	5.8039	5.8120	0.2893	7.5580	7.5750	7.5819	0.2893	12.5430	12.5413	12.5460
0.2196	4.2650	4.3047	4.3108	0.2196	5.6640	5.6827	5.6883	0.2198	7.4330	7.4373	7.4411	0.2198	12.3760	12.3891	12.3899
0.2073	4.2780	4.2811	4.2863	0.2073	5.6500	5.6544	5.6590	0.2073	7.4140	7.4041	7.4069	0.2073	12.3840	12.3501	12.3499
0.1784	4.1850	4.2167	4.2194	0.1783	5.5740	5.5767	5.5787	0.1786	7.3270	7.3153	7.3155	0.1786	12.3040	12.2441	12.2414
0.1504	4.1200	4.1400	4.1393	0.1504	5.4930	5.4850	5.4836	0.1504	7.1990	7.2084	7.2053	0.1504	12.1900	12.1145	12.1088
0.0961	3.9600	3.9352	3.9262	0.0961	5.2810	5.2414	5.2321	0.0963	6.9820	6.9307	6.9209	0.0963	11.8560	11.7757	11.7645
0.0689	3.8140	3.7934	3.7809	0.0689	5.1360	5.0750	5.0626	0.0689	6.8170	6.7417	6.7294	0.0689	11.6440	11.5461	11.5334

Table E.1.9 P (kPa) of 1,2-epoxybutane (1) and methanol (2) system at 298.15 K (Comelli, et al., 1996).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0270	18.7000	18.5302	18.5011	0.4960	27.7000	27.7254	27.7562
0.0470	19.6500	19.5752	19.5370	0.5290	27.8000	27.8423	27.8888
0.0660	20.5000	20.4612	20.4212	0.5710	27.9000	27.9489	27.9705
0.0870	21.2500	21.3342	21.2975	0.6380	27.9500	28.0227	28.0379
0.1060	21.9000	22.0391	22.0086	0.6970	27.9500	27.9789	27.9889
0.1320	22.7000	22.8895	22.8704	0.7480	27.7500	27.8372	27.8409
0.1690	23.7000	23.9070	23.9057	0.7910	27.6000	27.6174	27.6125
0.1930	24.3000	24.4651	24.4750	0.8400	27.3000	27.2109	27.1912
0.2490	25.4000	25.5186	25.5490	0.8900	26.7000	26.5467	26.5081
0.2990	26.1000	26.2277	26.2686	0.9310	25.8500	25.7226	25.6727
0.3610	26.7500	26.8826	26.9268	0.9580	25.0500	24.9842	24.9371
0.4280	27.3000	27.3828	27.4223	0.9830	24.3000	24.1146	24.0863

Table E.1.10 P (kPa) of 1,2-epoxybutane (1) and ethanol (2) system at 298.15 K (Comelli, et al., 1996).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0170	8.7500	8.7904	8.7729	0.6300	22.2000	22.2218	22.2242
0.0390	9.9500	9.9251	9.8943	0.6610	22.6000	22.5741	22.5630
0.0740	11.5500	11.5476	11.5113	0.7370	22.9000	22.9143	22.8921
0.1030	12.7000	12.7407	12.7099	0.7940	23.2000	23.2114	23.1823
0.1490	14.4000	14.3906	14.3787	0.8360	23.4000	23.3928	23.3611
0.1860	15.6000	15.5318	15.5386	0.8730	23.6000	23.5171	23.4844
0.2230	16.4500	16.5316	16.5567	0.9050	23.8000	23.5869	23.5544
0.2780	17.7500	17.7973	17.8443	0.9330	23.8500	23.6074	23.5770
0.3250	18.5000	18.7047	18.7630	0.9500	23.8500	23.5950	23.5675
0.3730	19.3000	19.4955	19.5578	0.9620	23.8000	23.5720	23.5478
0.4280	20.1000	20.2631	20.3213	0.9740	23.7000	23.5350	23.5158
0.4910	20.9000	20.9964	21.0413	0.9810	23.6000	23.5060	23.4906
0.5680	21.7000	21.7301	21.7517				

Table E.1.11 P (kPa) of 1,2-epoxybutane (1) and 2-propanol (2) system at 298.15 K (Comelli, et al., 1996).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0170	6.5000	6.6984	6.6797	0.4920	18.6500	18.5762	18.5981
0.0280	7.0500	7.2782	7.2518	0.5770	19.6000	19.5250	19.5257
0.0610	8.3500	8.8567	8.8216	0.6300	20.2000	20.0693	20.0587
0.0760	9.0000	9.5028	9.4691	0.6710	20.7000	20.4736	20.4563
0.0940	9.6500	10.2260	10.1989	0.7290	21.4000	21.0277	21.0044
0.1390	11.2000	11.8173	11.8073	0.7770	21.8000	21.4747	21.4498
0.1960	12.9500	13.4724	13.4893	0.8230	22.2500	21.8949	21.8707
0.2360	14.1000	14.4462	14.4760	0.8560	22.5000	22.1914	22.1691
0.2780	15.0000	15.3376	15.3798	0.8830	22.7000	22.4301	22.4102
0.3090	15.7000	15.9245	15.9708	0.9100	22.9000	22.6848	22.6477
0.3800	16.8500	17.0904	17.1347	0.9300	23.1000	22.8348	22.8207
0.4390	17.9000	17.9155	17.9499	0.9650	23.3000	23.1231	23.1149

Table E.1.12 P (kPa) of ethyl formate (1) and benzene (2) system at 323.15 K (Ohta et al., 1980).

x_1	Exp	Wilson	UNIQUAC
0.0260	38.6500	38.4755	38.4782
0.1620	48.3300	48.7215	48.7232
0.2940	56.8200	56.7202	56.7168
0.3560	59.8500	60.0051	60.0008
0.4700	64.9700	65.4895	65.4860
0.5940	70.7100	70.7881	70.7873
0.6790	74.7100	74.1652	74.1662
0.7420	77.3000	76.5619	76.5638
0.8300	80.6500	79.7888	79.7911
0.9390	84.8600	83.6265	83.6278

Table E.1.13 P (kPa) of ethyl formate (1) and cyclohexane (2) system at 323.15 K (Ohta et al., 1980).

x_1	Exp	Wilson	UNIQUAC
0.0690	55.3400	56.2670	55.7151
0.2070	73.6300	73.6025	74.0556
0.3670	83.2600	81.5957	82.0468
0.4570	85.8700	84.2348	84.4560
0.5730	88.4100	86.7738	86.7511
0.6260	89.9700	87.6978	87.6052
0.7960	91.5900	89.4691	89.2527
0.8500	91.1400	89.4197	89.1737
0.9780	88.6100	86.7512	86.6337

E.2 Heat of mixing data

Table E.2.1 H^E (J/mol) of benzene (1) and cyclohexane (2) system at 298.15 K (Hsu et al., 1975).

x_1	Exp	Wilson	UNIQUAC
0.1036	288.1100	321.8489	288.8247
0.1845	475.3000	480.1703	470.4462
0.3078	671.6200	623.1625	672.4925
0.3839	750.4400	669.2242	751.5530
0.4656	796.0100	690.9186	796.9290
0.5490	801.0700	687.0727	800.2967
0.6293	758.9400	659.4313	761.3887
0.7040	687.4300	611.0099	686.9579
0.7692	590.3600	547.3593	590.8556
0.8875	388.0200	398.6539	388.7049
0.9276	236.2700	258.9817	229.5711

Table E.2.2 H^E (J/mol) of benzene (1) and cyclohexane (2) system at 298.15 K (Kuus et al., 1996).

x_1	Exp	Wilson	UNIQUAC
0.1150	312.0000	353.1754	314.5954
0.1970	494.0000	502.1098	491.7797
0.3390	700.0000	642.4608	704.6955
0.3750	738.0000	661.1230	739.5037
0.4480	786.0000	682.5784	785.8819
0.4670	799.0000	684.8704	792.5801
0.4720	795.0000	685.2593	793.9708
0.5990	776.0000	668.3290	776.5082
0.7030	688.0000	608.1701	684.3736
0.7350	635.0000	581.2334	641.3946
0.8770	364.0000	385.1017	363.4571

Table E.2.3 H^E (J/mol) of benzene (1) and cyclohexane (2) system at 298.15 K (Meyer et al., 1977).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1924	476.5000	503.1486	473.2741	0.5587	779.0000	858.2589	781.2800
0.2130	514.0000	529.8934	511.4935	0.5758	774.5000	853.8570	775.8531
0.2519	583.0000	572.0309	577.0733	0.5923	766.5000	848.6566	768.6903
0.3278	680.8000	628.5142	679.8155	0.6088	758.8000	842.6654	759.8210
0.3464	704.3000	638.0486	699.8522	0.6253	747.7000	835.8814	749.2667
0.3832	733.5000	652.6481	733.4378	0.6416	738.4000	828.3049	737.0610
0.4014	748.0000	657.9348	747.0637	0.6578	722.6000	819.9167	723.2139
0.4194	757.0000	662.0056	758.6328	0.6739	710.0000	810.7114	707.7675
0.4373	767.0000	664.9383	768.1805	0.6899	693.0000	800.6555	690.7271
0.4551	773.3000	666.8008	775.7418	0.7215	654.0000	577.8790	651.9759
0.4901	781.6000	667.5434	785.0451	0.7371	632.6000	565.0771	630.3111
0.5008	782.5000	667.0348	786.3549	0.7984	532.0000	502.9993	528.8329
0.5075	784.7000	666.5163	786.8537	0.8285	474.0000	464.1714	469.4676
0.5247	785.0000	664.6080	788.8082	0.8872	335.0000	365.0367	334.0929
0.5418	782.0000	661.8476	784.9404				

Table E.2.4 H^E (J/mol) of benzene (1) and cyclohexane (2) system at 298.15 K (Stokes et al., 1969).

x_1	Exp	Wilson	UNIQUAC
0.1150	318.4000	356.4838	316.0575
0.1970	496.1000	504.4238	493.8421
0.3390	707.5000	642.0248	707.0919
0.3750	741.7000	660.0707	741.8684
0.4480	786.9000	680.5160	788.0692
0.4670	793.3000	682.6051	794.7001
0.4720	794.6000	682.9450	796.0718
0.5990	776.8000	663.4223	777.9918
0.7030	685.9000	605.7685	685.2588
0.7350	643.5000	579.1710	642.1004
0.8770	365.5000	385.3634	363.5372

Table E.2.5 H^E (J/mol) of 1,2-epoxybutane (1) and methanol (2) system at 298.15 K (Comelli et al., 1996).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0374	86.0000	102.1247	101.2999	0.4823	796.0000	724.8244	788.1854
0.0550	101.0000	146.3225	146.6506	0.5829	804.0000	738.8309	797.2204
0.0721	150.0000	187.1526	189.3033	0.6508	788.0000	716.8368	766.4355
0.1344	307.0000	320.3877	333.0268	0.7388	694.0000	646.2214	679.9690
0.1689	438.0000	419.5984	443.7709	0.7885	595.0000	576.3820	599.1728
0.2369	537.0000	495.1988	529.6441	0.8483	450.0000	465.9881	476.5416
0.3178	666.0000	599.6154	649.1256	0.9179	244.0000	289.7503	289.6963
0.4114	762.0000	685.4874	746.1085				

Table E.2.6 H^E (J/mol) of 1,2-epoxybutane (1) and ethanol (2) system at 298.15 K (Comelli et al., 1996).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0218	54.0000	84.4117	78.4485	0.5017	1102.0000	484.8923	1090.6422
0.0529	137.0000	173.5353	185.2818	0.5730	1133.0000	464.8128	1116.4537
0.0774	207.0000	226.3170	265.2632	0.6681	1101.0000	455.0410	1085.5561
0.1006	268.0000	266.4316	337.7098	0.7285	1037.0000	441.7394	1019.7271
0.1436	437.0000	322.9814	463.6067	0.8010	888.0000	414.4757	881.9758
0.1828	553.0000	360.5516	569.0239	0.8429	760.0000	389.4256	766.9516
0.2512	744.0000	405.7270	731.8227	0.8895	579.0000	346.8257	601.8363
0.3090	868.0000	430.6247	848.3994	0.9415	327.0000	260.8440	361.2938
0.4015	1020.0000	454.3913	993.9085				

Table E.2.7 H^E (J/mol) of 1,2-epoxybutane (1) and 2-propanol (2) system at 298.15 K (Comelli et al., 1996).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0354	109.0000	150.6138	190.3151	0.5690	1507.0000	405.3049	1467.4280
0.0683	260.0000	235.4510	353.2939	0.6376	1454.0000	392.4855	1430.1128
0.0991	394.0000	288.8613	494.3201	0.7252	1301.0000	369.9024	1302.2603
0.1279	532.0000	324.6518	616.5080	0.7787	1166.0000	351.4506	1172.4160
0.1603	772.0000	367.8957	815.9083	0.8407	946.0000	322.4254	962.3343
0.2267	974.0000	391.3340	968.9236	0.8756	788.0000	299.6445	810.6232
0.3055	1235.0000	412.4658	1180.6804	0.9135	588.0000	264.5159	613.3091
0.3696	1383.0000	418.8793	1309.9452	0.9548	329.0000	198.5119	352.5498
0.4680	1496.0000	417.1451	1434.6847				

Table E.2.8 H^E (J/mol) of ethyl formate (1) and benzene (2) system (Ohta et al., 1980).

	T = 298.15 K				T = 308.15 K				T = 318.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0691	143.9000	139.9395	132.6309	0.1094	169.0000	162.4847	158.9834	0.1133	160.7000	154.1914	151.7012
0.1609	284.5000	274.6818	265.3788	0.2112	272.4000	269.0402	265.5376	0.2036	243.5000	243.1047	240.5919
0.2089	331.8000	325.5593	317.0759	0.3063	331.4000	333.9344	331.5795	0.2531	282.0000	280.0285	277.8730
0.3142	389.9000	397.8591	392.7788	0.3985	363.0000	367.8056	366.6867	0.2978	307.1000	306.5517	304.8222
0.3826	399.2000	419.8271	417.0117	0.4044	362.8000	369.0541	368.0046	0.4126	339.3000	346.5697	345.9593
0.4555	407.5000	424.5395	423.5837	0.4909	374.5000	376.2689	374.9997	0.4284	341.8000	349.0411	348.5586
0.4969	406.7000	419.4211	419.1787	0.5797	352.3000	359.0871	359.0552	0.5558	341.4000	343.5567	343.6689
0.6999	330.5000	323.3334	323.2246	0.5869	350.2000	356.7885	356.7731	0.6019	326.9000	330.8141	330.9340
0.8093	238.1000	228.5210	227.3692	0.6938	311.3000	306.6436	306.2395	0.7139	274.9000	277.0878	276.8612
0.8478	200.8000	188.6788	187.2810	0.7963	236.8000	230.2517	229.2142	0.7973	221.3000	216.7414	216.1237
0.8891	149.8000	142.3380	140.8664	0.8991	136.4000	126.0000	125.7884	0.7995	221.8000	214.9191	214.2922
0.9485	77.8000	69.3008	68.2455					0.8963	130.5000	123.1675	122.3640

Table E.2.9 H^E (J/mol) of ethyl formate (1) and cyclohexane (2) system (Ohta et al., 1980).

	T = 298.15 K				T = 308.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0518	405.0000	237.3589	382.0073	0.0345	278.2000	186.8620	260.8119
0.1083	749.4000	358.8257	723.2678	0.0720	533.0000	287.9121	510.5719
0.1723	1041.8000	428.6426	1028.3798	0.1123	764.4000	348.8257	743.4436
0.2331	1261.4000	463.8018	1248.9864	0.1552	969.9000	387.4716	954.6605
0.2987	1410.8000	483.1856	1420.8904	0.2003	1146.8000	412.3840	1139.6843
0.3639	1516.7000	490.7479	1531.2154	0.2473	1294.9000	428.2480	1295.7252
0.4296	1571.9000	490.4193	1587.0980	0.2958	1413.4000	437.7700	1420.7198
0.4841	1582.0000	485.5635	1594.3459	0.3453	1501.2000	442.6326	1513.5041
0.5272	1566.9000	479.2210	1578.1706	0.3955	1558.5000	443.9459	1574.2198
0.5528	1548.9000	474.4725	1555.6447	0.4464	1587.0000	442.4034	1603.5408
0.5844	1515.0000	467.6121	1520.4555	0.4833	1589.9000	439.7613	1605.4392
0.6041	1489.9000	462.7658	1493.0492	0.5082	1583.2000	437.3171	1597.8114
0.6469	1419.6000	450.6385	1419.0858	0.6163	1482.4000	420.6808	1484.1159
0.6942	1319.6000	434.3715	1314.3095	0.6469	1429.3000	414.0478	1428.5665
0.7448	1184.5000	412.8030	1175.0760	0.6820	1356.0000	405.1769	1352.2120
0.7957	1018.0000	385.0510	1005.9143	0.7174	1267.8000	394.5998	1261.4459
0.8462	819.6000	348.1360	808.0050	0.7534	1163.6000	381.7256	1154.7913
0.8525	792.9000	342.5850	781.1342	0.7891	1044.7000	366.1633	1034.4804
0.9025	559.4000	286.7415	549.9379	0.8247	910.0000	346.7677	899.6512
0.9515	295.0000	195.0605	290.8377	0.8602	759.8000	321.7047	750.0141
				0.8956	593.3000	287.6230	585.0949
				0.9308	411.3000	237.8931	404.8627
				0.9657	213.4000	157.0286	209.3621

Table E.2.10 H^E (J/mol) of butanenitrile (1) and 2-butanol (2) system at 298.15 K (Garriga et al., 1997).

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.9045	696.0000	299.8319	750.5359	0.4666	1977.0000	451.8461	1939.8985
0.8563	1011.0000	357.9019	1036.9429	0.4169	1953.0000	447.2866	1913.0413
0.7804	1337.0000	409.2257	1390.7081	0.4146	1961.0000	447.0158	1911.0455
0.7443	1476.0000	424.0413	1523.2489	0.3238	1806.0000	431.5268	1775.4747
0.6916	1682.0000	438.8766	1680.5904	0.2329	1462.0000	403.5718	1517.4305
0.6232	1867.0000	449.7562	1826.8621	0.1244	963.0000	334.5616	1002.0290
0.5757	1938.0000	453.2670	1892.8707	0.0764	657.0000	270.4275	671.8207
0.5490	1970.0000	454.0597	1917.7294	0.0702	616.0000	261.0436	632.3868

Table E.2.11 H^E (J/mol) of 1-chloropentane (1) and di-n-butyl ether (2) system (Paul et al., 1986).

	T = 288.15 K				T = 298.15 K				T = 313.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1807	13.1000	10.1881	12.6841	0.1663	20.0000	22.0567	19.2612	0.1807	33.5000	41.4989	31.1850
0.2243	14.9000	12.0629	14.6305	0.2118	23.2000	25.3878	22.7159	0.2243	38.1000	45.5549	36.0564
0.2271	14.9000	12.1752	14.7415	0.2561	25.8000	27.7009	25.3794	0.2671	41.1000	47.8460	39.8956
0.2671	16.3000	13.6724	16.1461	0.2989	27.5000	29.1478	27.3232	0.3084	43.2000	48.6872	42.7446
0.3084	17.4000	15.0040	17.2509	0.3443	28.3000	29.9224	28.7388	0.3526	44.5000	48.3173	44.8971
0.3526	18.0000	16.1825	18.0594	0.3833	29.1000	30.0279	29.4482	0.3912	45.2000	47.0870	46.0482
0.3912	18.3000	16.9986	18.4630	0.4214	29.3000	29.6852	29.7120	0.4288	45.4000	45.2100	46.5434
0.4288	18.4000	17.5985	18.5975	0.4595	29.2000	28.9498	29.5737	0.4664	45.2000	42.7803	46.4472
0.4664	18.2000	18.0019	18.4892	0.4930	28.8000	28.0154	29.1379	0.4995	44.6000	40.2701	45.8948
0.4995	17.9000	18.1913	18.2032	0.5308	28.1000	26.8770	28.3146	0.5369	43.7000	37.1063	44.7694
0.5369	17.5000	18.2148	17.8776	0.5631	27.1000	25.3250	27.3503	0.5695	42.5000	34.1353	43.3766
0.5695	16.9000	18.0674	17.0550	0.5968	25.9000	23.7387	26.1061	0.6034	40.8000	30.9010	41.5443
0.6034	16.1000	17.7451	16.2561	0.6296	24.7000	22.0483	24.8794	0.6363	38.9000	27.6786	39.4140
0.6363	15.3000	17.2644	15.3442	0.6618	23.2000	20.2726	23.0894	0.6684	37.1000	24.5066	37.0230
0.6684	14.4000	16.6333	14.3356	0.6934	21.6000	18.4402	21.3641	0.6999	34.8000	21.4124	34.3978
0.6999	13.4000	15.8553	13.2424	0.7232	19.8000	16.6494	19.6030	0.7295	32.6000	18.5589	31.6984
0.7295	12.3000	14.9786	12.1315	0.7535	17.9000	14.7840	17.6950	0.7604	29.8000	15.6721	28.6603
0.7604	11.1000	13.9102	10.8958	0.7838	16.0000	12.8909	15.6853	0.7908	26.9000	12.9573	25.4727
0.7908	9.8000	12.7037	9.6149	0.8142	13.9000	10.9806	13.5839	0.8212	23.7000	10.3986	22.1094
0.8212	8.5000	11.3405	8.2806								

Table E.2.12 H^E (J/mol) of 1,2-dichloroethane (1) and di-n-butyl ether (2) system (Paul et al., 1986).

	T = 288.15 K				T = 298.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1681	202.6000	208.2093	203.3786	0.1681	216.8000	224.7708	217.5145
0.2237	284.6000	286.2627	281.5987	0.2237	281.7000	287.3152	280.1709
0.2802	323.2000	319.0993	315.2951	0.2802	343.1000	344.2048	338.1985
0.3355	370.6000	364.3509	361.9074	0.3355	398.0000	392.9210	388.6230
0.3860	407.4000	399.6587	398.7407	0.3860	436.7000	430.9546	429.0746
0.4395	433.4000	430.2827	431.0844	0.4395	466.4000	464.0138	464.7183
0.4843	450.4000	450.1285	452.2768	0.4843	486.5000	485.5315	488.3594
0.5244	463.1000	463.0373	466.1887	0.5244	501.0000	499.6585	504.1661
0.5638	468.8000	470.9058	474.7278	0.5638	509.8000	508.4518	514.2393
0.6012	469.7000	473.6001	477.6602	0.6012	511.6000	511.7754	518.2707
0.6328	468.5000	471.9579	475.6367	0.6328	512.4000	510.4659	517.0588
0.6654	461.9000	466.1899	469.4468	0.6654	507.1000	504.8380	510.9384
0.6942	453.1000	457.3669	459.6618	0.6942	497.9000	495.9521	501.0445
0.7251	440.1000	443.6613	444.4608	0.7251	482.7000	481.9606	485.3059
0.7511	425.8000	428.4168	427.5793	0.7518	465.3000	465.7986	467.0478
0.7780	408.1000	408.7205	405.8425	0.7780	444.0000	445.8880	444.5523
0.8006	388.3000	388.7656	383.9577	0.8006	423.8000	425.1529	421.1982
0.8272	362.8000	360.9265	353.6142	0.8272	395.5000	398.0264	388.6184
0.8508	337.7000	331.7686	322.2070	0.8508	365.8000	365.3843	354.7066

Table E.2.13 H^E (J/mol) of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system (Paul et al., 1986).

	T = 283.15 K				T = 298.15 K				T = 308.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.2469	-82.2000	-74.8008	-72.1840	0.1773	-54.1000	-51.5879	-48.9830	0.2931	-63.7000	-62.0722	-60.2540
0.2931	-88.7000	-83.3273	-81.3206	0.2308	-66.0000	-62.7952	-60.4683	0.3349	-67.9000	-66.4175	-65.1570
0.3349	-93.1000	-89.5379	-88.2175	0.2819	-73.0000	-71.5875	-69.8321	0.3770	-70.4000	-69.6745	-69.0238
0.3770	-95.7000	-94.3450	-93.7746	0.3305	-78.7000	-78.2070	-77.1852	0.4177	-71.8000	-71.7650	-71.6943
0.4177	-96.8000	-97.6087	-97.7519	0.3771	-82.6000	-82.9531	-82.7260	0.4513	-72.4000	-72.7150	-73.0773
0.4513	-97.6000	-99.2778	-99.9538	0.4216	-85.4000	-86.0195	-86.5588	0.4992	-71.9000	-72.8721	-73.7173
0.4992	-96.8000	-100.0560	-101.3240	0.4642	-86.6000	-87.6129	-88.8243	0.5298	-71.4000	-72.2462	-73.2831
0.5298	-96.0000	-99.5699	-101.0694	0.5051	-86.5000	-87.9093	-89.6479	0.5626	-70.1000	-70.9569	-72.0712
0.5626	-94.9000	-98.2007	-99.7859	0.6061	-82.2000	-83.4932	-85.6885	0.5935	-68.3000	-69.1662	-70.2134
0.5935	-93.9000	-96.1114	-97.5985	0.6527	-77.8000	-79.0096	-80.8877	0.6241	-66.3000	-66.8519	-67.6850
0.6241	-91.3000	-93.2820	-94.4812	0.7794	-59.2000	-59.2051	-58.2262	0.6549	-63.7000	-63.9897	-64.4504
0.6549	-88.1000	-89.6752	-90.3796	0.8176	-51.2000	-51.1145	-48.9181	0.6842	-61.1000	-60.7816	-60.7404
0.6989	-82.8000	-83.2136	-82.8484	0.8542	-42.5000	-42.4770	-39.1786	0.7133	-57.4000	-57.1383	-56.4631
0.7409	-76.1000	-75.6273	-73.8733					0.7409	-53.3000	-53.2730	-51.8867
0.7686	-70.9000	-69.8769	-67.0543					0.7686	-49.2000	-49.0037	-46.8224
0.8077	-62.5000	-60.7665	-56.3408								

Table E.2.14 H^E (J/mol) of toluene (1) and 1-chlorohexane (2) system (Paul et al., 1988).

	T = 288.15 K				T = 298.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1408	-100.9000	-105.8054	-104.0588	0.1857	-116.9000	-121.3458	-120.0032
0.1857	-127.2000	-132.1825	-130.3109	0.2298	-138.3000	-142.2153	-140.8954
0.2298	-150.5000	-154.6393	-152.7954	0.2729	-156.6000	-159.6470	-158.4330
0.2729	-169.9000	-173.2906	-171.5906	0.3151	-172.0000	-173.8663	-172.8179
0.3151	-186.0000	-188.4020	-186.9301	0.3565	-184.1000	-185.0683	-184.2257
0.3565	-200.0000	-200.2032	-199.0172	0.3970	-193.2000	-193.3843	-192.7701
0.3970	-208.7000	-208.8545	-207.9882	0.4368	-200.0000	-199.0013	-198.6250
0.4368	-215.6000	-214.5723	-214.0413	0.4758	-204.0000	-202.0390	-201.8974
0.4758	-219.6000	-217.5009	-217.3036	0.5140	-205.7000	-202.6384	-202.7186
0.5140	-220.7000	-217.8054	-217.9267	0.5638	-202.5000	-199.8727	-200.2161
0.5638	-217.8000	-214.3945	-214.8993	0.6124	-195.3000	-193.2828	-193.8405
0.6124	-209.8000	-208.9120	-207.7359	0.6597	-184.8000	-183.1565	-183.8704
0.6597	-197.7000	-195.6899	-196.7543	0.7059	-170.6000	-169.7081	-170.5163
0.7059	-182.4000	-180.9754	-182.1947	0.7510	-153.1000	-153.1666	-154.0062
0.7510	-163.4000	-163.0306	-164.3150	0.7950	-132.2000	-133.7565	-134.5669
0.7950	-141.0000	-142.1103	-143.3704	0.8379	-109.4000	-111.6981	-112.4238
0.8379	-116.1000	-118.4622	-119.8120	0.8799	-84.0000	-87.0833	-87.6756
0.8799	-89.6000	-92.1946	-93.1538				
0.9107	-67.9000	-70.9684	-71.7374				

Table E.2.15 H^E (J/mol) of 1-chlorohexane (1) and ethylbenzene (2) system (Paul et al., 1988).

	T = 288.15 K				T = 298.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1474	-83.6000	-86.2670	-86.3298	0.1474	-78.0000	-79.8058	-79.8272
0.1822	-99.8000	-101.9764	-102.0860	0.1822	-93.0000	-94.4772	-94.5221
0.2173	-114.6000	-116.0580	-116.1713	0.2173	-108.0000	-107.6808	-107.7487
0.2526	-127.1000	-128.4515	-128.5825	0.2526	-119.2000	-119.3527	-119.4413
0.3243	-148.5000	-148.2356	-148.3761	0.2883	-130.1000	-129.5270	-129.6310
0.3971	-162.9000	-161.0475	-161.1540	0.3243	-138.8000	-138.1350	-138.2474
0.4340	-166.7000	-164.7833	-164.8562	0.3605	-145.2000	-145.1262	-145.2387
0.4712	-169.3000	-166.6924	-166.7188	0.3971	-150.9000	-150.5055	-150.6088
0.5088	-168.7000	-166.7431	-166.7140	0.4340	-154.8000	-154.2170	-154.3014
0.5466	-166.3000	-164.9053	-164.8127	0.4712	-156.9000	-156.2261	-156.2819
0.5848	-161.9000	-161.1390	-160.9774	0.5088	-156.8000	-156.4961	-156.5143
0.6234	-155.2000	-155.3988	-155.1656	0.5466	-155.1000	-154.9901	-154.9830
0.6622	-146.9000	-147.6834	-147.3806	0.5848	-152.0000	-151.6643	-151.5857
0.7015	-136.2000	-137.8943	-137.5276	0.6234	-146.8000	-146.4679	-146.3341
0.7410	-123.9000	-126.0672	-125.6489	0.6622	-139.5000	-139.3911	-139.2015
0.7809	-109.6000	-112.1100	-111.6577	0.7015	-130.2000	-130.3345	-130.0919
0.8212	-93.2000	-95.9750	-95.5137	0.7410	-118.3000	-119.3220	-119.0341
				0.7809	-105.0000	-106.2594	-105.9387
				0.8212	-89.4000	-91.0930	-90.7580

Table E.2.16 H^E (J/mol) of 1-chlorohexane (1) and n-propylbenzene (2) system (Paul et al., 1988).

	T = 288.15 K				T = 298.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1266	-79.7000	-81.3008	-81.0117	0.1266	-70.6000	-74.6151	-74.2957
0.1644	-99.2000	-100.6604	-100.3619	0.1644	-87.9000	-92.5161	-92.1715
0.2023	-116.3000	-117.8494	-117.5638	0.2023	-104.5000	-108.4697	-108.1215
0.2401	-131.9000	-132.8019	-132.5453	0.2401	-119.8000	-122.4051	-122.0700
0.2778	-145.0000	-145.5592	-145.3421	0.2778	-133.5000	-134.3511	-134.0410
0.3156	-156.0000	-156.2116	-156.0401	0.3156	-144.3000	-144.3832	-144.1063
0.3532	-164.9000	-164.7049	-164.5606	0.3532	-153.2000	-152.4414	-152.2019
0.3909	-171.3000	-171.1360	-171.0577	0.3909	-160.3000	-158.6085	-158.4081
0.4285	-176.6000	-175.4908	-175.4542	0.4285	-165.0000	-162.8625	-162.6999
0.4660	-178.8000	-177.8047	-177.8034	0.4657	-168.3000	-165.2168	-165.0887
0.5035	-179.4000	-178.1099	-178.1362	0.5035	-169.3000	-166.7290	-166.6314
0.5410	-177.4000	-176.4239	-176.4692	0.5410	-167.0000	-164.3735	-164.3005
0.5785	-173.3000	-172.7630	-172.8183	0.5785	-163.0000	-161.1699	-161.1152
0.6159	-167.4000	-167.1608	-167.2171	0.6159	-156.7000	-156.1420	-156.0991
0.6532	-160.2000	-159.6472	-159.6969	0.6532	-149.0000	-149.3115	-149.2742
0.6905	-150.3000	-150.2245	-150.2606	0.6905	-140.4000	-140.6741	-140.6369
0.7278	-138.3000	-138.9058	-138.9232	0.7278	-128.1000	-130.2359	-130.1945
0.7651	-124.7000	-125.7039	-125.6996	0.7651	-115.1000	-118.0025	-117.9541
0.8023	-109.3000	-110.6736	-110.6475	0.8023	-100.2000	-104.0191	-103.9628
0.8394	-91.8000	-93.8413	-93.7962	0.8394	-84.3000	-88.3047	-88.2419

E.3 Calculated H^E based on parameters from VLE data

Table E.3.1 H^E (J/mol) of benzene (1) and cyclohexane (2) system at 298.15 K based on parameters from VLE data at 323.15 K.

	Hsu et al., 1975				Kuus et al., 1996				Stokes et al., 1969		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1036	288.1102	100.1126	95.9629	0.1150	312.0000	108.7326	104.9865	0.1150	316.4000	108.7326	104.9865
0.1845	475.3024	156.8640	153.5543	0.1970	494.0000	163.4228	161.1281	0.1970	496.1000	163.4228	161.1281
0.3078	671.6157	208.5405	213.1659	0.3390	700.0000	215.1098	223.0266	0.3390	707.5000	215.1098	223.0266
0.3839	750.4422	225.0792	233.6197	0.3750	738.0000	224.2164	231.8538	0.3750	741.7000	224.2164	231.8538
0.4655	796.0060	227.3984	242.2670	0.4480	786.0000	228.1287	241.5447	0.4480	786.9000	228.1287	241.5447
0.5490	801.0686	223.0504	237.4390	0.4670	799.0000	234.0841	242.3006	0.4670	793.3000	234.0841	242.3006
0.6293	758.9358	206.1798	220.3139	0.4720	795.0000	238.7500	242.3802	0.4720	794.6000	238.7500	242.3802
0.7040	687.4312	181.2481	193.9062	0.5990	776.0000	219.1036	228.1767	0.5990	776.8000	219.1036	228.1767
0.7692	590.3624	151.3459	162.9940	0.7030	688.0000	182.7597	194.3242	0.7030	685.9000	182.7597	194.3242
0.8675	388.0242	98.5283	103.3200	0.7350	635.0000	171.9609	180.1001	0.7350	643.5000	171.9609	180.1001
0.9276	236.2705	55.5931	59.5549	0.8770	364.0000	90.7373	96.7581	0.8770	365.5000	90.7373	96.7581

Table E.3.1 (continued)

	Meyer et al., 1977				Meyer et al., 1977		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1924	476.5000	156.7821	158.3757	0.5587	779.0000	251.7674	236.0024
0.2130	514.0000	171.1934	170.3011	0.5756	774.5000	248.9647	233.0988
0.2519	583.0000	191.4298	190.2679	0.5923	768.5000	245.8025	229.6947
0.3278	680.8000	217.0467	219.7339	0.6088	758.8000	241.9895	225.8071
0.3464	704.3000	221.6170	225.0736	0.6253	747.7000	237.9793	221.4504
0.3832	733.5000	233.6276	233.4908	0.6416	738.4000	231.8026	216.6435
0.4014	748.0000	240.3404	236.6136	0.6578	722.6000	226.3302	211.3959
0.4194	757.0000	246.0847	239.0437	0.6739	710.0000	220.8221	205.7296
0.4373	767.0000	247.8156	240.8020	0.6899	693.0000	213.8598	199.6526
0.4551	773.3000	254.4818	241.9097	0.7215	654.0000	200.5977	186.3313
0.4901	781.8000	252.5524	242.2545	0.7371	632.6000	195.2004	179.1154
0.5006	782.5000	251.1372	241.8897	0.7984	532.0000	162.6198	146.8452
0.5075	784.7000	252.6231	241.5307	0.8285	474.0000	143.9020	128.8396
0.5247	785.0000	255.4521	240.2353	0.8872	335.0000	101.7526	89.5264
0.5418	782.0000	254.3618	238.3865				

Table E.3.2 H^E (J/mol) of benzene (1) and cyclohexane (2) system at 298.15 K based on parameters from VLE data at 333.15 K.

	Hsu et al., 1975				Kuus et al., 1996				Stokes et al., 1969		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1036	288.1102	97.2250	87.1487	0.1150	312.0000	105.5208	95.2081	0.1150	318.4000	105.5208	95.2081
0.1845	475.3024	148.1584	138.0348	0.1970	494.0000	154.3025	144.6112	0.1970	496.1000	154.3025	144.6112
0.3078	671.6157	195.4898	188.5630	0.3390	700.0000	201.5233	196.4622	0.3390	707.5000	201.5233	196.4622
0.3839	750.4422	209.7863	204.5416	0.3750	738.0000	209.0106	203.2429	0.3750	741.7000	209.0106	203.2429
0.4655	796.0060	216.5182	209.7175	0.4480	786.0000	217.3782	209.6084	0.4480	786.9000	217.3782	209.6084
0.5490	801.0686	208.5244	203.0857	0.4670	799.0000	219.2689	209.7021	0.4670	793.3000	219.2689	209.7021
0.6293	758.9358	191.7698	186.2015	0.4720	795.0000	222.8284	209.6225	0.4720	794.6000	222.8284	209.6225
0.7040	687.4312	168.3071	162.0103	0.5990	776.0000	203.9832	193.7271	0.5990	776.6000	203.9832	193.7271
0.7692	590.3624	143.5262	134.7799	0.7030	688.0000	173.9206	162.3850	0.7030	685.9000	173.9206	162.3850
0.8675	388.0242	89.9042	84.0587	0.7350	635.0000	160.9647	149.7420	0.7350	643.5000	160.9647	149.7420
0.9276	236.2705	51.8711	47.9540	0.8770	364.0000	84.8562	78.5933	0.8770	365.5000	84.8562	78.5933

Table E.3.2 (continued)

	Meyer et al., 1977				Meyer et al., 1977		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.1924	476.5000	151.4641	142.2250	0.5587	779.0000	241.4405	201.5691
0.2130	514.0000	161.5721	152.5301	0.5756	774.5000	237.9755	198.5962
0.2519	583.0000	179.6475	169.5544	0.5923	766.5000	234.2041	195.2117
0.3278	680.8000	202.4684	193.8527	0.6088	758.8000	229.8439	191.4332
0.3464	704.3000	212.1412	198.0664	0.6253	747.7000	224.9206	187.2755
0.3832	733.5000	219.3040	204.4476	0.6416	738.4000	219.7352	182.7578
0.4014	748.0000	224.6262	206.6854	0.6578	722.6000	213.5078	177.8903
0.4194	757.0000	229.9802	208.2675	0.6739	710.0000	206.9566	172.6941
0.4373	767.0000	239.3959	209.2771	0.6899	693.0000	200.5544	167.1795
0.4551	773.3000	240.5783	209.7168	0.7215	654.0000	185.7681	155.2551
0.4901	781.8000	240.1175	208.9735	0.7371	632.6000	182.2183	148.8742
0.5008	782.5000	248.9017	208.3478	0.7984	532.0000	151.9071	120.8511
0.5075	784.7000	249.2541	207.8320	0.8285	474.0000	134.5038	105.5094
0.5247	785.0000	247.4211	206.2048	0.8872	335.0000	94.3551	72.5921
0.5418	782.0000	244.9102	204.1109				

Table E.3.3 H^E (J/mol) of 1,2-epoxybutane (1) and methanol (2) system at 298.15 K based on parameters from VLE data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC
0.0374	66.0000	50.9419	48.2885
0.0550	101.0000	74.7024	71.0425
0.0721	150.0000	97.6319	93.1212
0.1344	307.0000	180.6939	172.7847
0.1889	438.0000	250.8590	240.5100
0.2369	537.0000	309.5524	297.6942
0.3178	666.0000	400.6043	386.5032
0.4114	762.0000	489.7515	472.5757
0.4823	796.0000	540.6374	521.6614
0.5829	804.0000	583.4517	559.7123
0.6508	788.0000	586.2934	558.9739
0.7368	694.0000	551.9526	519.5638
0.7885	595.0000	504.9327	470.6360
0.8483	450.0000	420.8871	386.2687
0.9179	244.0000	271.4079	243.5190

Table E.3.4 H^E (J/mol) of 1,2-epoxybutane (1) and ethanol (2) system at 298.15 K based on parameters from VLE data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC
0.0218	54.0000	25.9274	24.3359
0.0529	137.0000	62.3192	58.8699
0.0774	207.0000	90.3844	85.8597
0.1006	288.0000	116.4786	111.1875
0.1436	437.0000	163.5267	157.3675
0.1828	553.0000	204.7843	198.3605
0.2512	744.0000	272.6882	266.5031
0.3090	868.0000	324.9015	319.6876
0.4015	1020.0000	397.2621	393.4023
0.5017	1102.0000	455.2605	451.6857
0.5730	1133.0000	479.6482	474.8772
0.6681	1101.0000	483.7245	474.6123
0.7285	1037.0000	464.3073	451.2220
0.8010	888.0000	411.7980	393.3586
0.8429	760.0000	363.0568	342.3381
0.8895	579.0000	289.1420	267.8825
0.9415	327.0000	176.3519	159.4575

Table E.3.5 H^E (J/mol) of 1,2-epoxybutane (1) and 2-propanol (2) system at 298.15 K based on parameters from VLE data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC
0.0354	109.0000	69.4696	75.4261
0.0683	250.0000	127.6111	140.3805
0.0991	394.0000	178.6689	196.6743
0.1279	532.0000	221.4377	245.4412
0.1803	772.0000	288.9210	324.5984
0.2267	974.0000	342.5509	384.4688
0.3055	1235.0000	413.0006	464.3030
0.3696	1383.0000	453.0017	509.1673
0.4680	1496.0000	484.2443	543.2604
0.5690	1507.0000	480.5532	534.6885
0.6376	1454.0000	461.6200	503.7506
0.7252	1301.0000	407.5679	434.6584
0.7787	1166.0000	359.3851	376.0756
0.8407	946.0000	287.2614	292.5473
0.8756	788.0000	237.7505	238.1000
0.9135	588.0000	175.5207	172.8727
0.9548	329.0000	97.9830	94.5177

Table E.3.6 H^E (J/mol) of ethyl formate (1) and benzene (2) system based on parameters from VLE data at 323.15 K.

	T = 298.15 K				T = 308.15 K				T = 318.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0691	143.9000	63.0450	22.9663	0.1094	169.0000	91.5696	34.4658	0.1133	160.7000	94.2005	35.9126
0.1609	264.5000	134.0791	46.7737	0.2112	272.4000	157.1392	55.8042	0.2036	243.5000	154.5575	55.3227
0.2089	331.8000	174.4496	54.5605	0.3063	331.4000	201.8851	67.7233	0.2531	282.0000	190.8592	62.8984
0.3142	389.9000	212.7087	67.1860	0.3985	363.6000	217.7870	72.8826	0.2978	307.1000	211.9959	68.0349
0.3826	399.2000	238.0641	71.0222	0.4044	362.8000	238.2499	73.0183	0.4126	339.3000	238.8685	74.5193
0.4555	407.5000	256.2411	71.7823	0.4909	374.5000	249.7337	72.5593	0.4284	341.8000	264.5928	74.7173
0.4969	406.7000	265.5211	70.8239	0.5797	352.3000	237.4559	67.7291	0.5558	341.4000	248.6932	70.8917
0.6999	330.5000	188.8249	53.7431	0.5869	350.2000	247.2589	67.1611	0.6019	325.9000	242.2009	67.3372
0.8093	238.1000	133.4089	37.4497	0.6936	311.3000	207.7558	55.9413	0.7139	274.9000	197.1682	54.5188
0.8478	200.8000	116.3577	30.7409	0.7963	236.8000	155.5568	40.6960	0.7973	221.3000	158.3282	41.5503
0.8891	149.8000	89.3865	23.0358	0.8991	136.4000	82.3365	21.7151	0.7995	221.8000	162.7573	41.1724
0.9485	77.8000	41.9036	11.0990					0.8963	130.5000	85.4429	22.8750

Table E.3.7 H^E (J/mol) of ethyl formate (1) and cyclohexane (2) system based on parameters from VLE data at 323.15 K.

	T = 298.15 K				T = 308.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0518	405.0000	195.1253	183.0606	0.0345	276.2000	139.8189	126.7757
0.1083	749.4000	367.3773	340.3676	0.0720	533.0000	283.8557	245.4533
0.1723	1041.8000	519.9474	472.5435	0.1123	764.4000	433.4411	352.7506
0.2331	1251.4000	604.2044	559.3328	0.1552	969.9000	546.0160	446.0905
0.2987	1410.8000	666.2031	616.9181	0.2003	1146.8000	650.2250	523.2931
0.3639	1516.7000	677.1750	642.6255	0.2473	1294.9000	701.4359	583.2803
0.4296	1571.9000	702.3341	641.6500	0.2858	1413.4000	791.6303	625.6228
0.4841	1582.0000	679.8499	623.4145	0.3453	1501.2000	800.8823	650.6113
0.5272	1566.9000	676.5080	599.3199	0.3955	1568.5000	830.0400	659.2744
0.5528	1548.9000	656.1937	581.3958	0.4484	1587.0000	793.0062	652.8972
0.5844	1515.0000	622.5457	555.8905	0.4833	1589.9000	756.2921	639.7649
0.6041	1489.9000	600.8669	536.2343	0.5082	1583.2000	730.6355	627.2303
0.6469	1419.6000	551.7805	495.6368	0.6163	1482.4000	610.0186	543.1417
0.6942	1319.6000	494.1018	442.5193	0.6469	1429.3000	572.6281	511.7768
0.7448	1184.5000	427.9652	379.6541	0.6820	1356.0000	528.2992	472.3194
0.7957	1018.0000	356.2430	311.1049	0.7174	1267.8000	481.2114	429.1174
0.8462	819.6000	279.2613	238.7468	0.7534	1163.6000	430.8947	382.0404
0.8525	792.9000	269.2127	229.4582	0.7891	1044.7000	378.3681	332.5710
0.9025	559.4000	185.6219	153.9932	0.8247	910.0000	323.1495	280.8014
0.9515	295.0000	96.4244	77.5180	0.8602	759.8000	265.0051	227.0528
				0.8956	593.3000	203.6737	171.6250
				0.9308	411.3000	139.0511	114.9607
				0.9657	213.4000	71.0435	57.4972

Table E.3.8 H^E (J/mol) of butanenitrile and butane-2-ol system at 298.15 K based on parameters from VLE data at eight temperature.

x_1	Exp	T = 278.15 K		T = 288.15 K		T = 293.15 K		T = 298.15 K		T = 303.15 K		T = 308.15 K		T = 313.15 K		T = 323.15 K	
		Wilson	UNIQUAC	Wilson	UNIQUAC	Wilson	UNIQUAC	Wilson	UNIQUAC	Wilson	UNIQUAC	Wilson	UNIQUAC	Wilson	UNIQUAC	Wilson	UNIQUAC
0.9045	696.0000	215.3894	218.5532	188.7309	183.0972	184.3273	179.9664	175.3019	167.9106	170.0443	162.3058	169.3052	162.3671	167.5699	162.4678	159.0055	153.9190
0.8563	1011.0000	303.2659	318.2345	268.6580	268.0480	262.8057	262.9312	250.7138	245.7394	243.5745	237.5309	242.4280	237.1981	239.8175	236.7357	227.7742	223.9165
0.7804	1337.0000	417.6213	459.1973	375.6796	390.0768	368.2005	381.3671	352.8096	357.3924	343.4953	345.4274	341.6076	343.9543	337.5501	341.8650	320.9043	322.4986
0.7443	1476.0000	462.6882	518.8288	418.9536	442.5157	410.8823	431.9319	394.4558	405.2952	384.3788	391.7046	382.0823	389.4896	377.2908	386.3453	358.7644	363.9843
0.6916	1682.0000	518.5734	596.5873	473.6887	511.8484	464.8642	498.3873	447.4215	468.5219	436.4793	452.7639	433.5082	449.2684	427.5781	444.3100	406.5995	417.7754
0.6232	1867.0000	574.6069	679.7209	530.1785	587.6663	520.4371	570.3257	502.3848	537.4394	490.6663	519.2709	486.6682	513.8337	479.1293	506.1413	455.4087	474.6569
0.5757	1938.0000	603.0191	724.5758	559.8314	629.8030	549.4135	609.7624	531.3095	575.5590	519.2282	556.0158	514.4120	549.1041	505.6695	539.3487	480.3013	504.8332
0.5490	1970.0000	615.2769	744.8027	573.0272	649.3362	562.1953	627.8084	544.1707	593.1464	531.9357	572.9495	526.6229	565.1850	517.1760	554.2421	490.9692	518.2020
0.4666	1977.0000	636.1268	782.6361	597.5059	688.7153	585.1789	662.9372	567.7936	628.1397	555.2664	606.5318	548.2752	596.1558	538.5701	581.6063	508.1892	541.8668
0.4169	1953.0000	635.8553	785.8791	599.7518	695.4954	586.3448	667.5804	569.5785	633.6353	556.9897	611.6774	548.9129	599.8552	535.8385	583.3339	506.4962	542.2607
0.4146	1961.0000	635.5970	785.6454	599.6134	695.4713	586.1533	667.4683	569.4193	633.5797	556.8297	611.6157	548.7022	599.7310	535.5656	583.1250	506.1862	542.0092
0.3236	1808.0000	606.4198	746.8424	575.3094	668.0711	559.6045	637.6634	544.3921	607.2075	531.9410	585.8163	521.8654	571.9503	508.4849	552.7072	476.3492	511.5138
0.2329	1462.0000	534.4504	644.1935	508.4026	582.3707	490.6771	552.5724	477.5225	527.8432	465.7335	508.8799	454.2660	494.5611	437.6605	474.8384	408.8011	437.4116
0.1244	963.0000	369.8475	421.2548	351.2039	385.7702	333.9567	363.1725	324.5915	348.2333	315.2605	335.3595	304.5732	324.0039	290.0106	308.5190	267.7754	282.4890
0.0754	657.0000	254.7510	278.7233	241.1214	258.7652	227.0887	240.7957	220.4121	231.2860	213.4697	222.6069	205.0795	214.4592	193.9607	203.4036	177.8861	185.6984
0.0702	616.0000	240.5558	261.8984	227.5803	241.4192	214.0876	226.3087	207.7547	217.4108	201.1417	209.2387	193.1095	201.5182	182.4971	191.0478	167.2418	174.3627

Table E.3.9 H^E (J/mol) of 1-chloropentane (1) and di-n-butyl ether (2) system based on parameters from VLE data at 313.15 K.

x_1	T = 288.15 K			x_1	T = 298.15 K			x_1	T = 313.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.1807	13.1000	-74.9142	-25.8719	0.1663	20.0000	-61.7513	-19.8282	0.1807	33.5000	-60.1395	-15.8232
0.2243	14.9000	-67.6372	-31.8725	0.2118	23.2000	-74.6461	-25.4060	0.2243	38.1000	-70.8588	-20.0434
0.2271	14.9000	-65.1093	-32.2482	0.2561	25.8000	-70.5135	-30.5721	0.2671	41.1000	-64.2631	-24.0339
0.2671	16.3000	-66.5276	-37.4894	0.2989	27.5000	-72.0848	-35.3184	0.3084	43.2000	-64.0846	-27.7695
0.3084	17.4000	-65.2842	-42.5690	0.3443	28.6000	-71.6097	-39.9937	0.3526	44.5000	-62.1358	-31.5283
0.3526	18.0000	-71.2894	-47.5427	0.3833	29.1000	-74.3690	-43.6376	0.3912	45.2000	-64.1541	-34.5662
0.3912	18.3000	-34.0834	-51.4188	0.4214	29.3000	-37.2615	-46.7978	0.4288	45.4000	-25.5049	-37.2374
0.4288	18.4000	-45.4434	-54.7088	0.4595	29.2000	-47.8531	-49.5001	0.4664	45.2000	-36.8302	-39.5666
0.4664	18.2000	-17.8628	-57.4557	0.4930	28.8000	-18.9601	-51.4475	0.4995	44.6000	-5.7765	-41.2879
0.4995	17.9000	-27.5888	-59.3747	0.5308	28.1000	-29.9289	-53.1081	0.5369	43.7000	-16.6769	-42.6091
0.5369	17.5000	-11.4272	-60.9235	0.5631	27.1000	-11.8169	-54.0248	0.5695	42.5000	1.5868	-43.7241
0.5695	16.9000	-9.3905	-61.8899	0.5968	25.9000	-10.0345	-54.4477	0.6034	40.8000	3.1049	-44.2250
0.6034	16.1000	5.3285	-61.8628	0.6296	24.7000	4.6938	-54.2910	0.6363	38.9000	17.9618	-44.2295
0.6363	15.3000	2.1695	-61.3772	0.6618	23.2000	2.2532	-53.5500	0.6684	37.1000	16.0133	-43.7360
0.6684	14.4000	13.7111	-60.2405	0.6934	21.6000	13.4629	-52.2172	0.6999	34.8000	26.1148	-42.7351
0.6999	13.4000	-0.5052	-58.4482	0.7232	19.8000	0.9144	-50.3752	0.7295	32.6000	12.4889	-41.2942
0.7295	12.3000	-11.1985	-56.1174	0.7535	17.9000	-9.1974	-47.8852	0.7604	29.8000	0.9981	-39.2375
0.7604	11.1000	-19.6792	-52.9796	0.7838	16.0000	-16.7047	-44.7378	0.7908	26.9000	-7.6482	-36.6282
0.7908	9.8000	-25.4189	-49.1538	0.8142	13.9000	-21.6830	-40.8835	0.8212	23.7000	-13.7101	-33.4020
0.8212	8.5000	-28.6431	-44.5587								

Table E.3.10 H^E (J/mol) of 1-chloropentane (1) and di-n-butyl ether (2) system based on parameters from VLE data at 323.15 K.

x_1	T = 288.15 K			x_1	T = 298.15 K			x_1	T = 313.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.1807	13.1000	-46.0576	-5.7114	0.1663	20.0000	-36.9974	-2.5112	0.1807	33.5000	-36.1677	0.8919
0.2243	14.9000	-47.4711	-7.6431	0.2118	23.2000	-38.4063	-3.9048	0.2243	38.1000	-35.8702	0.2320
0.2271	14.9000	-21.5287	-7.7713	0.2561	25.8000	-25.6613	-5.4502	0.2671	41.1000	-21.5321	-0.6561
0.2671	16.3000	-12.1099	-9.6418	0.2989	27.5000	-16.9560	-7.0682	0.3084	43.2000	-11.5611	-1.6955
0.3084	17.4000	-2.6017	-11.6163	0.3443	28.6000	-9.0241	-8.8602	0.3526	44.5000	-2.5403	-2.9573
0.3526	18.0000	22.5452	-13.7226	0.3833	29.1000	17.3683	-10.4145	0.3912	45.2000	24.8081	-4.1440
0.3912	18.3000	27.3092	-15.5085	0.4214	29.3000	22.0580	-11.9044	0.4288	45.4000	30.0842	-5.3388
0.4288	18.4000	19.8232	-17.1576	0.4595	29.2000	14.6159	-13.3258	0.4664	45.2000	22.9353	-6.5357
0.4664	18.2000	16.3595	-18.6768	0.4930	28.8000	13.1056	-14.4866	0.4995	44.6000	21.6775	-7.5621
0.4995	17.9000	17.4783	-19.8732	0.5308	28.1000	12.2667	-15.8592	0.5369	43.7000	21.0243	-8.6571
0.5369	17.5000	34.2354	-21.0289	0.5631	27.1000	30.4585	-16.5154	0.5695	42.5000	39.4525	-9.5270
0.5695	16.9000	45.6998	-21.8344	0.5968	25.9000	40.7421	-17.2349	0.6034	40.8000	49.7605	-10.3184
0.6034	16.1000	53.5548	-22.4400	0.6296	24.7000	48.6041	-17.7351	0.6363	38.9000	57.5656	-10.9481
0.6363	15.3000	53.8559	-22.7705	0.6618	23.2000	49.1192	-18.0056	0.6684	37.1000	57.8695	-11.4037
0.6684	14.4000	52.0339	-22.8187	0.6934	21.6000	47.4989	-18.0306	0.6999	34.8000	55.8980	-11.6720
0.6999	13.4000	40.8409	-22.5739	0.7232	19.8000	37.7215	-17.8109	0.7295	32.6000	45.6379	-11.7392
0.7295	12.3000	27.2113	-22.0548	0.7535	17.9000	24.6308	-17.3205	0.7604	29.8000	31.3474	-11.5936
0.7604	11.1000	15.3342	-21.1874	0.7838	16.0000	13.8319	-16.5355	0.7908	26.9000	19.7281	-11.2103
0.7908	9.8000	5.9498	-19.9828	0.8142	13.9000	5.2617	-15.4256	0.8212	23.7000	10.3907	-10.5634
0.8212	8.5000	-1.1950	-18.4026								

Table E.3.11 H^E (J/mol) of 1,2-dichloroethane (1) and di-n-butyl ether (2) system based on parameters from VLE data at 330.00 K.

x_1	T = 288.15 K			T = 298.15 K		
	Exp	Wilson	UNIQUAC	Exp	Wilson	UNIQUAC
0.1681	202.6000	141.8571	141.4757	216.8000	143.4257	143.4605
0.2237	264.6000	180.1536	183.5285	281.7000	182.1877	186.0293
0.2802	323.2000	214.7464	223.2633	343.1000	217.2142	226.2068
0.3355	370.8000	242.6525	258.7853	396.0000	245.4929	262.0757
0.3860	407.4000	271.4250	287.8684	436.7000	274.5825	291.3951
0.4395	433.4000	305.4354	314.6366	466.4000	308.9132	318.3236
0.4843	450.4000	330.9818	333.3642	486.5000	334.6747	337.1095
0.5244	463.1000	344.4185	348.8565	501.0000	348.2668	350.6922
0.5638	468.8000	356.7016	356.6912	509.8000	360.6580	360.3581
0.6012	469.7000	367.6008	362.4677	511.6000	371.6342	366.0132
0.6328	468.5000	395.0345	364.2999	512.4000	399.2968	367.6995
0.6654	461.9000	413.9195	362.8993	507.1000	418.3729	366.1066
0.6942	453.1000	429.5685	358.5542	497.9000	434.2246	361.5566
0.7251	440.1000	435.4877	350.2576	482.7000	440.2740	353.0048
0.7511	425.8000	424.2533	340.0242	465.3000	428.1114	342.2032
0.7780	408.1000	392.6107	325.9416	444.0000	396.8278	328.1739
0.8006	388.3000	364.4499	311.0648	423.8000	368.2607	313.0512
0.8272	362.8000	329.1571	289.5889	395.5000	332.4601	291.2710
0.8508	337.7000	295.5781	266.5437	365.8000	298.4060	267.9468

Table E.3.12 H^E (J/mol) of 1,2-dichloroethane (1) and di-n-butyl ether (2) system based on parameters from VLE data at 350.00 K.

x_1	T = 288.15 K			T = 298.15 K		
	Exp	Wilson	UNIQUAC	Exp	Wilson	UNIQUAC
0.1681	202.6000	160.0579	181.1350	216.8000	160.7078	181.3120
0.2237	264.6000	198.5478	231.5853	281.7000	199.4193	231.8328
0.2802	323.2000	231.5435	277.3010	343.1000	232.6301	277.6243
0.3355	370.8000	266.6100	316.1177	396.0000	267.9350	316.5178
0.3860	407.4000	330.2230	345.9611	436.7000	332.0139	346.4317
0.4395	433.4000	380.5014	371.1853	466.4000	382.7974	371.7291
0.4843	450.4000	410.8037	386.7847	486.5000	413.5048	387.3866
0.5244	463.1000	456.6465	396.1041	501.0000	460.2514	396.7539
0.5638	468.8000	477.6109	400.6433	509.8000	481.7072	401.3348
0.6012	469.7000	490.4327	400.3872	511.6000	494.7753	401.1118
0.6328	468.5000	498.8715	396.4490	512.4000	503.6351	397.1953
0.6654	461.9000	491.3225	388.5583	507.1000	496.2640	389.3207
0.6942	453.1000	468.5520	378.1406	497.9000	473.3345	378.9078
0.7251	440.1000	453.3194	363.1205	482.7000	458.1798	363.8851
0.7511	425.8000	423.8089	347.2035	465.3000	427.3714	347.4852
0.7780	408.1000	391.1142	327.3790	444.0000	395.3273	328.1124
0.8006	388.3000	362.0990	307.9287	423.8000	366.0062	308.6368
0.8272	362.8000	320.0582	281.5873	395.5000	323.4306	282.2348
0.8508	337.7000	281.5227	254.8520	365.8000	284.4182	255.4724

Table E.3.13 H^E (J/mol) of 1,2-dichloroethane (1) and di-n-butyl ether (2) system based on parameters from VLE data at 370.00 K.

x_1	T = 288.15 K			T = 298.15 K		
	Exp	Wilson	UNIQUAC	Exp	Wilson	UNIQUAC
0.1681	202.6000	149.9985	169.4490	216.8000	150.4612	169.5538
0.2237	264.6000	188.5208	216.2674	281.7000	189.1641	216.4339
0.2802	323.2000	220.7486	258.4717	343.1000	221.5694	258.7123
0.3356	370.8000	251.4463	294.0734	396.0000	252.4574	294.3959
0.3880	407.4000	291.9486	321.2201	436.7000	293.2422	321.6236
0.4395	433.4000	312.1190	343.8957	466.4000	313.6119	344.3886
0.4843	450.4000	325.4056	357.6576	486.5000	327.0611	358.2261
0.5244	463.1000	336.2435	365.6089	501.0000	338.0603	366.2412
0.5638	468.8000	340.3883	369.0968	509.8000	342.3222	369.7923
0.6012	469.7000	347.0117	368.1819	511.6000	349.1201	368.9098
0.6328	468.5000	353.7223	363.9273	512.4000	356.0274	364.7135
0.6654	461.9000	389.5820	356.0358	507.1000	392.6134	356.8538
0.6942	453.1000	397.7893	345.9054	497.9000	401.2087	346.7438
0.7251	440.1000	401.7972	331.5372	482.7000	405.6484	332.3871
0.7511	425.8000	405.6688	316.4765	465.3000	409.0127	316.8815
0.7780	408.1000	372.9231	297.8696	444.0000	376.9302	298.7077
0.8006	388.3000	339.3402	279.7313	423.8000	342.9334	280.5496
0.8272	362.8000	298.8443	255.2895	395.5000	301.9485	256.0706
0.8508	337.7000	261.9472	230.6535	365.8000	264.8165	231.3880

Table E.3.14 H^E (J/mol) of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system based on parameters from VLE data at 323.15 K.

x_1	T = 283.15 K			x_1	T = 298.15 K			x_1	T = 313.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.2469	-82.2000	-1122.2917	-326.4605	0.1773	-54.1000	-846.9191	-219.1402	0.2931	-63.7000	-1042.4877	-309.4968
0.2931	-88.7000	-1185.9606	-371.1976	0.2308	-65.0000	-979.9581	-276.3032	0.3349	-67.9000	-1076.6884	-340.8700
0.3349	-93.1000	-1219.2455	-407.2138	0.2819	-73.0000	-1067.7821	-323.1451	0.3770	-70.4000	-1095.0197	-368.0209
0.3770	-95.7000	-1217.9459	-437.9068	0.3305	-78.7000	-1099.4966	-362.6852	0.4177	-71.8000	-1080.1612	-389.6529
0.4177	-96.8000	-1210.6179	-461.8741	0.3771	-82.6000	-1120.2142	-394.5422	0.4513	-72.4000	-1068.0690	-403.8374
0.4513	-97.6000	-1190.4764	-477.1796	0.4216	-85.4000	-1116.9223	-418.9206	0.4992	-71.9000	-1036.8243	-417.9015
0.4992	-98.6000	-1149.4860	-491.5877	0.4642	-86.6000	-1098.2101	-436.2914	0.5298	-71.4000	-1006.7281	-422.8680
0.5298	-98.0000	-1112.5931	-498.0101	0.5051	-86.5000	-1066.3479	-447.1017	0.5626	-70.1000	-968.3748	-424.5180
0.5626	-94.9000	-1068.9446	-496.4257	0.6061	-82.2000	-945.8330	-446.9656	0.5935	-68.3000	-926.6286	-422.4406
0.5935	-93.9000	-1016.3680	-492.5794	0.6527	-77.8000	-885.5967	-432.9731	0.6241	-66.3000	-878.2943	-416.7647
0.6241	-91.3000	-962.4518	-484.5839	0.7794	-59.2000	-602.9421	-345.7509	0.6549	-63.7000	-826.6954	-407.2726
0.6549	-88.1000	-902.9171	-472.1999	0.8176	-51.2000	-508.8741	-304.3405	0.6842	-61.1000	-772.6507	-394.5947
0.6989	-82.6000	-811.4652	-446.7113	0.8542	-42.5000	-414.1509	-257.6823	0.7133	-57.4000	-715.1887	-378.3610
0.7409	-76.1000	-716.9695	-413.5282					0.7409	-53.3000	-658.4638	-359.5032
0.7686	-70.9000	-649.0239	-386.7613					0.7686	-49.2000	-596.7355	-337.0875
0.8077	-62.5000	-551.9695	-342.1854								

Table E.3.15 H^E (J/mol) of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system based on parameters from VLE data at 343.15 K.

x_1	T = 283.15 K			x_1	T = 298.15 K			x_1	T = 313.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.2469	-82.2000	-116.0217	-464.7752	0.1773	-54.1000	-94.2760	-325.4158	0.2931	-63.7000	-101.1879	-476.9523
0.2931	-88.7000	-131.9749	-535.2316	0.2308	-65.0000	-117.3491	-410.2563	0.3349	-67.9000	-112.0187	-527.4825
0.3349	-93.1000	-148.2253	-593.2734	0.2819	-73.0000	-138.1441	-484.2770	0.3770	-70.4000	-122.4470	-572.6498
0.3770	-95.7000	-164.7686	-645.6609	0.3305	-76.7000	-157.9477	-547.5591	0.4177	-71.8000	-133.3800	-610.3061
0.4177	-96.8000	-183.3964	-689.8963	0.3771	-82.6000	-178.8933	-600.9545	0.4513	-72.4000	-148.7385	-636.5160
0.4513	-97.6000	-202.6102	-721.1823	0.4216	-85.4000	-197.6550	-644.5204	0.4992	-71.9000	-156.1550	-665.4777
0.4992	-96.8000	-258.2901	-756.6945	0.4642	-86.6000	-259.3008	-678.6606	0.5298	-71.4000	-211.6638	-678.3096
0.5298	-96.0000	-295.1869	-773.2092	0.5051	-86.5000	-293.5957	-703.6991	0.5626	-70.1000	-240.2497	-686.6844
0.5626	-94.9000	-274.5796	-785.0086	0.6061	-82.2000	-218.8628	-727.4536	0.5935	-68.3000	-218.0086	-689.0625
0.5935	-93.9000	-316.0916	-790.0329	0.6527	-77.8000	-233.2252	-716.8700	0.6241	-66.3000	-251.6415	-685.7107
0.6241	-91.3000	-341.3526	-788.6507	0.7794	-59.2000	-120.5609	-600.3942	0.6549	-63.7000	-269.0478	-676.1346
0.6549	-88.1000	-330.1251	-780.2900	0.8176	-51.2000	-86.6385	-535.2136	0.6842	-61.1000	-255.7388	-660.7884
0.6889	-82.8000	-355.8703	-764.9356	0.8542	-42.5000	-61.9970	-457.8503	0.7133	-57.4000	-294.5057	-639.0612
0.7409	-76.1000	-357.9887	-714.2638					0.7409	-53.3000	-319.0619	-612.0456
0.7686	-70.9000	-320.3125	-677.6947					0.7686	-49.2000	-282.9653	-576.2274
0.8077	-62.5000	-254.8730	-611.4581								

Table E.3.16 H^E (J/mol) of toluene (1) and 1-chlorohexane (2) system based on parameters from VLE data at 323.15 K.

x_1	T = 288.15 K			x_1	T = 298.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.1408	-100.9000	-106.4255	-248.5425	0.1857	-116.9000	-133.5847	-306.3938
0.1857	-127.2000	-135.0241	-319.0571	0.2298	-138.3000	-157.4751	-368.0882
0.2298	-150.5000	-154.0903	-383.5820	0.2729	-156.6000	-171.7023	-423.5469
0.2729	-169.9000	-166.5723	-441.7115	0.3151	-172.0000	-179.8785	-472.8151
0.3151	-186.0000	-181.4502	-493.4847	0.3565	-184.1000	-190.7047	-515.8924
0.3565	-200.0000	-180.9802	-538.8929	0.3970	-193.2000	-186.9443	-552.5691
0.3970	-208.7000	-170.7868	-577.6953	0.4368	-200.0000	-171.4460	-582.8604
0.4368	-215.6000	-153.5422	-609.9297	0.4758	-204.0000	-155.6230	-606.5634
0.4758	-219.6000	-129.5782	-635.3382	0.5140	-205.7000	-130.9148	-623.5349
0.5140	-220.7000	-105.8426	-653.7662	0.5638	-202.5000	-111.8600	-635.4844
0.5638	-217.8000	-97.6334	-667.2322	0.6124	-195.3000	-100.7368	-634.8650
0.6124	-209.8000	-100.2893	-667.5837	0.6597	-184.8000	-99.1147	-621.2757
0.6597	-197.7000	-112.8286	-654.3413	0.7059	-170.6000	-105.9591	-594.2394
0.7059	-182.4000	-117.5089	-626.9411	0.7510	-153.1000	-105.8145	-553.2876
0.7510	-163.4000	-115.3240	-584.8099	0.7950	-132.2000	-99.5539	-498.0145
0.7950	-141.0000	-107.1538	-527.4254	0.8379	-109.4000	-87.9561	-428.1241
0.8379	-116.1000	-93.7807	-454.3635	0.8799	-84.0000	-71.6291	-343.0527
0.8799	-89.6000	-75.8055	-364.9011				
0.9107	-67.9000	-59.7053	-287.1734				

Table E.3.17 H^E (J/mol) of toluene (1) and 1-chlorohexane (2) system based on parameters from VLE data at 343.15 K.

x_1	T = 288.15 K			x_1	T = 298.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.1408	-100.9000	-47.0535	-264.9635	0.1857	-116.9000	-49.0116	-327.3888
0.1857	-127.2000	-62.5215	-340.4026	0.2298	-138.3000	-61.1222	-393.6413
0.2298	-150.5000	-77.6722	-409.5807	0.2729	-156.6000	-72.9159	-453.3488
0.2729	-169.9000	-94.0672	-472.0565	0.3151	-172.0000	-86.0472	-506.5518
0.3151	-186.0000	-113.9454	-527.8640	0.3565	-184.1000	-102.6292	-553.2416
0.3565	-200.0000	-132.5993	-576.9860	0.3970	-193.2000	-117.8222	-593.1709
0.3970	-208.7000	-153.4896	-619.1530	0.4368	-200.0000	-134.9996	-626.3788
0.4368	-215.6000	-160.6164	-654.3966	0.4758	-204.0000	-138.8608	-652.5998
0.4758	-219.8000	-163.4878	-682.4250	0.5140	-205.7000	-138.8642	-671.6743
0.5140	-220.7000	-190.9155	-703.0559	0.5638	-202.5000	-154.3228	-685.7356
0.5638	-217.8000	-219.1170	-718.7613	0.6124	-195.3000	-174.8989	-686.3618
0.6124	-209.8000	-239.9932	-720.4756	0.6597	-184.8000	-188.3150	-673.0522
0.6597	-197.7000	-244.1458	-707.6132	0.7059	-170.6000	-186.7278	-645.2160
0.7059	-182.4000	-254.9109	-679.4890	0.7510	-153.1000	-189.9715	-602.2464
0.7510	-163.4000	-259.8444	-636.3799	0.7950	-132.2000	-187.2684	-543.5740
0.7950	-141.0000	-239.3769	-574.5892	0.8379	-109.4000	-163.9643	-468.7218
0.8379	-116.1000	-195.0335	-496.4911	0.8799	-84.0000	-123.0402	-376.8789
0.8799	-89.6000	-128.6131	-400.0927				
0.9107	-67.9000	-66.0261	-315.7639				

Table E.3.18 H^E (J/mol) of 1-chlorohexane (1) and ethylbenzene (2) system based on parameters from VLE data at 323.15 K.

x_1	T = 288.15 K			x_1	T = 298.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.1474	-83.6000	-11.7382	-53.7304	0.1474	-78.0000	-11.7234	-53.4507
0.1822	-99.8000	-13.9228	-63.6564	0.1822	-93.0000	-13.9059	-63.3128
0.2173	-114.6000	-16.7382	-72.6043	0.2173	-108.0000	-16.7164	-72.1983
0.2526	-127.1000	-19.9119	-80.5277	0.2526	-119.2000	-19.8840	-80.0618
0.3243	-148.5000	-23.9379	-93.3107	0.2883	-130.1000	-23.8913	-86.9233
0.3971	-162.9000	-26.4586	-101.7678	0.3243	-138.8000	-27.1580	-92.7346
0.4340	-166.7000	-27.8598	-104.3215	0.3805	-145.2000	-29.3742	-97.4595
0.4712	-169.3000	-28.1142	-105.7199	0.3971	-150.9000	-30.3584	-101.0997
0.5088	-168.7000	-26.9203	-105.9369	0.4340	-154.6000	-29.7023	-103.6161
0.5466	-166.3000	-27.7451	-104.9460	0.4712	-156.9000	-31.3802	-104.9843
0.5848	-161.9000	-25.6973	-102.7169	0.5088	-156.8000	-29.7035	-105.1789
0.6234	-155.2000	-26.4534	-99.2148	0.5466	-155.1000	-31.4665	-104.1744
0.6622	-146.9000	-27.7014	-94.4322	0.5848	-152.0000	-34.0513	-101.9414
0.7015	-136.2000	-28.6836	-88.3027	0.6234	-146.8000	-36.6469	-98.4458
0.7410	-123.9000	-28.9597	-80.8430	0.6622	-139.5000	-38.7301	-93.6818
0.7809	-109.6000	-26.3896	-71.9902	0.7015	-130.2000	-37.1391	-87.5834
0.8212	-93.2000	-21.4371	-61.7095	0.7410	-118.3000	-32.1338	-80.1683
				0.7809	-105.0000	-26.6795	-71.3750
				0.8212	-89.4000	-21.3598	-61.1699

Table E.3.19 H^E (J/mol) of 1-chlorohexane (1) and ethylbenzene (2) system based on parameters from VLE data at 343.15 K.

x_1	T = 288.15 K			x_1	T = 298.15 K		
	Exp	Wilson	UNIQUAC		Exp	Wilson	UNIQUAC
0.1474	-83.6000	-70.1493	-341.3401	0.1474	-78.0000	-67.0400	-322.3006
0.1822	-99.8000	-77.4614	-396.9877	0.1822	-93.0000	-73.8278	-375.3200
0.2173	-114.6000	-82.0759	-444.3721	0.2173	-108.0000	-77.9669	-420.6308
0.2526	-127.1000	-85.8547	-483.6384	0.2526	-119.2000	-81.3699	-458.3343
0.3243	-148.5000	-90.9574	-539.3945	0.2883	-130.1000	-80.1082	-488.8564
0.3971	-162.9000	-112.8049	-566.1920	0.3243	-138.8000	-88.1751	-512.3012
0.4340	-166.7000	-114.6043	-569.4128	0.3605	-145.2000	-92.4877	-528.8583
0.4712	-169.3000	-116.7218	-566.1628	0.3971	-150.9000	-100.0979	-538.8441
0.5088	-168.7000	-115.2217	-556.6482	0.4340	-154.8000	-98.9831	-542.4267
0.5466	-166.3000	-116.8013	-541.1508	0.4712	-156.9000	-104.6077	-539.8251
0.5848	-161.9000	-112.7110	-519.8110	0.5088	-156.8000	-103.6753	-531.2217
0.6234	-155.2000	-110.3971	-492.7985	0.5466	-155.1000	-105.5464	-516.6689
0.6622	-146.9000	-105.9374	-460.4570	0.5848	-152.0000	-105.2541	-496.6911
0.7015	-136.2000	-95.1328	-422.7125	0.6234	-146.8000	-96.9669	-471.4398
0.7410	-123.9000	-79.0191	-380.0201	0.6622	-139.5000	-81.3075	-440.8317
0.7809	-109.6000	-65.3210	-332.3414	0.7015	-130.2000	-68.9697	-404.9907
0.8212	-93.2000	-51.6859	-279.8120	0.7410	-118.3000	-56.6577	-364.3428
				0.7809	-105.0000	-45.9186	-318.8481
				0.8212	-89.4000	-42.0374	-268.6248

Table E.3.20 H^E (J/mol) of 1-chlorohexane (1) and n-propylbenzene (2) system based on parameters from VLE data at 363.15 K.

x_1	T = 288.15 K			T = 298.15 K		
	Exp	Wilson	UNIQUAC	Exp	Wilson	UNIQUAC
0.1268	-79.7000	-81.4337	-290.5499	-70.6000	-76.8778	-273.7951
0.1644	-99.2000	-82.9193	-356.4947	-87.9000	-76.9353	-336.3688
0.2023	-116.3000	-91.0365	-413.3953	-104.5000	-84.0621	-390.5423
0.2401	-131.9000	-93.9374	-461.2375	-119.8000	-86.0375	-436.2610
0.2778	-145.0000	-92.5500	-500.3970	-133.5000	-83.7707	-473.8443
0.3156	-156.0000	-100.6163	-531.3991	-144.3000	-91.3680	-503.7602
0.3532	-164.9000	-113.1739	-554.3493	-153.2000	-103.7976	-526.0758
0.3909	-171.3000	-111.1187	-569.7809	-160.3000	-101.3476	-541.2757
0.4285	-176.6000	-102.6270	-577.9246	-165.0000	-92.5828	-549.5535
0.4660	-178.6000	-93.6386	-579.1417	-168.3000	-83.0963	-551.2447
0.5035	-179.4000	-83.8874	-573.7572	-169.3000	-72.9481	-546.6062
0.5410	-177.4000	-71.4742	-562.0545	-167.0000	-60.2210	-535.9263
0.5785	-173.3000	-62.9459	-544.3068	-163.0000	-51.6775	-519.4456
0.6159	-167.4000	-62.5428	-520.6460	-158.7000	-51.8218	-497.4617
0.6532	-160.2000	-70.8734	-491.9659	-149.0000	-61.3358	-470.2471
0.6905	-150.3000	-75.6258	-457.8472	-140.4000	-67.2506	-437.9660
0.7278	-138.3000	-76.9966	-418.7148	-128.1000	-69.7580	-400.8257
0.7651	-124.7000	-75.1683	-374.7824	-115.1000	-69.0370	-359.0240
0.8023	-109.3000	-70.3274	-326.3909	-100.2000	-65.2678	-312.8801
0.8394	-91.8000	-62.6542	-273.7688	-84.3000	-58.6284	-262.6087

E.4 Calculated pressure based on parameters from H^E data

Table E.4.1 P (kPa) of benzene (1) and cyclohexane (2) system based on parameters from H^E data at 298.15 K (Kuus et al., 1996).

	T = 323.15 K				T = 333.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0340	36.8800	43.9610	38.7768	0.0700	53.5600	68.9843	58.5280
0.0740	37.4800	49.1737	41.2661	0.0760	53.6800	69.8299	59.0000
0.1070	37.9400	51.7884	42.9760	0.1020	54.1000	72.8530	60.8915
0.1380	38.3100	53.4422	44.3370	0.1260	54.4800	74.9308	62.4317
0.1470	38.4200	53.8207	44.6920	0.1780	56.4800	77.9251	66.1780
0.2010	39.0500	55.4515	46.4893	0.2020	55.6100	78.8474	66.2079
0.2390	39.3600	56.1591	47.4584	0.2340	56.1900	79.7623	67.3807
0.2740	39.5700	56.6146	48.1720	0.2700	56.2800	80.5435	68.4600
0.2870	39.6700	56.7485	48.3988	0.3360	56.9300	81.4200	69.8939
0.3350	39.9900	57.1217	49.0803	0.3510	57.0200	81.5638	70.1371
0.3470	40.0300	57.1910	49.2165	0.3740	57.0300	81.7234	70.4591
0.3480	39.9600	57.1984	49.2273	0.4400	57.4400	82.0188	71.0865
0.3650	40.0900	57.2803	49.3981	0.4500	57.4600	82.0426	71.1480
0.4040	40.2100	57.4226	49.7070	0.4610	57.4900	82.0630	71.2065
0.4220	40.2700	57.4679	49.8148	0.4710	57.5200	82.0764	71.2516
0.4340	40.2700	57.4917	49.8753	0.4780	57.5600	82.0829	71.2787
0.4480	40.3100	57.5132	49.9354	0.4880	57.5900	82.0881	71.3113
0.4630	40.4000	57.5291	49.9879	0.4990	57.6000	82.0882	71.3389
0.4770	40.3200	57.5374	50.0261	0.5090	57.6100	82.0831	71.3566
0.4930	40.3300	57.5390	50.0577	0.5180	57.6200	82.0744	71.3668
0.4970	40.3300	57.5381	50.0636	0.5280	57.6200	82.0598	71.3716
0.5090	40.3500	57.5323	50.0768	0.5330	57.6100	82.0508	71.3715
0.5240	40.3500	57.5181	50.0838	0.5380	57.6000	82.0401	71.3697
0.5310	40.3300	57.5088	50.0835	0.5470	57.5900	82.0178	71.3623
0.5600	40.3100	57.4509	50.0584	0.5580	57.5700	81.9910	71.3494
0.5910	40.2700	57.3507	49.9884	0.6020	57.4300	81.7764	71.1977
0.6570	40.0700	56.9872	49.6753	0.6730	57.1300	81.1159	70.6459
0.6900	39.9500	56.6578	49.4173	0.7090	56.8900	80.5821	70.1803
0.7550	39.5500	55.8941	48.6309	0.7640	56.4200	79.2775	69.1294
0.7950	39.2200	54.7524	47.8885	0.7880	56.1300	78.4851	68.5010
0.8120	39.0200	54.2369	47.4915	0.8280	55.6900	76.7133	67.1427
0.8440	38.6800	53.0183	46.5767	0.8700	54.9800	73.9869	65.1591
0.8970	38.0500	49.9766	44.4178	0.8950	54.4300	71.7553	63.6166
0.9140	37.8100	48.8125	43.4998	0.9030	54.3000	70.9159	63.0532
0.9340	37.4700	46.6706	42.2400	0.9170	54.1000	69.2727	61.9746
				0.9440	53.5800	65.3398	59.5114

Table E.4.2 P (kPa) of benzene (1) and cyclohexane (2) system based on parameters from H^E data at 298.15 K (Stokes et al., 1969).

	T = 323.15 K				T = 333.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0340	38.8800	44.2473	38.7952	0.0700	53.5600	69.5142	58.5723
0.0740	37.4800	49.5642	41.3000	0.0760	53.6800	70.3717	59.0469
0.1070	37.9400	52.1973	43.0188	0.1020	54.1000	73.4233	60.9462
0.1380	38.3100	53.8484	44.3856	0.1260	54.4800	75.5068	62.4954
0.1470	38.4200	54.2245	44.7419	0.1760	56.4800	78.4860	65.2513
0.2010	39.0500	55.8361	46.5444	0.2020	55.6100	79.3971	66.2838
0.2390	39.3600	56.5302	47.5150	0.2340	56.1900	80.3170	67.4587
0.2740	39.5700	56.9750	48.2291	0.2700	56.2800	81.0628	68.5389
0.2870	39.6700	57.1055	48.4658	0.3360	56.9300	81.9177	69.9722
0.3350	39.9900	57.4683	49.1388	0.3510	57.0200	82.0477	70.2151
0.3470	40.0300	57.5355	49.2727	0.3740	57.0300	82.2125	70.5363
0.3480	39.9600	57.5407	49.2835	0.4400	57.4400	82.4989	71.1617
0.3650	40.0900	57.6221	49.4539	0.4500	57.4600	82.5220	71.2228
0.4040	40.2100	57.7600	49.7618	0.4610	57.4900	82.5417	71.2810
0.4220	40.2700	57.8039	49.8690	0.4710	57.5200	82.5548	71.3258
0.4340	40.2700	57.8269	49.9294	0.4780	57.5600	82.5609	71.3527
0.4480	40.3100	57.8477	49.9892	0.4880	57.5900	82.5658	71.3850
0.4630	40.4000	57.8631	50.0413	0.4990	57.6000	82.5658	71.4123
0.4770	40.3200	57.8710	50.0792	0.5090	57.6100	82.5609	71.4298
0.4930	40.3300	57.8726	50.1105	0.5180	57.6200	82.5523	71.4397
0.4970	40.3300	57.8717	50.1164	0.5280	57.6200	82.5380	71.4443
0.5090	40.3500	57.8660	50.1294	0.5330	57.6100	82.5290	71.4441
0.5240	40.3500	57.8522	50.1361	0.5380	57.6000	82.5188	71.4422
0.5310	40.3300	57.8431	50.1357	0.5470	57.5900	82.4989	71.4346
0.5600	40.3100	57.7867	50.1102	0.5560	57.5700	82.4708	71.4216
0.5910	40.2700	57.6889	50.0398	0.6020	57.4300	82.2609	71.2689
0.6570	40.0700	57.3135	49.7258	0.6730	57.1300	81.6128	70.7155
0.6900	39.9500	57.0095	49.4672	0.7090	56.8900	81.0870	70.2486
0.7550	39.5500	56.0579	48.6785	0.7640	56.4200	79.7955	69.1943
0.7950	39.2200	55.1229	47.9335	0.7880	56.1300	79.0081	68.5638
0.8120	39.0200	54.6094	47.5351	0.8280	55.6900	77.2402	67.2005
0.8440	38.6800	53.3912	46.6167	0.8700	54.9600	74.5041	65.2090
0.8970	38.0500	50.3293	44.4491	0.8950	54.4300	72.2526	63.6602
0.9140	37.8100	48.9478	43.5275	0.9030	54.3000	71.4033	63.0946
0.9340	37.4700	46.9734	42.2625	0.9170	54.1000	69.7370	62.0116
				0.9440	53.5800	65.7312	59.5388

Table E.4.3 P (kPa) of benzene (1) and cyclohexane (2) system based on parameters from H^E data at 298.15 K (Hsu et al., 1975).

	T = 323.15 K				T = 333.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0340	36.6800	43.2921	38.8068	0.0700	53.5600	67.6800	58.6022
0.0740	37.4800	48.1968	41.3228	0.0760	53.6800	68.4847	59.0789
0.1070	37.9400	50.7151	43.0492	0.1020	54.1000	71.3859	60.9884
0.1380	38.3100	52.3347	44.4219	0.1260	54.4800	73.4050	62.5422
0.1470	38.4200	52.7089	44.7797	0.1780	55.4800	76.3602	65.3094
0.2010	39.0500	54.3400	46.5894	0.2020	55.6100	77.2842	66.3459
0.2390	39.3600	55.0596	47.5638	0.2340	56.1900	78.2294	67.5252
0.2740	39.5700	55.5281	48.2803	0.2700	56.2800	79.0067	68.6092
0.2870	39.6700	55.6668	48.5078	0.3360	56.9300	79.9131	70.0469
0.3350	39.9900	56.0558	49.1908	0.3510	57.0200	80.0525	70.2904
0.3470	40.0300	56.1284	49.3271	0.3740	57.0300	80.2300	70.6125
0.3480	39.9600	56.1341	49.3379	0.4400	57.4400	80.5390	71.2393
0.3650	40.0900	56.2222	49.5087	0.4500	57.4600	80.5635	71.3006
0.4040	40.2100	56.3720	49.8174	0.4610	57.4900	80.5844	71.3589
0.4220	40.2700	56.4195	49.9248	0.4710	57.5200	80.5977	71.4039
0.4340	40.2700	56.4443	49.9854	0.4780	57.5600	80.6040	71.4309
0.4480	40.3100	56.4665	50.0453	0.4880	57.5900	80.6085	71.4633
0.4630	40.4000	56.4826	50.0978	0.4990	57.6000	80.6073	71.4907
0.4770	40.3200	56.4904	50.1358	0.5090	57.6100	80.6007	71.5083
0.4930	40.3300	56.4908	50.1670	0.5180	57.6200	80.5902	71.5184
0.4970	40.3300	56.4895	50.1729	0.5280	57.6200	80.5732	71.5231
0.5090	40.3500	56.4820	50.1860	0.5330	57.6100	80.5626	71.5229
0.5240	40.3500	56.4652	50.1930	0.5380	57.6000	80.5506	71.5211
0.5310	40.3300	56.4545	50.1926	0.5470	57.5900	80.5253	71.5136
0.5600	40.3100	56.3885	50.1674	0.5560	57.5700	80.4951	71.5007
0.5910	40.2700	56.2761	50.0975	0.6020	57.4300	80.2566	71.3490
0.6570	40.0700	55.8536	49.7849	0.6730	57.1300	79.5362	70.7975
0.6900	39.9500	55.5178	49.5272	0.7090	56.8900	78.9415	70.3317
0.7550	39.5500	54.4914	48.7401	0.7640	56.4200	77.5856	69.2789
0.7950	39.2200	53.5104	47.9955	0.7880	56.1300	76.7626	68.6484
0.8120	39.0200	52.9808	47.5969	0.8280	55.6900	74.9523	67.2839
0.8440	38.6800	51.7486	46.6773	0.8700	54.9600	72.2324	65.2878
0.8970	38.0500	48.7542	44.5031	0.8950	54.4300	70.0547	63.7335
0.9140	37.8100	47.4456	43.5773	0.9030	54.3000	69.2455	63.1655
0.9340	37.4700	45.6127	42.3059	0.9170	54.1000	67.8753	62.0775
				0.9440	53.5800	63.9856	59.5911

Table E.4.4 P (kPa) of benzene (1) and cyclohexane (2) system based on parameters from H^E data at 298.15 K (Meyer et al., 1977).

	T = 323.15 K				T = 333.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0340	36.6800	45.5238	38.6901	0.0700	53.5600	71.6236	58.3154
0.0740	37.4800	51.2585	41.1033	0.0760	53.6800	72.7257	58.7740
0.1070	37.9400	53.9484	42.7673	0.1020	54.1000	75.8754	60.6150
0.1380	38.3100	56.5753	44.0962	0.1260	54.4800	77.9671	62.1179
0.1470	38.4200	55.9388	44.4435	0.1780	55.4800	80.8626	64.8078
0.2010	39.0500	57.4608	46.2080	0.2020	55.6100	81.7223	65.8205
0.2390	39.3600	58.0987	47.1642	0.2340	56.1900	82.5758	66.9772
0.2740	39.5700	58.4969	47.8713	0.2700	56.2800	83.2559	68.0454
0.2870	39.6700	58.6131	48.0966	0.3360	56.9300	84.0207	69.4723
0.3350	39.9900	58.9331	48.7761	0.3510	57.0200	84.1355	69.7154
0.3470	40.0300	58.9919	48.9123	0.3740	57.0300	84.2804	70.0380
0.3480	39.9600	58.9965	48.9231	0.4400	57.4400	84.5309	70.6698
0.3850	40.0900	59.0675	49.0943	0.4500	57.4600	84.5610	70.7321
0.4040	40.2100	59.1874	49.4049	0.4610	57.4900	84.5682	70.7914
0.4220	40.2700	59.2255	49.5138	0.4710	57.5200	84.5795	70.8373
0.4340	40.2700	59.2455	49.5750	0.4780	57.5600	84.5850	70.8649
0.4480	40.3100	59.2638	49.6360	0.4880	57.5900	84.5893	70.8982
0.4630	40.4000	59.2771	49.6893	0.4990	57.6000	84.5894	70.9266
0.4770	40.3200	59.2841	49.7283	0.5090	57.6100	84.5850	70.9450
0.4930	40.3300	59.2858	49.7607	0.5180	57.6200	84.5775	70.9557
0.4970	40.3300	59.2849	49.7669	0.5280	57.6200	84.5651	70.9611
0.5090	40.3500	59.2800	49.7808	0.5330	57.6100	84.5572	70.9612
0.5240	40.3500	59.2682	49.7882	0.5380	57.6000	84.5482	70.9597
0.5310	40.3300	59.2604	49.7882	0.5470	57.5900	84.5290	70.9527
0.5600	40.3100	59.2114	49.7639	0.5660	57.5700	84.5059	70.9403
0.5910	40.2700	59.1258	49.8944	0.6020	57.4300	84.3200	70.7902
0.6570	40.0700	58.7909	49.3820	0.6730	57.1300	83.7350	70.2409
0.6900	39.9500	58.5152	49.1248	0.7090	56.8900	83.2337	69.7780
0.7550	39.5500	57.8331	48.3439	0.7640	56.4200	82.0418	68.7367
0.7950	39.2200	56.7441	47.6101	0.7680	56.1300	81.2697	68.1161
0.8120	39.0200	56.2480	47.2188	0.8280	55.6900	79.5689	66.7785
0.8440	38.6800	55.0517	46.3190	0.8700	54.9800	76.8314	64.8320
0.8970	38.0500	51.9429	44.2040	0.8950	54.4300	74.5207	63.3222
0.9140	37.8100	50.4985	43.3070	0.9030	54.3000	73.6368	62.7714
0.9340	37.4700	48.3942	42.0775	0.9170	54.1000	71.8841	61.7178
				0.9440	53.5800	67.5774	59.3152

Table E.4.5 P (kPa) of 1-chloropentane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 288.15 K.

	T = 313.15 K				T = 323.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0774	25.5000	24.6119	25.4598	0.0831	40.7000	39.4108	40.5002
0.1209	28.5000	27.1382	28.3374	0.1416	48.5000	46.3461	48.3934
0.2242	35.3000	33.3820	35.1122	0.2652	60.9000	57.8534	60.6823
0.2877	39.2000	37.3600	39.2399	0.3509	69.3000	66.1516	69.1168
0.3549	43.5000	41.6801	43.5814	0.4291	76.8000	73.8886	76.7609
0.3978	46.4000	44.4449	46.3402	0.5480	88.0000	85.6565	88.1150
0.5515	56.1000	54.5993	56.1591	0.5990	93.3000	91.0439	93.2405
0.5678	56.9000	55.6874	57.1956	0.6220	95.4000	93.3882	95.4615
0.6810	64.2000	63.2743	64.3781	0.6552	98.7000	98.7771	98.6847
0.6964	65.2000	64.3087	65.3537	0.6952	102.7000	100.8651	102.5203
0.7793	70.4000	69.8764	70.6027	0.7789	110.7000	109.4238	110.5811
0.8225	73.1000	72.7738	73.3378	0.8443	117.0000	116.1017	116.8784
0.8985	78.1000	77.8563	78.1534	0.9042	122.7000	122.2002	122.6504
0.9307	80.1000	80.0020	80.1982	0.9474	126.6000	126.5836	126.6180
				0.9860	130.6000	130.4874	130.5464

Table E.4.6 P (kPa) of 1-chloropentane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 298.15 K.

	T = 313.15 K				T = 323.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0774	25.5000	24.0858	25.6643	0.0831	40.7000	38.7582	40.7624
0.1209	28.5000	26.3985	28.6308	0.1416	48.5000	45.1314	48.8996
0.2242	35.3000	32.3358	35.5501	0.2652	60.9000	56.2164	61.4113
0.2877	39.2000	36.2407	39.7255	0.3509	69.3000	64.4727	69.9018
0.3549	43.5000	40.5367	44.0881	0.4291	76.8000	72.2969	77.5402
0.3978	46.4000	43.3500	46.8467	0.5480	88.0000	84.3386	88.8051
0.5515	56.1000	53.7376	56.5947	0.5990	93.3000	89.8837	93.8661
0.5678	56.9000	54.8581	57.6187	0.6220	95.4000	92.3000	96.0555
0.6810	64.2000	62.6859	64.6989	0.6552	98.7000	95.7952	99.2101
0.6964	65.2000	63.7538	65.6565	0.6952	102.7000	100.0129	103.0034
0.7793	70.4000	69.4982	70.8170	0.7789	110.7000	108.8396	110.9251
0.8225	73.1000	72.4825	73.5056	0.8443	117.0000	115.7145	117.1123
0.8985	78.1000	77.7046	78.2428	0.9042	122.7000	121.9777	122.7872
0.9307	80.1000	79.9031	80.2548	0.9474	126.6000	126.4683	126.8895
				0.9860	130.6000	130.4585	130.5645

Table E.4.7 P (kPa) of 1-chloropentane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 313.15 K.

	T = 313.15 K				T = 323.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0774	26.5000	24.1125	25.6552	0.0631	40.7000	38.8137	41.0061
0.1209	28.5000	26.4156	28.9039	0.1416	48.5000	45.1738	49.3877
0.2242	35.3000	32.3101	35.9553	0.2652	60.9000	56.1894	62.0807
0.2877	39.2000	36.1903	40.1734	0.3509	69.3000	64.4063	70.6203
0.3549	43.5000	40.4678	44.5543	0.4291	76.8000	72.2101	78.2514
0.3978	46.4000	43.2736	47.3119	0.5460	88.0000	84.2477	89.4336
0.5515	56.1000	53.6809	56.9937	0.5990	93.3000	89.7990	94.4358
0.5678	56.9000	54.7834	58.0062	0.6220	95.4000	92.2192	96.5966
0.6810	64.2000	62.6299	64.9890	0.6552	98.7000	95.7208	99.7071
0.6964	65.2000	63.7009	65.9343	0.6952	102.7000	99.9475	103.4439
0.7793	70.4000	69.4624	71.0141	0.7789	110.7000	108.7948	111.2399
0.8225	73.1000	72.4554	73.6604	0.8443	117.0000	115.6857	117.3271
0.8985	78.1000	77.6913	78.3258	0.9042	122.7000	121.9621	122.9135
0.9307	80.1000	79.8947	80.3095	0.9474	126.8000	126.4607	126.9558
				0.9860	130.6000	130.4567	130.5813

Table E.4.8 P (kPa) of 1,2-dichloroethane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 288.15 K.

	T = 330.00 K				T = 350.00 K				T = 370.00 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0374	64.8000	87.2503	66.6242	0.0163	129.1000	149.3542	130.2520	0.0097	264.1000	285.4241	265.3008
0.0895	79.2000	113.3948	82.4274	0.0340	144.7000	182.6662	147.2364	0.0502	326.6000	413.8104	333.5507
0.1046	95.2000	136.4927	99.4091	0.0578	166.5000	221.4571	169.8696	0.0842	380.0000	498.8711	389.9991
0.1272	103.5000	149.1443	110.1708	0.1362	232.9000	316.6091	244.4703	0.1490	473.3000	624.7623	495.2541
0.2073	138.3000	184.8752	147.1548	0.3871	416.5000	479.1638	438.3561	0.2902	680.6000	815.6982	712.5462
0.3339	191.5000	226.0939	201.5625	0.5089	520.6000	553.0623	540.8432	0.3475	758.1000	877.8193	795.3885
0.4304	218.6000	252.3152	239.3540	0.5908	577.6000	595.9656	595.9931	0.3999	828.5000	930.9554	868.1728
0.4817	248.0000	265.5425	258.0636	0.7080	653.9000	656.6270	665.3444	0.4571	902.3000	986.5328	944.2129
0.5424	267.4000	280.9852	278.9368	0.7754	693.1000	692.5070	701.7943	0.5032	957.6000	1030.2541	1002.8136
0.6096	288.6000	298.0425	300.4621	0.8334	725.3000	724.1884	731.8395	0.5690	1040.3000	1091.9125	1082.2219
0.7350	329.2000	330.7040	336.5586	0.8843	754.2000	752.6992	757.8459	0.6368	1119.2000	1155.1773	1158.6460
0.8277	355.8000	358.0216	360.7301	0.9197	773.8000	772.9537	776.1453	0.7851	1282.8000	1298.9165	1310.0974
0.9060	375.6000	378.4361	380.7345	0.9337	783.0000	781.0653	783.5123	0.8555	1357.5000	1366.4146	1376.4044
0.9700	396.9000	397.5634	398.0149	0.9692	803.0000	801.9015	802.7335	0.9259	1432.5000	1437.8255	1442.2507
				0.9768	808.1000	807.6036	808.1047	0.9899	1505.2000	1504.5929	1504.9155
				0.9896	815.7000	814.0535	814.2559				

Table E.4.9 P (kPa) of 1,2-dichloroethane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 298.15 K.

	T = 330.00 K				T = 350.00 K				T = 370.00 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0374	64.8000	94.9383	87.5436	0.0163	129.1000	156.4783	131.0195	0.0097	284.1000	292.9711	266.0948
0.0695	79.2000	125.1654	84.0837	0.0340	144.7000	195.9598	148.8119	0.0502	326.6000	444.3680	337.5129
0.1046	95.2000	151.0550	101.8140	0.0578	166.5000	241.0689	172.4887	0.0842	380.0000	541.2908	398.4326
0.1272	103.5000	164.8651	113.0262	0.1382	232.9000	349.0780	250.2371	0.1490	473.3000	678.8373	505.8967
0.2073	138.3000	202.2595	151.3884	0.3871	418.6000	509.0468	449.5567	0.2902	680.6000	872.3591	729.9094
0.3339	191.5000	242.3292	207.2641	0.6089	620.6000	576.6440	552.5447	0.3475	768.1000	931.6975	814.4519
0.4304	218.6000	268.4574	245.5272	0.6908	577.6000	615.3372	606.9458	0.3999	828.5000	981.4140	888.2454
0.4817	248.0000	278.3938	264.2848	0.7080	653.9000	670.0631	674.0418	0.4571	902.3000	1032.8691	964.7801
0.5424	267.4000	292.2127	284.9677	0.7754	693.1000	702.8185	708.6731	0.5032	957.8000	1072.6263	1023.3150
0.6096	288.6000	307.4748	306.0548	0.8334	725.3000	731.5271	736.9549	0.5690	1040.3000	1128.6640	1101.9180
0.7350	329.2000	336.7928	340.7090	0.8843	754.2000	757.6920	761.3482	0.6368	1119.2000	1186.0112	1176.8749
0.8277	355.8000	359.7822	363.4362	0.9197	773.8000	776.3673	778.5347	0.7851	1282.8000	1314.7781	1321.9057
0.9060	375.6000	380.3825	382.1431	0.9337	783.0000	783.8687	785.4703	0.8555	1357.5000	1378.2838	1384.4288
0.9700	396.9000	398.1547	398.4369	0.9692	803.0000	803.1828	803.6278	0.9259	1432.5000	1443.8424	1446.3374
				0.9768	808.1000	808.4817	808.7165	0.9899	1505.2000	1505.4055	1505.4768
				0.9898	815.7000	814.4822	814.5567				

Table E.4.10 P (kPa) of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 283.15 K.

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0141	39.5000	38.6557	35.6082	0.0380	114.4000	102.3642	96.3548
0.0335	46.8000	40.9329	38.2370	0.0955	155.2000	131.8813	113.9978
0.0517	53.6000	45.3009	40.6577	0.1557	203.2000	168.7198	135.9730
0.1152	78.8000	63.0435	51.2648	0.2194	252.8000	213.2094	163.6234
0.1575	95.3000	76.7976	59.3884	0.2889	308.7000	266.8583	199.5648
0.3082	155.7000	135.2738	97.4458	0.3538	359.4000	320.5731	239.1233
0.3813	176.4000	158.3768	114.7131	0.4870	468.9000	437.6542	340.1892
0.4270	206.7000	188.0671	139.1646	0.5616	533.4000	505.2853	408.8761
0.4821	228.8000	213.5896	162.4020	0.5884	535.3000	509.6571	413.5855
0.5387	253.2000	239.2316	187.9020	0.6444	602.0000	580.7446	494.6520
0.5861	272.8000	262.5526	213.0307	0.7002	650.8000	631.3995	567.2278
0.6558	303.7000	295.4442	251.5136	0.7246	673.1000	653.4325	585.5155
0.7065	326.0000	319.2297	281.3573	0.7979	739.1000	719.0089	672.4477
0.7656	352.1000	346.6898	317.4652	0.8533	792.7000	767.8138	738.2105
0.8271	377.9000	374.8599	355.5357	0.8685	800.4000	779.3318	753.6186
0.8707	397.4000	394.5341	382.0533	0.8795	822.3000	790.6309	768.6273
0.9492	432.6000	429.2533	426.4935	0.9223	851.4000	827.5074	816.4285
0.9544	434.5000	431.5192	429.2025	0.9506	870.7000	851.6058	846.1811
0.9771	442.6000	441.3593	440.5737	0.9631	875.5000	862.1750	858.7193
				0.9776	884.1000	874.3766	872.7285
				0.9904	889.6000	885.0946	884.5700

Table E.4.11 P (kPa) of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 298.15 K.

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0141	39.5000	36.7068	39.4688	0.0380	114.4000	102.6190	116.0400
0.0335	46.8000	41.0505	47.3000	0.0955	155.2000	132.4573	161.5147
0.0517	53.6000	45.4771	54.6797	0.1557	203.2000	169.5399	209.6901
0.1152	78.8000	63.3905	80.6655	0.2194	252.8000	214.1865	261.2256
0.1575	95.3000	77.2276	98.1690	0.2889	306.7000	267.9028	318.0031
0.3082	155.7000	135.8159	161.5747	0.3538	359.4000	321.6018	371.4184
0.3613	178.4000	158.9049	184.2119	0.4870	468.9000	438.4949	481.6360
0.4270	208.7000	188.5527	212.3429	0.5616	533.4000	505.9730	543.2813
0.4821	228.8000	214.0344	235.9794	0.5684	535.3000	510.3348	547.2367
0.5367	253.2000	239.6083	259.3606	0.6444	602.0000	581.2534	611.2066
0.5861	272.8000	262.8736	280.4844	0.7002	650.8000	631.7924	656.5043
0.6558	303.7000	295.6866	310.0575	0.7248	673.1000	653.7774	678.1605
0.7065	326.0000	319.4181	331.3566	0.7979	739.1000	719.2233	734.5947
0.7656	352.1000	346.8210	355.9019	0.8533	792.7000	767.9465	778.1650
0.8271	377.9000	374.9408	381.0957	0.8665	800.4000	779.4473	788.4847
0.8707	397.4000	394.5858	398.7651	0.8795	822.3000	790.7306	798.6313
0.9492	432.6000	429.2671	430.4273	0.9223	851.4000	827.5617	831.9812
0.9544	434.5000	431.5312	432.5336	0.9506	870.7000	851.6360	854.0750
0.9771	442.6000	441.3644	441.7721	0.9631	875.5000	862.1962	863.8752
				0.9776	884.1000	874.3884	875.2961
				0.9904	889.6000	885.0993	885.4414

Table E.4.12 P (kPa) of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system based on parameters from H^E data at 308.15 K.

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0141	39.5000	36.6402	39.4817	0.0380	114.4000	102.3222	116.0969
0.0335	46.6000	40.9032	47.3302	0.0956	155.2000	131.8569	161.6477
0.0517	53.6000	45.2646	54.7253	0.1557	203.2000	168.7822	209.8892
0.1152	76.8000	63.0233	80.7594	0.2194	252.8000	213.3883	261.4789
0.1575	95.3000	76.8098	98.2899	0.2889	306.7000	267.1500	318.2966
0.3082	155.7000	135.4228	161.7575	0.3538	359.4000	320.9411	371.7313
0.3613	178.4000	158.5580	184.4032	0.4870	468.9000	438.0618	481.9357
0.4270	206.7000	188.2694	212.5352	0.5616	533.4000	505.6553	543.5461
0.4821	228.8000	213.8038	236.1647	0.5664	535.3000	510.0236	547.4987
0.5367	253.2000	239.4256	259.5525	0.6444	602.0000	581.0408	611.4152
0.5861	272.8000	262.7291	280.6394	0.7002	650.8000	631.6361	656.6689
0.6558	303.7000	295.5871	310.1824	0.7248	673.1000	653.6422	676.3053
0.7065	326.0000	319.3446	331.4566	0.7979	739.1000	719.1403	734.6822
0.7656	352.1000	346.7714	355.9725	0.8533	792.7000	767.8933	778.2156
0.8271	377.9000	374.9101	381.1380	0.8685	800.4000	779.4002	788.5279
0.8707	397.4000	394.5652	398.7908	0.8795	822.3000	790.6892	798.6678
0.9492	432.6000	429.2603	430.4334	0.9223	851.4000	827.5370	831.9997
0.9544	434.5000	431.5251	432.5388	0.9508	870.7000	851.6210	854.0851
0.9771	442.6000	441.3615	441.7745	0.9831	875.5000	862.1852	863.8824
				0.9776	884.1000	874.3819	875.3003
				0.9904	889.6000	885.0965	885.4431

Table E.4.13 P (kPa) of toluene (1) and 1-chlorohexane (2) system based on parameters from H^E data at 288.15 K.

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0560	5.0500	4.8643	5.0123	0.0389	11.9400	11.6502	11.8810
0.1859	5.9500	5.4681	5.8370	0.1029	12.8400	12.1621	12.7011
0.2877	6.6800	6.0980	6.5347	0.1647	13.7400	12.7721	13.5269
0.3200	6.9300	6.3226	6.7651	0.2306	14.7300	13.5404	14.4436
0.3691	7.3100	6.6840	7.1233	0.3046	15.8700	14.5342	15.5160
0.4230	7.6900	7.1052	7.5272	0.3707	16.8900	15.5244	16.5111
0.4578	8.0000	7.3889	7.7935	0.4388	17.9700	16.6299	17.5706
0.5248	8.5100	7.9587	8.3176	0.4783	18.5800	17.3045	18.2006
0.6070	9.1700	8.6832	8.9790	0.5129	19.1300	17.9125	18.7607
0.6979	9.9000	9.5111	9.7295	0.5900	20.4000	19.3144	20.0353
0.7969	10.6900	10.4253	10.5624	0.6739	21.7900	20.6939	21.4580
0.8898	11.4000	11.2815	11.3503	0.7464	22.9900	22.2857	22.7109
0.9600	11.9700	11.9206	11.9441	0.8017	23.9000	23.3549	23.6770
				0.8666	24.9800	24.6100	24.8175
				0.9288	26.0300	25.8063	25.9122
				0.9731	26.7600	26.6510	26.6897

Table E.4.14 P (kPa) of toluene (1) and 1-chlorohexane (2) system based on parameters from H^E data at 298.15 K.

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0560	5.0600	4.8791	5.0141	0.0389	11.9400	11.6723	11.8831
0.1859	5.9500	5.5073	5.8412	0.1029	12.8400	12.2155	12.7058
0.2877	6.6800	6.1461	6.5393	0.1647	13.7400	12.8487	13.5331
0.3200	6.9300	6.3719	6.7696	0.2306	14.7300	13.6341	14.4504
0.3691	7.3100	6.7337	7.1276	0.3046	15.8700	14.6383	15.5227
0.4230	7.6900	7.1537	7.5309	0.3707	16.8900	15.6309	16.5169
0.4578	8.0000	7.4359	7.7969	0.4388	17.9700	16.7332	17.5754
0.5248	8.5100	7.9994	8.3203	0.4783	18.5800	17.4038	18.2043
0.6070	9.1700	8.7190	8.9807	0.5129	19.1300	18.0073	18.7637
0.6979	9.9000	9.5381	9.7302	0.5900	20.4000	19.3984	20.0367
0.7969	10.6900	10.4428	10.5625	0.6739	21.7900	20.9591	21.4580
0.8898	11.4000	11.2902	11.3503	0.7464	22.9900	22.3353	22.7102
0.9600	11.9700	11.9235	11.9441	0.8017	23.9000	23.3927	23.6760
				0.8666	24.9800	24.6343	24.8166
				0.9288	26.0300	25.8186	25.9117
				0.9731	26.7600	26.6554	26.6896

Table E.4.15 P (kPa) of 1-chlorohexane (1) and ethylbenzene (2) system based on parameters from H^E data at 288.15 K.

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0331	4.6400	4.6180	4.6279	0.0351	11.2500	11.1684	11.2127
0.0683	4.6300	4.5855	4.6058	0.1054	11.2500	11.0501	11.1289
0.1376	4.6200	4.5264	4.5673	0.1768	11.2400	10.9292	11.0596
0.2182	4.6100	4.4670	4.5309	0.2394	11.2400	10.8398	11.0124
0.3132	4.6000	4.4122	4.5001	0.3187	11.2400	10.7509	10.9710
0.3942	4.6000	4.3801	4.4843	0.3397	11.2400	10.7324	10.9635
0.4482	4.5900	4.3669	4.4792	0.3752	11.2400	10.7061	10.9540
0.4825	4.5900	4.3621	4.4780	0.3859	11.2400	10.6995	10.9519
0.4903	4.5900	4.3614	4.4780	0.4399	11.2400	10.6750	10.9472
0.5537	4.5900	4.3613	4.4810	0.4468	11.2400	10.6730	10.9472
0.5554	4.6000	4.3615	4.4811	0.4860	11.2400	10.6666	10.9504
0.6356	4.5900	4.3763	4.4928	0.4973	11.2400	10.6664	10.9522
0.7358	4.6000	4.4178	4.5188	0.5119	11.2500	10.6671	10.9551
0.8389	4.6100	4.4664	4.5578	0.5803	11.2500	10.6868	10.9771
0.9377	4.6300	4.5747	4.6054	0.7059	11.2800	10.7937	11.0525
0.9915	4.6400	4.6307	4.6351	0.8037	11.3100	10.9398	11.1398
				0.9029	11.3400	11.1398	11.2512
				0.9909	11.3700	11.3559	11.3672

Table E.4.16 P (kPa) of 1-chlorohexane (1) and ethylbenzene (2) system based on parameters from H^E data at 298.15 K.

	T = 323.15 K				T = 343.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0331	4.6400	4.6195	4.6311	0.0351	11.2500	11.1899	11.2209
0.0683	4.6300	4.5884	4.6124	0.1054	11.2500	11.0601	11.1518
0.1376	4.6200	4.5319	4.5795	0.1768	11.2400	10.9450	11.0948
0.2182	4.6100	4.4752	4.5484	0.2394	11.2400	10.8598	11.0560
0.3132	4.6000	4.4226	4.5218	0.3187	11.2400	10.7752	11.0221
0.3942	4.6000	4.3917	4.5079	0.3397	11.2400	10.7576	11.0159
0.4482	4.5900	4.3789	4.5031	0.3752	11.2400	10.7324	11.0083
0.4825	4.5900	4.3742	4.5019	0.3859	11.2400	10.7280	11.0066
0.4903	4.5900	4.3735	4.5018	0.4399	11.2400	10.7026	11.0030
0.5537	4.5900	4.3731	4.5039	0.4468	11.2400	10.7007	11.0031
0.5554	4.6000	4.3732	4.5040	0.4860	11.2400	10.6944	11.0061
0.6356	4.5900	4.3870	4.5135	0.4973	11.2400	10.6942	11.0077
0.7358	4.6000	4.4263	4.5353	0.5119	11.2500	10.6948	11.0102
0.8389	4.6100	4.4919	4.5686	0.5803	11.2500	10.7134	11.0294
0.9377	4.6300	4.5769	4.6098	0.7059	11.2800	10.8152	11.0944
0.9915	4.6400	4.6310	4.6357	0.8037	11.3100	10.9550	11.1700
				0.9029	11.3400	11.1477	11.2671
				0.9909	11.3700	11.3566	11.3687

Table E.4.17 P (kPa) of 1-chlorohexane (1) and n-propylbenzene (2) system based on parameters from H^E data at 288.15 K.

x_1	Exp	Wilson	UNIQUAC
0.0416	11.6700	11.6735	11.7404
0.1609	13.7100	13.0256	13.2710
0.2603	14.6500	13.7925	14.0986
0.3289	15.6700	14.7311	15.0825
0.4125	16.7800	15.8045	16.1770
0.4528	17.3200	16.3472	16.7203
0.4699	17.5100	16.5821	16.9537
0.5375	18.4600	17.5352	17.8909
0.6230	19.5800	18.7900	19.1053
0.7083	20.6900	20.0543	20.3125
0.7899	21.8300	21.3518	21.5404
0.8803	23.0400	22.7717	22.8779
0.9560	24.0600	23.9620	23.9996

Table E.4.18 P (kPa) of 1-chlorohexane (1) and n-propylbenzene (2) system based on parameters from H^E data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC
0.0416	11.6700	11.6861	11.7557
0.1809	13.7100	13.0698	13.3232
0.2503	14.6600	13.8465	14.1615
0.3289	15.6700	14.7915	15.1519
0.4125	16.7800	15.8668	16.2478
0.4526	17.3200	16.4068	16.7900
0.4699	17.5100	16.6431	17.0226
0.5375	18.4800	17.5924	17.9552
0.6230	19.5800	18.8394	19.1607
0.7063	20.6900	20.0938	20.3568
0.7899	21.8300	21.3801	21.5723
0.8803	23.0400	22.7874	22.8958
0.9560	24.0600	23.9875	24.0060

Table E.4.19 P (kPa) of 1,2-epoxybutane (1) and methanol (2) system at 298.15 K based on parameters from H^E data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0270	18.7000	17.5873	19.6769	0.4960	27.7000	25.5663	29.9614
0.0470	19.6500	18.0754	21.3304	0.5290	27.8000	25.8509	30.0168
0.0660	20.5000	18.5271	22.6483	0.5710	27.9000	26.1604	30.0566
0.0870	21.2500	19.0129	23.8679	0.6380	27.9500	26.5325	30.0359
0.1060	21.9000	19.4400	24.7929	0.6970	27.9500	26.7363	29.8977
0.1320	22.7000	20.0055	25.8343	0.7480	27.7500	26.8177	29.6418
0.1690	23.7000	20.7722	26.9667	0.7910	27.6000	26.8142	29.2640
0.1930	24.3000	21.2454	27.5322	0.8400	27.3000	26.7174	28.6521
0.2490	25.4000	22.2753	28.4847	0.8900	26.7000	26.4739	27.6598
0.2990	26.1000	23.1067	29.0365	0.9310	25.8500	26.0604	26.4802
0.3610	26.7500	24.0214	29.4805	0.9580	25.0500	25.5385	25.4650
0.4280	27.3000	24.8847	29.7785	0.9830	24.3000	24.6085	24.3142

Table E.4.20 P (kPa) of 1,2-epoxybutane (1) and ethanol (2) system at 298.15 K based on parameters from H^E data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0170	8.7500	10.8760	11.7864	0.6300	22.2000	28.5568	29.7678
0.0390	9.9500	14.0500	16.0346	0.6810	22.6000	28.6078	29.6400
0.0740	11.5500	17.8274	21.1943	0.7370	22.9000	28.6386	29.6028
0.1030	12.7000	20.1184	24.3087	0.7940	23.2000	28.6487	29.6251
0.1490	14.4000	22.7159	27.6749	0.8360	23.4000	28.6427	29.5956
0.1860	15.6000	24.1784	29.3680	0.8730	23.6000	28.6228	29.4211
0.2230	16.4500	25.2634	30.4263	0.9050	23.8000	28.5807	29.0157
0.2780	17.7500	26.4006	31.2000	0.9330	23.8500	28.4890	28.2979
0.3250	18.5000	27.0687	31.3715	0.9500	23.8500	28.3609	27.5971
0.3730	19.3000	27.5518	31.2707	0.9620	23.8000	28.1838	26.9321
0.4280	20.1000	27.9400	30.9705	0.9740	23.7000	27.8310	26.0858
0.4910	20.9000	28.2350	30.5380	0.9810	23.6000	27.4435	25.4906
0.5680	21.7000	28.4542	30.0479				

Table E.4.21 P (kPa) of 1,2-epoxybutane (1) and 2-propanol (2) system at 298.15 K based on parameters from H^E data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0170	6.5000	11.9145	13.0786	0.4920	18.6500	27.5864	34.6975
0.0260	7.0500	14.7117	17.1039	0.5770	19.6000	27.6568	32.9156
0.0610	8.3500	19.9741	26.4259	0.6300	20.2000	27.6835	32.1420
0.0760	9.0000	21.4422	29.5505	0.6710	20.7000	27.6986	31.7483
0.0940	9.6500	22.7614	32.5729	0.7290	21.4000	27.7140	31.5134
0.1390	11.2000	24.8017	37.4689	0.7770	21.8000	27.7224	31.5932
0.1960	12.9500	26.0968	40.0398	0.8230	22.2500	27.7256	31.8384
0.2360	14.1000	26.6034	40.4014	0.8560	22.5000	27.7215	32.0202
0.2780	15.0000	26.9490	40.0358	0.8830	22.7000	27.7086	32.0604
0.3090	15.7000	27.1272	39.4636	0.9100	22.9000	27.6741	31.8378
0.3800	16.8500	27.3886	37.6803	0.9300	23.1000	27.6145	31.3440
0.4390	17.9000	27.5139	36.0618	0.9650	23.3000	27.2455	29.1420

Table E.4.22 P (kPa) of ethyl formate (1) and benzene (2) system at 323.15 K based on parameters from H^E data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0260	38.6500	40.3700	41.0882	0.5940	70.7100	75.3423	79.0833
0.1620	48.3300	55.0063	58.4186	0.6790	74.7100	77.9538	81.2371
0.2940	56.8200	63.3802	67.7507	0.7420	77.3000	79.7438	82.6255
0.3560	59.8600	66.3848	70.8355	0.8300	80.6500	82.0394	84.2284
0.4700	64.9700	71.0549	75.3037	0.9390	84.8800	84.5211	85.4897

Table E.4.23 P (kPa) of ethyl formate (1) and benzene (2) system at 323.15 K based on parameters from H^E data at 308.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0260	38.6500	39.5246	40.2519	0.5940	70.7100	73.8329	77.4897
0.1620	48.3300	52.5422	55.8160	0.6790	74.7100	76.6988	79.8888
0.2940	56.8200	60.9917	65.2024	0.7420	77.3000	78.6871	81.4661
0.3560	59.8500	64.1631	68.4757	0.8300	80.6500	81.2881	83.3710
0.4700	64.9700	69.1764	73.3278	0.9390	84.8600	84.2208	85.1258

Table E.4.24 P (kPa) of ethyl formate (1) and benzene (2) system at 323.15 K based on parameters from H^E data at 318.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0260	38.6500	39.2907	40.0328	0.5940	70.7100	73.1457	76.8721
0.1620	48.3300	51.7120	55.0304	0.6790	74.7100	76.1171	79.3600
0.2940	56.8200	60.0659	64.3410	0.7420	77.3000	78.1927	81.0086
0.3560	59.8500	63.2580	67.6432	0.8300	80.6500	80.9326	83.0293
0.4700	64.9700	68.3578	72.5885	0.9390	84.8600	84.0763	84.9775

Table E.4.25 P (kPa) of ethyl formate (1) and cyclohexane (2) system at 323.15 K based on parameters from H^E data at 298.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0690	55.3400	97.1869	127.9228	0.6260	89.9700	108.9420	130.5238
0.2070	73.6300	108.4938	160.4406	0.7960	91.5900	108.6920	132.9339
0.3670	83.2600	107.9989	145.8620	0.8500	91.1400	107.8066	132.5538
0.4570	85.8700	108.3977	137.3927	0.9780	88.6100	94.3796	102.0513
0.5730	88.4100	108.7996	131.3851				

Table E.4.26 P (kPa) of ethyl formate (1) and cyclohexane (2) system at 323.15 K based on parameters from H^E data at 308.15 K.

x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.0690	55.3400	103.7083	124.7193	0.6260	89.9700	111.1790	129.2761
0.2070	73.6300	109.6619	157.2585	0.7960	91.5900	110.9397	131.3643
0.3670	83.2600	110.5372	143.6773	0.8500	91.1400	110.1571	130.8283
0.4570	85.8700	110.7967	135.8444	0.9780	88.6100	96.2052	101.2440
0.5730	88.4100	111.0766	130.1132				

Table E.4.27 P (kPa) of butanenitrile (1) and 2-butanol (2) system based on parameters from H^E data at 298.15 K.

	T = 278.15 K				T = 288.15 K				T = 293.15 K				T = 298.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.9411	0.9090	1.1610	3.0042	0.9411	1.6570	2.2441	5.8146	0.9411	2.2300	3.0710	7.9897	0.9411	2.9140	4.1310	10.6801
0.9158	0.9270	1.1961	3.1850	0.9158	1.7130	2.3271	6.2156	0.9158	2.2880	3.1966	8.5766	0.9158	3.0250	4.3131	11.5065
0.8745	0.9250	1.2232	3.1504	0.8745	1.7450	2.3940	6.2078	0.8745	2.3490	3.2995	8.6064	0.8745	3.0980	4.4647	11.6002
0.7794	0.9710	1.2420	2.6788	0.7794	1.8270	2.4433	5.3291	0.7794	2.4660	3.3777	7.4214	0.7794	3.2930	4.5828	10.0612
0.7500	0.9670	1.2438	2.5405	0.7500	1.8350	2.4486	5.0551	0.7500	2.4760	3.3865	7.0400	0.7500	3.2960	4.5963	9.5506
0.6382	0.9880	1.2461	2.1918	0.6382	1.8610	2.4563	4.3271	0.6382	2.5330	3.3999	6.0003	0.6382	3.3930	4.6180	8.1307
0.6056	0.9970	1.2462	2.1438	0.6056	1.8720	2.4568	4.2139	0.6056	2.5490	3.4011	5.8300	0.6056	3.4060	4.6200	7.8898
0.5541	0.9840	1.2460	2.1149	0.5541	1.8530	2.4569	4.1225	0.5541	2.5460	3.4017	5.6784	0.5541	3.3920	4.6214	7.6637
0.5315	1.0000	1.2458	2.1199	0.5315	1.8790	2.4568	4.1153	0.5315	2.5340	3.4017	5.6562	0.5315	3.3860	4.6216	7.6227
0.4304	0.9840	1.2448	2.2795	0.4304	1.8570	2.4551	4.3329	0.4304	2.4960	3.3999	5.8891	0.4304	3.3640	4.6196	7.8732
0.4298	0.9810	1.2448	2.2812	0.4298	1.8670	2.4551	4.3355	0.4298	2.5040	3.3998	5.8922	0.4298	3.3920	4.6196	7.8769
0.3716	0.9610	1.2438	2.4865	0.3716	1.8240	2.4533	4.6618	0.3716	2.4810	3.3975	6.2902	0.3716	3.3570	4.6166	8.3621
0.3037	0.9240	1.2421	2.8524	0.3036	1.7920	2.4499	5.2583	0.3036	2.4520	3.3929	7.0313	0.3036	3.2900	4.6103	9.2791
0.2892	0.9430	1.2416	2.9505	0.2892	1.7970	2.4488	5.4172	0.2892	2.4140	3.3914	7.2295	0.2892	3.3280	4.6083	9.5248
0.2197	0.8910	1.2377	3.5255	0.2197	1.7210	2.4407	6.3474	0.2197	2.3650	3.3801	8.3859	0.2196	3.1730	4.5925	10.9553
0.2072	0.9090	1.2365	3.6460	0.2071	1.7650	2.4383	6.5412	0.2071	2.3620	3.3768	8.6253	0.2071	3.2010	4.5879	11.2467
0.1785	0.8760	1.2330	3.9355	0.1785	1.6810	2.4310	6.9955	0.1784	2.3080	3.3665	9.1850	0.1784	3.1140	4.5736	11.9283
0.1503	0.8680	1.2276	4.2211	0.1502	1.6560	2.4197	7.4343	0.1502	2.2840	3.3506	9.7140	0.1502	3.0620	4.5516	12.5631
0.0962	0.8040	1.2041	4.5967	0.0962	1.5710	2.3712	7.9385	0.0962	2.1660	3.2628	10.2791	0.0962	2.9260	4.4575	13.1839
0.0689	0.7560	1.1743	4.4920	0.0688	1.4630	2.3103	7.6813	0.0688	2.0350	3.1983	9.9057	0.0688	2.8220	4.3413	12.6571

Table E.4.27 (continued)

	T = 303.15 K				T = 308.15 K				T = 313.15 K				T = 323.15 K		
x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC	x_1	Exp	Wilson	UNIQUAC
0.9412	3.8450	5.4874	14.1547	0.9413	4.9410	7.1787	18.3998	0.9413	6.3140	9.3287	23.7758	0.9414	9.9370	15.2175	38.1788
0.9158	3.9200	5.7506	15.3151	0.9158	5.0660	7.5494	19.9883	0.9160	6.4710	9.8401	25.9082	0.9161	10.2390	16.1558	41.8833
0.8747	4.1200	5.9716	15.5127	0.8748	5.2810	7.8630	20.3373	0.8749	6.7590	10.2837	26.4868	0.8754	10.7870	16.9850	43.1942
0.7795	4.2980	6.1489	13.5269	0.7796	5.6100	8.1207	17.8393	0.7796	7.1980	10.6545	23.3660	0.7798	11.5390	17.7139	38.5659
0.7500	4.3420	6.1698	12.8446	0.7500	5.6320	8.1520	16.9495	0.7502	7.2930	10.7001	22.2254	0.7505	11.7240	17.8063	36.7584
0.6383	4.4720	6.2043	10.9147	0.6383	5.8530	8.2046	14.3943	0.6384	7.5430	10.7793	18.8620	0.6387	12.2260	17.9733	31.2207
0.6056	4.5130	6.2079	10.5738	0.6056	5.8890	8.2104	13.9298	0.6058	7.6140	10.7885	18.2380	0.6060	12.3760	17.9941	30.1387
0.5541	4.5290	6.2107	10.2383	0.5542	5.9280	8.2154	13.4561	0.5542	7.6430	10.7969	17.5724	0.5544	12.4630	18.0146	28.9394
0.5315	4.5020	6.2112	10.1668	0.5315	5.9090	8.2165	13.3442	0.5316	7.6770	10.7989	17.4049	0.5318	12.5000	18.0202	28.6057
0.4304	4.5050	6.2095	10.4078	0.4304	5.9050	8.2155	13.5599	0.4304	7.6890	10.7996	17.5586	0.4305	12.5950	18.0283	28.5082
0.4298	4.4900	6.2095	10.4121	0.4298	5.9090	8.2155	13.5647	0.4298	7.6530	10.7995	17.5640	0.4299	12.6350	18.0283	28.5144
0.3716	4.4530	6.2058	10.9863	0.3716	5.8520	8.2110	14.2375	0.3717	7.6570	10.7944	18.3379	0.3717	12.5790	18.0224	29.5038
0.3035	4.4120	6.1976	12.0978	0.3035	5.8020	8.2004	15.5684	0.3038	7.5980	10.7811	19.9076	0.3038	12.5300	18.0024	31.6375
0.2893	4.3980	6.1950	12.3921	0.2893	5.7900	8.1970	15.9221	0.2893	7.5580	10.7767	20.3371	0.2893	12.5430	17.9954	32.2277
0.2196	4.2650	6.1738	14.1274	0.2196	5.6640	8.1688	18.0016	0.2198	7.4330	10.7398	22.7992	0.2198	12.3760	17.9347	35.5985
0.2073	4.2780	6.1676	14.4725	0.2073	5.6500	8.1605	18.4125	0.2073	7.4140	10.7288	23.2919	0.2073	12.3840	17.9163	36.2645
0.1784	4.1850	6.1480	15.2933	0.1783	5.5740	8.1342	19.3863	0.1786	7.3270	10.6943	24.4217	0.1786	12.3040	17.8584	37.7693
0.1504	4.1200	6.1183	16.0358	0.1504	5.4930	8.0944	20.2466	0.1504	7.1990	10.6412	25.4242	0.1504	12.1900	17.7687	39.0554
0.0961	3.9600	5.9901	16.6996	0.0961	5.2810	7.9230	20.9297	0.0963	6.9820	10.4160	26.1047	0.0963	11.8560	17.3906	39.6128
0.0689	3.8140	5.8350	15.9859	0.0689	5.1360	7.7174	19.9773	0.0689	6.8170	10.1449	24.8519	0.0689	11.6440	16.9419	37.5613

E.5 Sensitivity based on VLE data

Table E.5.1 Sensitivity of benzene (1) and cyclohexane (2) system at 323.15 K based on VLE data.

% Error of Parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	4.38	4.04
-20.00	1.85	1.68
-10.00	1.00	0.91
-5.00	0.58	0.53
0.00	0.15	0.15
5.00	0.27	0.22
10.00	0.70	0.59
20.00	1.55	1.32
50.00	4.10	3.42

Table E.5.2 Sensitivity of 1-chloropentane (1) and di-n-butyl ether (2) system at 323.15 K based on VLE data.

% Error of Parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	0.18	0.29
-20.00	0.15	0.11
-10.00	0.15	0.13
-5.00	0.14	0.13
0.00	0.12	0.13
5.00	0.10	0.12
10.00	0.09	0.10
20.00	0.16	0.10
50.00	0.81	0.48

Table E.5.3 Sensitivity of 1,2-dichloroethane (1) and di-n-butyl ether (2) system at 350.00 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	4.05	4.02
-20.00	1.79	1.81
-10.00	1.02	1.04
-5.00	0.63	0.65
0.00	0.34	0.35
5.00	0.40	0.41
10.00	0.64	0.66
20.00	1.38	1.42
50.00	3.76	3.94

Table E.5.4 Sensitivity of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system at 343.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	1.25	3.33
-20.00	0.91	2.09
-10.00	0.96	1.17
-5.00	1.07	0.95
0.00	1.21	1.22
5.00	1.39	1.88
10.00	1.62	2.65
20.00	2.16	4.34
50.00	4.19	10.36

Table E.5.5 Sensitivity of toluene (1) and 1-chlorohexane (2) system at 343.15 K based on VLE data.

% Error of Parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	0.96	4.50
-20.00	0.58	2.54
-10.00	0.37	1.42
-5.00	0.25	0.79
0.00	0.12	0.12
5.00	0.06	0.64
10.00	0.21	1.41
20.00	0.55	3.08
50.00	1.80	8.83

Table E.5.6 Sensitivity of 1-chlorohexane (1) and ethylbenzene (2) system at 343.15 K based on VLE data.

% Error of Parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	0.62	3.56
-20.00	0.36	1.98
-10.00	0.20	1.08
-5.00	0.11	0.57
0.00	0.03	0.03
5.00	0.11	0.58
10.00	0.22	1.21
20.00	0.48	2.57
50.00	1.44	7.39

Table E.5.7 Sensitivity of 1-chlorohexane (1) and n-propylbenzene (2) system at 363.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	0.94	3.38
-20.00	0.75	2.06
-10.00	0.58	1.28
-5.00	0.47	0.84
0.00	0.36	0.36
5.00	0.23	0.16
10.00	0.10	0.70
20.00	0.23	1.89
50.00	1.42	6.07

Table E.5.8 Sensitivity of 1,2-epoxybutane (1) and methanol (2) system at 298.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	11.02	10.13
-20.00	4.02	3.81
-10.00	1.89	1.82
-5.00	0.88	0.86
0.00	0.43	0.50
5.00	1.13	1.11
10.00	1.99	1.94
20.00	3.66	3.58
50.00	7.88	7.95

Table E.5.9 Sensitivity of 1,2-epoxybutane (1) and ethanol (2) system at 298.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	9.04	8.53
-20.00	3.44	3.32
-10.00	1.70	1.67
-5.00	0.87	0.87
0.00	0.46	0.58
5.00	1.01	1.04
10.00	1.64	1.65
20.00	3.01	2.94
50.00	6.89	6.84

Table E.5.10 Sensitivity of 1,2-epoxybutane (1) and 2-propanol (2) system at 298.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	8.40	8.29
-20.00	2.82	2.89
-10.00	1.92	1.79
-5.00	1.88	1.81
0.00	2.25	2.26
5.00	2.84	2.92
10.00	3.58	3.74
20.00	5.24	5.57
50.00	11.29	12.65

Table E.5.11 Sensitivity of ethyl formate (1) and benzene (2) system at 323.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	3.49	1.43
-20.00	1.56	0.77
-10.00	0.92	0.88
-5.00	0.73	0.66
0.00	0.68	0.68
5.00	0.79	0.69
10.00	0.94	0.73
20.00	1.33	0.82
50.00	3.02	1.07

Table E.5.12 Sensitivity of ethyl formate (1) and cyclohexane (2) system at 323.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	12.83	12.53
-20.00	5.85	5.85
-10.00	3.62	3.65
-5.00	2.52	2.56
0.00	1.81	1.76
5.00	1.67	1.65
10.00	1.71	1.95
20.00	3.09	3.29
50.00	8.67	9.06

Table E.5.13 Sensitivity of butanenitrile (1) and 2-butanol (2) system at 323.15 K based on VLE data.

% Error of parameters	% AAD (P)	
	Wilson	UNIQUAC
-50.00	11.34	11.77
-20.00	4.56	4.84
-10.00	2.31	2.46
-5.00	1.20	1.27
0.00	0.54	0.60
5.00	1.04	1.26
10.00	2.08	2.35
20.00	4.22	4.77
50.00	10.33	12.05

E.6 Sensitivity based on H^E data

Table E.6.1 Sensitivity of benzene (1) and cyclohexane (2) system at 298.15 K based on H^E data (Meyer et al., 1977).

% Error of Parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	19.55	45.98
-20.00	8.84	17.49
-10.00	9.67	8.64
-5.00	10.53	4.33
0.00	11.64	0.35
5.00	12.95	4.06
10.00	14.45	8.14
20.00	17.89	16.06
50.00	31.88	38.04

Table E.6.2 Sensitivity of 1-chloropentane (1) and di-n-butyl ether (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	69.36	36.13
-20.00	53.27	34.83
-10.00	28.85	20.63
-5.00	13.13	10.96
0.00	9.34	1.27
5.00	25.22	13.51
10.00	47.82	28.31
20.00	99.79	63.02
50.00	308.30	207.85

Table E.6.3 Sensitivity of 1,2-dichloroethane (1) and di-n-butyl ether (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	37.46	47.23
-20.00	12.42	18.36
-10.00	5.76	9.19
-5.00	2.77	4.66
0.00	0.62	0.95
5.00	2.80	4.16
10.00	5.32	8.51
20.00	9.89	17.03
50.00	20.36	41.33

Table E.6.4 Sensitivity of 1,1,1-trichloroethane (1) and di-n-butyl ether (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	61.59	144.56
-20.00	27.63	80.28
-10.00	14.44	44.43
-5.00	7.48	23.88
0.00	1.38	4.04
5.00	7.15	22.41
10.00	14.83	48.10
20.00	30.91	104.52
50.00	85.03	312.74

Table E.6.5 Sensitivity of toluene (1) and 1-chlorohexane (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	52.46	59.43
-20.00	21.29	25.78
-10.00	10.45	12.99
-5.00	4.94	6.30
0.00	1.41	1.27
5.00	6.24	7.67
10.00	11.92	14.95
20.00	23.45	30.10
50.00	59.41	80.32

Table E.6.6 Sensitivity of 1-chlorohexane (1) and ethylbenzene (2) system at 298.15 K based on H^E data.

% Error of Parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	51.47	52.86
-20.00	20.82	21.73
-10.00	10.34	10.86
-5.00	5.08	5.36
0.00	0.59	0.54
5.00	5.61	5.85
10.00	10.99	11.55
20.00	21.86	23.13
50.00	55.23	59.30

Table E.6.7 Sensitivity of 1-chlorohexane (1) and n-propylbenzene (2) system at 298.15 K based on H^E data.

% Error of Parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	51.08	49.97
-20.00	20.19	19.54
-10.00	9.64	9.33
-5.00	4.31	4.22
0.00	2.03	1.97
5.00	6.44	6.04
10.00	11.86	11.18
20.00	22.81	21.49
50.00	56.44	52.63

Table E.6.8 Sensitivity of 1,2-epoxybutane (1) and methanol (2) system at 298.15 K based on H^E data.

% Error of Parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	28.25	30.08
-20.00	16.12	14.79
-10.00	14.87	12.32
-5.00	14.51	11.59
0.00	14.61	11.51
5.00	14.79	12.26
10.00	15.13	13.97
20.00	16.20	17.29
50.00	20.23	23.11

Table E.6.9 Sensitivity of 1,2-epoxybutane (1) and ethanol (2) system at 298.15 K based on H^E data.

% Error of Parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	28.78	26.41
-20.00	33.67	12.37
-10.00	37.42	9.84
-5.00	39.47	9.43
0.00	41.60	9.58
5.00	43.77	10.32
10.00	45.94	11.67
20.00	50.20	14.25
50.00	61.12	18.73

Table E.6.10 Sensitivity of 1,2-epoxybutane (1) and 2-propanol (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	44.11	31.44
-20.00	48.09	14.21
-10.00	51.48	11.43
-5.00	53.36	10.96
0.00	55.32	11.66
5.00	57.31	13.25
10.00	59.31	15.08
20.00	63.26	19.08
50.00	73.46	28.48

Table E.6.11 Sensitivity of ethyl formate (1) and benzene (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	40.09	45.99
-20.00	14.89	19.05
-10.00	8.00	10.93
-5.00	5.32	7.04
0.00	4.23	5.24
5.00	4.02	4.46
10.00	5.48	5.45
20.00	9.38	11.42
50.00	20.21	29.62

Table E.6.12 Sensitivity of ethyl formate (1) and cyclohexane (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	52.95	37.34
-20.00	54.92	12.71
-10.00	57.78	6.31
-5.00	59.42	3.41
0.00	61.16	1.20
5.00	62.98	2.00
10.00	64.85	4.15
20.00	68.62	8.31
50.00	79.20	17.16

Table E.6.13 Sensitivity of butanenitrile (1) and 2-butanol (2) system at 298.15 K based on H^E data.

% Error of parameters	% AAD (H^E)	
	Wilson	UNIQUAC
-50.00	62.96	31.83
-20.00	65.11	8.63
-10.00	67.57	3.57
-5.00	68.98	2.51
0.00	70.45	2.86
5.00	71.98	3.59
10.00	73.53	4.42
20.00	76.65	6.19
50.00	85.09	9.84

APPENDIX F

COMPUTER PROGRAMS

In this section are presented the Pascal programs for convenience of calculation. There are two programs for obtaining parameters for the Wilson and UNIQUAC equations and two programs for calculation the pressure and excess enthalpy, respectively.

F.1 Calculate binary parameters based on VLE data

```
PROGRAM VLE;
USES CRT,PRINTER;
CONST RC = 8.314; {J/mol}
TYPE
    A1 = ARRAY[1..40] OF REAL;
    A2 = ARRAY[1..40,1..2] OF REAL;
    A3 = ARRAY[1..2,1..2] OF REAL;
    A4 = ARRAY[1..2] OF REAL;
VAR
   I,J,K,N : INTEGER;      {N_MAX = 40}
    SELECT,ANS : CHAR;
    DD,HH,KK,S,S1,S2,T,T1,T2,FF,RPD,AAD,CHK,LAM12,LAM21,TEMP,A,B : REAL;
    F,F1,F2,GEXP,GECAL,P,PC,DE,SXR,SXQ,SXQP,CC : A1;
    X,Y,G,GW,GC,PHI,TETA,TETAP,TTETAP,STTETAP,XR,XQ,XQP,PART,LNG : A2;
    SL,VIJ,U,TOR : A3;
    PSAT,V,R,Q,QP,L : A4;
    NAME : ARRAY[1..3] OF STRING;
    FILETEXT : TEXT; FREC:STRING;
PROCEDURE OUTPUT;
BEGIN
  WRITE('INPUT NAME FILE = ');
  READLN(FREC);
  FREC := FREC + '.DAT';
  ASSIGN(FILETEXT,FREC);
  REWRITE(FILETEXT);
  WRITELN(FILETEXT,NAME[1],'[1] + ',NAME[2],'[2] AT ',TEMP:7:2,' K');
  IF SELECT = '1' THEN
     BEGIN
      WRITELN(FILETEXT,'LAM12   LAM21       %AAD ');
      WRITELN(FILETEXT,LAM12:11:8,'  ',LAM21:11:8,'  ',AAD:11:7);
     END;
  IF SELECT = '2' THEN
     BEGIN
      WRITELN(FILETEXT,'U12   U21       %AAD ');
```

```
      WRITELN(FILETEXT,U[1,2]:11:8,' ',U[2,1]:11:8,' ',AAD:11:7);
    END;
  WRITELN(FILETEXT,' ');
  WRITELN(FILETEXT,'x1   Pexp   Pcal');
  FOR I:= 1 TO N DO
    WRITELN(FILETEXT,x[I,1]:5:4,'  ',P[I]:8:4,' ',Pc[I]:8:4);
  WRITELN(FILETEXT,'   ');
  CLOSE(FILETEXT);
END;
FUNCTION GCALW(I:INTEGER;SL:A3;X:A2):REAL;   (***)
(*** CALCULATES GE/RT BY WILSON EQUATION ***)
BEGIN
  GCALW := X[I,1]*LN(X[I,1]+SL[1,2]*X[I,2])+X[I,2]*LN(X[I,2]+SL[2,1]*X[I,1]);
END;
FUNCTION GCALU:REAL;   (***)
(*** CALCULATES GE/RT BY UNIQUAC EQUATION ***)
BEGIN
 GCALU := X[I,1]*(LN(PHI[I,1]/X[I,1])+5*Q[1]*LN(TETA[I,1]/PHI[I,1])-Q[1]*LN(STTETAP[I,1]))
     + X[I,2]*(LN(PHI[I,2]/X[I,2])+5*Q[2]*LN(TETA[I,2]/PHI[I,2])-Q[2]*LN(STTETAP[I,2]));
END;
PROCEDURE FUNC_GCAL;   (***)
BEGIN
  IF SELECT = '1' THEN FOR I:= 1 TO N DO GECAL[I] := GCALW(I,SL,X);
  IF SELECT = '2' THEN FOR I:= 1 TO N DO GECAL[I] := GCALU;
END;
PROCEDURE FUNC_SUMF;   (***)
BEGIN
  DD := 0.0;  HH := 0.0;    KK := 0.0;
  S := 0.0;   S1 := 0.0;    S2 := 0.0;  T := 0.0;   T1 := 0.0;    T2 := 0.0;
  FOR I:= 1 TO N DO
    BEGIN
     S  := S  + F[I]*F1[I];
     T  := T  + F[I]*F2[I];
     S1 := S1 + Sqr(F1[I]);
     S2 := S2 + F1[I]*F2[I];
     T1 := S2;
     T2 := T2 + Sqr(F2[I]);
    END;
  DD := S1*T2 - S2*T1;
  HH := (S*T2 - T*T1)/DD;
  KK := (S1*T - T1*S)/DD;
END;
PROCEDURE FUNC_DGW;   (***)
(*** DERIVATIES OF GE/RT BY WILSON MODEL ***)
BEGIN
 FUNC_GCAL;
 FOR I:= 1 TO N DO
  BEGIN
   GEXP[I] := X[I,1]*LN(G[I,1])+X[I,2]*LN(G[I,2]);
   F[I] := GEXP[I]+GECAL[I];
```

```
  END;
 S1 := 0.0;  S2 := 0.0;    S := 0.0;  T1 := 0.0;  T2 := 0.0;    T := 0.0;
 FF := 0.0;  KK := 0.0;    DD:= 0.0;     HH := 0.0;
 FOR I:= 1 TO N DO
    BEGIN
     FF := FF+SQR(F[I]);
     F1[I] :=( X[I,1]*X[I,2]/(X[I,1]+SL[1,2]*X[I,2]));
     F2[I] :=( X[I,1]*X[I,2]/(X[I,2]+SL[2,1]*X[I,1]));
    END;
END;
PROCEDURE FUNC_DGU;   (***)
(*** DERIVATIES OF GE/RT BY UNIQUAC MODEL ***)
BEGIN
 FUNC_GCAL;
 FOR I:= 1 TO N DO
  BEGIN
   GEXP[I] := X[I,1]*LN(G[I,1])+X[I,2]*LN(G[I,2]);
   F[I] := GEXP[I]-GECAL[I];
  END;
 S1 := 0.0;  S2 := 0.0;  S := 0.0;  T := 0.0;  T1 := 0.0;  T2 := 0.0;
 FF := 0.0;  KK := 0.0;  DD := 0.0; HH := 0.0;
 FOR I:= 1 TO N DO
    BEGIN
     FF := FF+SQR(F[I]);
     F1[I] := PART[I,2];
     F2[I] := PART[I,1];
    END;
END;
PROCEDURE WILSONCA;   (***)
(*CALCULATE THE ACTIVITY COEFFICIENTS WHEN KNOWN ALL PARAMETERS*)
VAR
  IS,IT : INTEGER;
  SXV,SXL,SXK,G11 : REAL;
BEGIN
   IS := 2;
   FOR IT:= 1 TO N DO
    BEGIN
     FOR I:= 1 TO IS DO
      BEGIN
       SXV := 0.0; SXL := 0.0;
       FOR J:= 1 TO IS DO
        BEGIN
         SXV := SXV + X[IT,J];
         SXL := SXL + X[IT,J]*SL[I,J];
        END;
       G11 := LN(SXV/SXL);
       SXK := 0.0;
       FOR K:= 1 TO IS DO
        BEGIN
         SXV := 0.0; SXL := 0.0;
```

```
          FOR J:= 1 TO IS DO
           BEGIN
            SXV := SXV + X[IT,J];
            SXL := SXL + X[IT,J]*SL[K,J];
           END;
          SXK := SXK + X[IT,K]*((1/SXV)-(SL[K,I]/SXL));
         END;
        GW[IT,I] := EXP(G11+SXK);
       END;
    END;
END;
PROCEDURE FUNC_AADW;   (***)
BEGIN
  FOR I:= 1 TO N DO
    BEGIN
      PC[I] := 0.0;
      DE[I] := 0.0;
    END;
  WILSONCA;
  WRITELN('GW[',I,' 1] = ',GW[I,1]:7:4,'    GW[',I,' 2] = ',GW[I,2]:7:4);
  FOR I:= 1 TO N DO
    PC[I] := GW[I,1]*X[I,1]*PSAT[1] + GW[I,2]*X[I,2]*PSAT[2];
  FOR I:= 1 TO N DO
    DE[I] := (PC[I]-P[I])/P[I];
  RPD := 0.0; AAD := 0.0;
  FOR I:= 1 TO N DO
    RPD := RPD + ABS(DE[I]);
  AAD := (100/N)*RPD;
  WRITELN(' P_EXP       P_CAL');
  FOR I:= 1 TO N DO
    WRITELN(P[I]:8:4,'    ',PC[I]:8:4);
  WRITELN;
  WRITELN('%AAD = ',AAD:10:6);
  WRITELN('PRESS ENTER');
  READLN;
END;
PROCEDURE FUNC_AADU;   (***)
BEGIN
 FOR I:= 1 TO N DO
   BEGIN
    PC[I] := 0.0;
    DE[I] := 0.0;
   END;
 FOR I:= 1 TO 2 DO
   L[I]:= 5*(R[I]-Q[I])-(Q[I]-1);
 FOR K:= 1 TO N DO
   CC[K]:= (TOR[2,1]/STTETAP[K,1])-(TOR[1,2]/STTETAP[K,2]);
 FOR K:= 1 TO N DO
  BEGIN
   LNG[K,1] := LN(PHI[K,1]/X[K,1])+5*Q[1]*LN(TETA[K,1]/PHI[K,1])
```

```
+ PHI[K,2]*(L[1]-R[1]*L[2]/R[2])-QP[1]*LN(STTETAP(K,1))+TETAP[K,2]*QP[1]*CC[K];
    LNG[K,2] := LN(PHI[K,2]/X[K,2])+5*Q[2]*LN(TETA[K,2]/PHI[K,2])
+ PHI[K,1]*(L[2]-R[2]*L[1]/R[1])-QP[2]*LN(STTETAP[K,2])-TETAP[K,1]*QP[2]*CC[K];
   END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      GC[K,I] := EXP(LNG[K,I]);
  FOR I:= 1 TO N DO
    PC[I] := GC[I,1]*X[I,1]*PSAT[1] + GC[I,2]*X[I,2]*PSAT[2];
  FOR I:= 1 TO N DO
    DE[I] := (PC[I]-P[I])/P[I];
  RPD := 0.0; AAD := 0.0;
  FOR I:= 1 TO N DO
    RPD := RPD + ABS(DE[I]);
  AAD := (100/N)*RPD;
  WRITELN(' P_EXP       P_CAL');
  FOR I:= 1 TO N DO
    WRITELN(P[I]:8:4,'    ',PC[I]:8:4);
  WRITELN;
  WRITELN('%AAD = ',AAD:10:6);
  WRITELN('PRESS ENTER');
  READLN;
END;
PROCEDURE WILSONG;    (***)
(*THIS PROCEDURE CALCULATE THE WILSON PARAMETERS BASED ON VLE DATA*)
LABEL 70,200;
BEGIN
  FOR I:= 1 TO 2 DO
    BEGIN
     WRITE('ENTER V',I,' : '); READLN(V[I]);
    END;
  WRITELN;
  FOR I:= 1 TO 2 DO
    FOR J:= 1 TO 2 DO
     BEGIN
      IF I = J THEN
        BEGIN
         VIJ[I,J] := 1.0;
         SL[I,J] := 1.0;
        END
       ELSE
         VIJ[I,J] := V[J]/V[I];
     END;
  WRITELN('V12   = ',VIJ[1,2]:20:10);
  WRITELN(' SL12 = ',SL[1,2]:8:6,'    SL21 = ',SL[2,1]:8:6);
  FOR I:= 1 TO N DO
    BEGIN
      GEXP[I]:= 0.0;
      GECAL[I]:= 0.0;
      F[I] := 0.0;
```

```
      F1[I]:= 0.0;
      F2[I]:= 0.0;
    END;
70: FUNC_DGW;
  FUNC_SUMF;
  WRITELN('SL12 = ',SL[1,2]:20:10,'    SL21 = ',SL[2,1]:20:10);
  CHK := ABS(HH/SL[1,2])+ABS(KK/SL[2,1]);
  IF CHK <= 0.0001 THEN
    BEGIN
     WRITELN('-------------------------------------');
     WRITELN('SL12  = ',SL[1,2]:20:10,'   SL21  = ',SL[2,1]:20:10);
     LAM12 := -RC*TEMP*LN(SL[1,2]/VIJ[1,2]);
     LAM21 := -RC*TEMP*LN(SL[2,1]/VIJ[2,1]);
     WRITELN('LAM12 = ',LAM12:20:4,'   LAM21 = ',LAM21:20:4);
     WRITELN('-------------------------------------');
     WRITELN;
     REPEAT
      WRITE('DO YOU WANT TO PRINT BINARY PARAMETERS? [Y/N] ');
      READLN(ANS);
     UNTIL (ANS = 'Y') OR (ANS = 'y') OR (ANS = 'N') OR (ANS = 'n');
     IF (ANS = 'Y') OR (ANS = 'y') THEN
       WRITELN(LST,' LAM12 = ',LAM12:10:4,'    LAM21 = ',LAM21:10:4);
    END
  ELSE
    BEGIN
     SL[1,2] := SL[1,2]-HH;
     SL[2,1] := SL[2,1]-KK;
     GOTO 70;
    END;
END;
PROCEDURE UNIQG;     (***)
(*THIS PROCEDURE CALCULATE THE UNIQUAC PARAMETERS BASED ON VLE DATA*)
LABEL 10,20,30;
BEGIN
 FOR I:= 1 TO 2 DO
   BEGIN
    WRITE('ENTER R',I,' : '); READLN(R[I]);
    WRITE('ENTER Q',I,' : '); READLN(Q[I]);
    QP[I] := Q[I];
   END;
 FOR I:= 1 TO 2 DO
   FOR J:= 1 TO 2 DO
     IF I = J THEN
       TOR[I,J] := 1.0;
 WRITELN(' TOR12 = ',TOR[1,2]:8:6,'    TOR21 = ',TOR[2,1]:8:6);
 FOR I:= 1 TO N DO
   BEGIN
     GEXP[I]:= 0.0;
     GECAL[I]:= 0.0;
     F[I] := 0.0;
```

```
      F1[I]:= 0.0;
      F2[I]:= 0.0;
    END;
  FOR K:= 1 TO N DO
    BEGIN
      SXR[K]:= 0.0; SXQ[K]:= 0.0; SXQP[K]:= 0.0;
      FOR I:= 1 TO 2 DO
        BEGIN
          PHI[K,I]:= 0.0;  TETA[K,I]:= 0.0; TETAP[K,I]:= 0.0;
          XR[K,I]:= 0.0;   XQ[K,I]:= 0.0;  XQP[K,I]:= 0.0;
        END;
    END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      BEGIN
        XR[K,I] := X[K,I]*R[I];      XQ[K,I] := X[K,I]*Q[I];
        XQP[K,I]:= X[K,I]*QP[I];     SXR[K] := SXR[K] + XR[K,I];
        SXQ[K] := SXQ[K] + XQ[K,I]; SXQP[K] := SXQP[K] + XQP[K,I];
      END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      BEGIN
        PHI[K,I]:= XR[K,I]/SXR[K];
        TETA[K,I]:= XQ[K,I]/SXQ[K];
        TETAP[K,I]:= XQP[K,I]/SXQP[K];
      END;
10: FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      BEGIN
        TTETAP[K,I]:= 0.0;
        STTETAP[K,I] := 0.0;
      END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      FOR J:= 1 TO 2 DO
        IF I = J THEN GOTO 20 ELSE
          BEGIN
            TTETAP[K,I]:= TETAP[K,J]*TOR[J,I];
20:         END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      FOR J:= 1 TO 2 DO
        STTETAP[K,I] := STTETAP[K,I] + TETAP[K,J]*TOR[J,I];
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      FOR J:= 1 TO 2 DO
        IF I = J THEN GOTO 30 ELSE
          BEGIN
            PART[K,I] := (XQP[K,I]/STTETAP[K,I])*TETAP[K,J];
30:         END;
```

```
  FUNC_DGU;
  FUNC_SUMF;
  WRITELN('TOR12 = ',TOR[1,2]:20:10,'    TOR21 = ',TOR[2,1]:20:10);
  CHK := ABS(HH/TOR[1,2])+ABS(KK/TOR[2,1]);
  IF CHK <= 0.0001 THEN
    BEGIN
      WRITELN('-------------------------------------------------');
      WRITELN('TOR12  = ',TOR[1,2]:20:10,'   TOR21  = ',TOR[2,1]:20:10);
      U[1,2] := -RC*TEMP*LN(TOR[1,2]);
      U[2,1] := -RC*TEMP*LN(TOR[2,1]);
      WRITELN('U12 = ',U[1,2]:20:4,'    U21 = ',U[2,1]:20:4);
      WRITELN('-------------------------------------------------');
      WRITELN;
      REPEAT
       WRITE('DO YOU WANT TO PRINT BINARY PARAMETERS? [Y/N] ');
       READLN(ANS);
      UNTIL (ANS = 'Y') OR (ANS = 'y') OR (ANS = 'N') OR (ANS = 'n');
      IF (ANS = 'Y') OR (ANS = 'y') THEN
        WRITELN(LST,' U12 = ',U[1,2]:10:4,'   U[2,1] = ',U[2,1]:10:4);
    END
  ELSE
    BEGIN
      TOR[1,2] := TOR[1,2]-HH;
      TOR[2,1] := TOR[2,1]-KK;
      GOTO 10;
    END;
END;
PROCEDURE FUNC_AADP;   (***)
BEGIN
  IF SELECT = '1' THEN FUNC_AADW;
  IF SELECT = '2' THEN FUNC_AADU;
END;
(****** MAIN PROGRAM ******)
BEGIN
  CLRSCR;
  WRITELN('************************************************');
  WRITELN('              INPUT DATA');
  WRITELN('************************************************');
  WRITE('NAME OF COMPONENT 1 : '); READLN(NAME[1]);
  WRITE('NAME OF COMPONENT 2 : '); READLN(NAME[2]);
  WRITE('PSAT[1] : '); READLN(PSAT[1]);
  WRITE('PSAT[2] : '); READLN(PSAT[2]);
  WRITE('NO. OF DATA : '); READLN(N);
  WRITE('TEMPERATURE [K] : '); READLN(TEMP);
  WRITELN('PRESSURE, MOLE FRACTION OF COMPONENT 1, GAMMA1 AND GAMMA2 ');
  FOR I:= 1 TO N DO
    BEGIN
      WRITE('   P[',I:2,'] [kPa] : '); READLN(P[I]);
      WRITE('   X1[',I:2,'] : '); READLN(X[I,1]);
      WRITE('   GAMMA1[',I:2,'] : '); READLN(G[I,1]);
```

```
      WRITE('    GAMMA2[',I:2,'] : '); READLN(G[I,2]);
      WRITELN;
    END;
  FOR I:= 1 TO N DO
    X[I,2] := 1.0-X[I,1];
  WRITE('INITIAL GUESS PARAMETER A = 0.4 ');
  WRITE('INITIAL GUESS PARAMETER B = 0.4 ');
  A := 0.4;
  B := 0.4;
  WRITELN;
  REPEAT
   WRITELN('  ACTIVITY COEFFICIENT MODELS ');
   WRITELN('     1. WILSON ');
   WRITELN('     2. UNIQUAC ');
   WRITELN('     0. EXIT ');
   WRITELN;
   WRITE('SELECT =======> '); READLN(SELECT);
   CASE SELECT OF
     '1' : BEGIN
             SL[1,2] := A;              SL[2,1] := B;
             WILSONG;
           END;
     '2' : BEGIN
             TOR[1,2] := A;             TOR[2,1] := B;
             UNIQG;
           END;
   END; {END OF CASE}
   FUNC_AADP;
   IF (SELECT = '1') OR (SELECT = '2') THEN
    BEGIN
      REPEAT
        WRITE('DO YOU WANT TO PRINT RESULTS? [Y/N] ');
        READLN(ANS);
      UNTIL (ANS = 'Y') OR (ANS = 'y') OR (ANS = 'N') OR (ANS = 'n');
      IF (ANS = 'Y') OR (ANS = 'y') THEN
        BEGIN
          WRITELN(LST,' P_EXP       P_CAL    [kPa]');
          FOR I:= 1 TO N DO
            WRITELN(LST,P[I]:8:4,'     ',PC[I]:8:4);
          WRITELN(LST);
          WRITELN(LST,' %AAD = ',AAD:12:7  );
        END;
      REPEAT
        WRITE('DO YOU WANT OUTPUT FILE? (Y/N) ');
        READLN(ANS);
      UNTIL (ANS = 'Y') OR (ANS = 'y') OR (ANS = 'N') OR (ANS = 'n');
      IF (ANS = 'Y') OR (ANS = 'y') THEN OUTPUT;
    END;
  UNTIL SELECT = '0';
END.
```

F.2 Calculate binary parameters based on H^E data

```
PROGRAM HEAT;
USES CRT,PRINTER;
CONST RC = 8.314; {J/MOL}
TYPE
    A1 = ARRAY[1..40] OF REAL;
    A2 = ARRAY[1..40,1..2] OF REAL;
    A3 = ARRAY[1..2,1..2] OF REAL;
    A4 = ARRAY[1..2] OF REAL;
VAR
   I,J,K,N : INTEGER;      {N_MAX = 40}
   SELECT,ANS : CHAR;
   DD,HH,KK,S,S1,S2,T,T1,T2,FF,RPD,AAD,CHK,LAM12,LAM21,TEMP,A,B : REAL;
   F,F1,F2,HEXP,HECAL,HE,HEC,DE,SXR,SXQ,SXQP,CC,SFAC : A1;
   X,Y,PHI,TETA,TETAP,TTETAP,STTETAP,XR,XQ,XQP,PART : A2;
   SL,VIJ,U,TOR,AA : A3;
   PSAT,V,R,Q,QP,L : A4;
   NAME : ARRAY[1..3] OF STRING;
   FILETEXT : TEXT; FREC:STRING;
PROCEDURE OUTPUT;
BEGIN
  WRITE('INPUT NAME FILE = ');
  READLN(FREC);
  FREC := FREC + '.DAT';
  ASSIGN(FILETEXT,FREC);
  REWRITE(FILETEXT);
  WRITELN(FILETEXT,NAME[1],'[1] + ',NAME[2],'[2] AT ',TEMP:7:2,' K');
  IF SELECT = '1' THEN
    BEGIN
     WRITELN(FILETEXT,'LAM12   LAM21      %AAD ');
     WRITELN(FILETEXT,LAM12:11:8,'  ',LAM21:11:8,'  ',AAD:11:7);
    END;
  IF SELECT = '2' THEN
    BEGIN
     WRITELN(FILETEXT,'U12   U21      %AAD ');
     WRITELN(FILETEXT,U[1,2]:11:8,'  ',U[2,1]:11:8,'  ',AAD:11:7);
    END;
  WRITELN(FILETEXT,' ');
  WRITELN(FILETEXT,'X1    HEEXP    HECAL');
  FOR I:= 1 TO N DO
    WRITELN(FILETEXT,X[I,1]:5:4,'   ',HE[I]:12:4,'  ',HECAL[I]:12:4);
  WRITELN(FILETEXT,'    ');
  CLOSE(FILETEXT);
END;
FUNCTION HCALW(I:INTEGER;X:A2):REAL;     (***)
(*** CALCULATES GE/RT BY WILSON EQUATION ***)
BEGIN
  HCALW := X[I,1]*X[I,2]*(((LAM12*SL[1,2])/(X[I,1]+SL[1,2]*X[I,2]))
```

```
        +((LAM21*SL[2,1])/(X[I,2]+SL[2,1]*X[I,1])));
END;
PROCEDURE HCALU;      (***)
LABEL 10,400;
BEGIN
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      BEGIN
        TTETAP[K,I]:= 0.0;
        STTETAP[K,I] := 0.0;
      END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      FOR J:= 1 TO 2 DO
        IF I = J THEN GOTO 400 ELSE
          BEGIN
            TTETAP[K,I]:= TETAP[K,J]*TOR[J,I];
400:        END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      FOR J:= 1 TO 2 DO
        STTETAP[K,I] := STTETAP[K,I] + TETAP[K,J]*TOR[J,I];
  FOR K:= 1 TO N DO
    HECAL[K] := 0.0;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      FOR J:= 1 TO 2 DO
        IF I = J THEN GOTO 10 ELSE
          BEGIN
   HECAL[K] := HECAL[K]+RC*(XQP[K,I]/STTETAP[K,I])*TTETAP[K,I]*AA[J,I];
10:       END;
END;
PROCEDURE FUNC_HEATCAL;   (***)
BEGIN
  IF SELECT = '1' THEN FOR I:= 1 TO N DO HECAL[I] := HCALW(I,X);
  IF SELECT = '2' THEN HCALU;
END;
PROCEDURE FUNC_SUMF;   (***)
BEGIN
  DD := 0.0; HH := 0.0; KK := 0.0;
  S := 0.0; S1 := 0.0; S2 := 0.0;  T := 0.0; T1 := 0.0; T2 := 0.0;
  FOR I:= 1 TO N DO
    BEGIN
      S  := S  + F[I]*F1[I];
      T  := T  + F[I]*F2[I];
      S1 := S1 + SQR(F1[I]);
      S2 := S2 + F1[I]*F2[I];
      T1 := S2;
      T2 := T2 + SQR(F2[I]);
    END;
```

```
  DD := S1*T2 - S2*T1;
  HH := (S*T2 - T*T1)/DD;
  KK := (S1*T - T1*S)/DD;
END;
PROCEDURE FUNC_DHW;    (***)
(*** DERIVATIES OF GE/RT BY WILSON MODEL ***)
VAR   RT,RT2,LART,LBRT,DA12T,DA21T,DA12A,DA21B,DDA12TA,DDA21TB,A,B,A12,A21 : REAL;
      P1,P2,X1X2,Q,Q1 : A1;
BEGIN
  RT := RC*TEMP;
  RT2 := RC*SQR(TEMP);
    FOR I:= 1 TO N DO
     BEGIN
       X1X2[I] := X[I,1]*X[I,2];
       F[I] := 0.0;
     END;
  A := LAM12;
  B := LAM21;
  LART := A/RT;
  LBRT := B/RT;
  A12 := (V[2]/V[1])*EXP(-LART);
  A21 := (V[1]/V[2])*EXP(-LBRT);
  DA12T := (A*A12)/RT2;
  DA21T := (B*A21)/RT2;
  DA12A := (-1)*A12/RT;
  DA21B := (-1)*A21/RT;
  DDA12TA := (A12/RT2)*(1 - LART);
  DDA21TB := (A21/RT2)*(1 - LBRT);
  FOR I:= 1 TO N DO
     BEGIN
       P1[I] := X1X2[I]/(X[I,1] + (A12*X[I,2]));
       P2[I] := X1X2[I]/(X[I,2] + (A21*X[I,1]));
       Q1[I] := P1[I]*DA12T + P2[I]*DA21T;
     END;
  FOR I:= 1 TO N DO
     BEGIN
       Q[I] := (-1)*(HE[I]/RT2);
       F[I] := Q[I] + Q1[I];
     END;
  FF := 0.0;
  FOR I:= 1 TO N DO
     BEGIN
       FF := FF + SQR(F[I]);
       F1[I] := P1[I]*DDA12TA - DA12A*DA12T*SQR((P1[I]/X[I,1]));
       F2[I] := P2[I]*DDA21TB - DA21B*DA21T*SQR((P2[I]/X[I,2]));
     END;
  S1 := 0.0;  S2 := 0.0;    S := 0.0;  T := 0.0;   T1 := 0.0;    T2 := 0.0;
  DD := 0.0;   HH := 0.0;    FF := 0.0;    KK := 0.0;
END;
PROCEDURE FUNC_DHU;    (***)
```

```
(*** DERIVATIES OF GE/RT BY UNIQUAC MODEL ***)
LABEL 40;
VAR  DA,DRR,DR : A2;
BEGIN
  FUNC_HEATCAL;
  FOR I:= 1 TO N DO
    BEGIN
      HEXP[I] := HE[I];
      F[I] := HEXP[I]-HECAL[I];
      FOR J:= 1 TO 2 DO
        BEGIN
          DA[I,J] := 0.0;
          DR[I,J] := 0.0;
          DRR[I,J] := 0.0;
        END;
    END;
  S1 := 0.0;  S2 := 0.0;    S := 0.0;  T := 0.0;   T1 := 0.0;    T2 := 0.0;
  DD:= 0.0;   HH := 0.0;    FF := 0.0;    KK := 0.0;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      FOR J:= 1 TO 2 DO
        IF I = J THEN GOTO 40 ELSE
          BEGIN
            DA[K,I] := STTETAP[K,I] - (TETAP[K,I]*AA[J,I]/TEMP);
40:       END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      BEGIN
        DR[K,I] := (XQP[K,I]/SQR(STTETAP[K,I]))*TTETAP[K,I];
        DRR[K,I]:= DR[K,I]*DA[K,I];
      END;
  FOR I:= 1 TO N DO
    BEGIN
      FF := FF+SQR(F[I]);
      F1[I] := RC*DRR[I,2];
      F2[I] := RC*DRR[I,1];
    END;
END;
PROCEDURE WILSON;    (***)
(*THIS PROCEDURE CALCULATE THE WILSON PARAMETERS BASED ON HE DATA*)
LABEL 70,200;
BEGIN
  FOR I:= 1 TO 2 DO
    BEGIN
      WRITE('ENTER V',I,' : '); READLN(V[I]);
    END;
  WRITELN;
  FOR I:= 1 TO 2 DO
    FOR J:= 1 TO 2 DO
      BEGIN
```

```
      IF I = J THEN
       BEGIN
        VIJ[I,J] := 1.0;
        SL[I,J] := 1.0;
       END
      ELSE
        VIJ[I,J] := V[J]/V[I];
    END;
  WRITELN;
  WRITELN('V12   = ',VIJ[1,2]:20:10);
  WRITELN(' SL12 = ',SL[1,2]:8:6,'    SL21 = ',SL[2,1]:8:6);
  LAM12 := -RC*TEMP*LN(SL[1,2]/VIJ[1,2]);
  LAM21 := -RC*TEMP*LN(SL[2,1]/VIJ[2,1]);
  FOR I:= 1 TO N DO
    BEGIN
     HEXP[I]:= 0.0;
     HECAL[I]:= 0.0;
     F[I] := 0.0;
     F1[I]:= 0.0;
     F2[I]:= 0.0;
    END;
70: FUNC_DHW;
   FUNC_SUMF;
   WRITELN('LAM12 = ',LAM12:20:10,'     LAM21 = ',LAM21:20:10);
   CHK := ABS(HH/LAM12)+ABS(KK/LAM21);
   IF CHK <= 0.0001 THEN
     BEGIN
      WRITELN('-------------------------------------');
      WRITELN('LAM12  = ',LAM12:20:10,'    LAM21  = ',LAM21:20:10);
      SL[1,2] := VIJ[1,2]*EXP(-LAM12/(RC*TEMP));
      SL[2,1] := VIJ[2,1]*EXP(-LAM21/(RC*TEMP));
      WRITELN('SL12 = ',SL[1,2]:20:4,'   SL21 = ',SL[2,1]:20:4);
      WRITELN('-------------------------------------');
      WRITELN;
      BEGIN
       REPEAT
        WRITE('DO YOU WANT TO PRINT BINARY PARAMETERS? [Y/N] ');
        READLN(ANS);
       UNTIL (ANS = 'Y') OR (ANS = 'y') OR (ANS = 'N') OR (ANS = 'n');
       IF (ANS = 'Y') OR (ANS = 'y') THEN
         WRITELN(LST,' LAM12 = ',LAM12:10:4,'    LAM21 = ',LAM21:10:4);
      END;
      FUNC_HEATCAL;
     END
   ELSE
     BEGIN
      LAM12 := LAM12-HH;
      LAM21 := LAM21-KK;
      GOTO 70;
     END;
```

```
END;
PROCEDURE UNIQ;      (***)
(*THIS PROCEDURE CALCULATE THE UNIQUAC PARAMETERS BASED ON VLE DATA*)
LABEL 10,20,30;
BEGIN
 FOR I:= 1 TO 2 DO
   BEGIN
    WRITE('ENTER R',I,' : '); READLN(R[I]);
    WRITE('ENTER Q',I,' : '); READLN(Q[I]);
    QP[I] := Q[I];
   END;
 FOR I:= 1 TO 2 DO
   FOR J:= 1 TO 2 DO
     IF I = J THEN
       TOR[I,J] := 1.0;
 AA[1,2] := -TEMP*LN(TOR[1,2]);
 AA[2,1] := -TEMP*LN(TOR[2,1]);
 U[1,2] := AA[1,2]*RC;
 U[2,1] := AA[2,1]*RC;
 WRITELN(' TOR12 = ',TOR[1,2]:8:6,'    TOR21 = ',TOR[2,1]:8:6);
 FOR I:= 1 TO N DO
   BEGIN
    HEXP[I]:= 0.0;
    HECAL[I]:= 0.0;
    F[I] := 0.0;
    F1[I]:= 0.0;
    F2[I]:= 0.0;
   END;
 FOR K:= 1 TO N DO
    BEGIN
     SXR[K]:= 0.0;  SXQ[K]:= 0.0;  SXQP[K]:= 0.0;
     FOR I:= 1 TO 2 DO
       BEGIN
         PHI[K,I]:= 0.0;   TETA[K,I]:= 0.0; TETAP[K,I]:= 0.0;
         XR[K,I]:= 0.0;    XQ[K,I]:= 0.0;   XQP[K,I]:= 0.0;
       END;
    END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      BEGIN
       XR[K,I] := X[K,I]*R[I];      XQ[K,I] := X[K,I]*Q[I];
       XQP[K,I]:= X[K,I]*QP[I];     SXR[K]  := SXR[K] + XR[K,I];
       SXQ[K]  := SXQ[K] + XQ[K,I];  SXQP[K] := SXQP[K] + XQP[K,I];
      END;
  FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
      BEGIN
        PHI[K,I]:= XR[K,I]/SXR[K];
        TETA[K,I]:= XQ[K,I]/SXQ[K];
        TETAP[K,I]:= XQP[K,I]/SXQP[K];
```

```
        END;
10:  TOR[1,2] := EXP(-AA[1,2]/TEMP);
     TOR[2,1] := EXP(-AA[2,1]/TEMP);
   FOR K:= 1 TO N DO
     FOR I:= 1 TO 2 DO
       BEGIN
         TTETAP[K,I]:= 0.0;
         STTETAP[K,I] := 0.0;
       END;
   FOR K:= 1 TO N DO
     FOR I:= 1 TO 2 DO
       FOR J:= 1 TO 2 DO
         IF I = J THEN GOTO 20 ELSE
           BEGIN
             TTETAP[K,I]:= TETAP[K,J]*TOR[J,I];
20:          END;
   FOR K:= 1 TO N DO
     FOR I:= 1 TO 2 DO
       FOR J:= 1 TO 2 DO
         STTETAP[K,I] := STTETAP[K,I] + TETAP[K,J]*TOR[J,I];
   FOR K:= 1 TO N DO
     FOR I:= 1 TO 2 DO
       FOR J:= 1 TO 2 DO
         IF I = J THEN GOTO 30 ELSE
           BEGIN
             PART[K,I] := (XQP[K,I]/STTETAP[K,I])*TETAP[K,J];
30:          END;
   FUNC_DHU;
   FUNC_SUMF;
   WRITELN('AA12 = ',AA[1,2]:20:10,'     AA21 = ',AA[2,1]:20:10);
   CHK := ABS(HH/AA[1,2])+ABS(KK/AA[2,1]);
   IF CHK <= 0.0001 THEN
     BEGIN
       WRITELN('-------------------------------------------');
       WRITELN('AA12  = ',AA[1,2]:20:10,'    AA21  = ',AA[2,1]:20:10);
       U[1,2] := RC*AA[1,2];
       U[2,1] := RC*AA[2,1];
       WRITELN('U12 = ',U[1,2]:20:4,'      U21 = ',U[2,1]:20:4);
       WRITELN('-------------------------------------------');
       WRITELN;
       BEGIN
         REPEAT
           WRITE('DO YOU WANT TO PRINT BINARY PARAMETERS? [Y/N] ');
           READLN(ANS);
         UNTIL (ANS = 'Y') OR (ANS = 'Y') OR (ANS = 'N') OR (ANS = 'N');
         IF (ANS = 'Y') OR (ANS = 'Y') THEN
           WRITELN(LST,' U12 = ',U[1,2]:10:4,'    U[2,1] = ',U[2,1]:10:4);
       END;
       FUNC_HEATCAL;
     END
```

```
    ELSE
      BEGIN
        AA[1,2] := AA[1,2]+HH;
        AA[2,1] := AA[2,1]+KK;
        GOTO 10;
      END;
  END;
  PROCEDURE FUNC_AADW;   (***)
  BEGIN
     FUNC_HEATCAL;
     FOR I:= 1 TO N DO
       DE[I] := 0.0;
     FOR I:= 1 TO N DO
       DE[I] := (HECAL[I]-HE[I])/HE[I];
     RPD := 0.0; AAD := 0.0;
     FOR I:= 1 TO N DO
       RPD := RPD + ABS(DE[I]);
     AAD := (100/N)*RPD;
     WRITELN(' HE_EXP       HE_CAL');
     FOR I:= 1 TO N DO
       WRITELN(HE[I]:12:4,'    ',HECAL[I]:12:4);
     WRITELN;
     WRITELN('%AAD = ',AAD:10:6);
     WRITELN('PRESS ENTER');
     READLN;
  END;
  PROCEDURE FUNC_AADU;   (***)
  BEGIN
     FUNC_HEATCAL;
     FOR I:= 1 TO N DO
       DE[I] := 0.0;
     FOR I:= 1 TO N DO
       DE[I] := (HECAL[I]-HE[I])/HE[I];
     RPD := 0.0; AAD := 0.0;
     FOR I:= 1 TO N DO
       RPD := RPD + ABS(DE[I]);
     AAD := (100/N)*RPD;
     WRITELN(' HE_EXP       HE_CAL');
     FOR I:= 1 TO N DO
       WRITELN(HE[I]:12:4,'    ',HECAL[I]:12:4);
     WRITELN;
     WRITELN('%AAD = ',AAD:10:6);
     WRITELN('PRESS ENTER');
     READLN;
  END;
  PROCEDURE FUNC_AAD;
  BEGIN
     IF SELECT = '1' THEN FUNC_AADW;
     IF SELECT = '2' THEN FUNC_AADU;
  END;
```

```
BEGIN                    (****** MAIN PROGRAM *****)
  CLRSCR;
  WRITELN('************************************************');
  WRITELN('              INPUT DATA');
  WRITELN('************************************************');
  WRITE('NAME OF COMPONENT 1 : '); READLN(NAME[1]);
  WRITE('NAME OF COMPONENT 2 : '); READLN(NAME[2]);
  WRITE('NO. OF DATA : '); READLN(N);
  WRITE('TEMPERATURE [K] : '); READLN(TEMP);
  WRITELN('EXCESS ENTHALPY, MOLE FRACTION OF COMPONENT 1 ');
  FOR I:= 1 TO N DO
    BEGIN
      WRITE('    HE[',I:2,']  [KPA] : '); READLN(HE[I]);
      WRITE('    X1[',I:2,'] : '); READLN(X[I,1]);
      WRITELN;
    END;
  FOR I:= 1 TO N DO
    X[I,2] := 1.0-X[I,1];
  WRITELN('INITIAL GUESS PARAMETER A = 0.4 ');
  WRITELN('INITIAL GUESS PARAMETER B = 0.4 ');
  A := 0.4;
  B := 0.4;
  REPEAT
   WRITELN('  ACTIVITY COEFFICIENT MODELS ');
   WRITELN('     1. WILSON ');
   WRITELN('     2. UNIQUAC ');
   WRITELN('     0. EXIT ');
   WRITELN;
   WRITE('SELECT =======> '); READLN(SELECT);
   CASE SELECT OF
     '1' : BEGIN
             SL[1,2] := A;
             SL[2,1] := B;
             WILSON;
           END;
     '2' : BEGIN
             TOR[1,2] := A;
             TOR[2,1] := B;
             UNIQ;
           END;
   END; {END OF CASE}
   IF (SELECT = '1') OR (SELECT = '2') THEN
    BEGIN
      FUNC_AAD;
      REPEAT
        WRITE('DO YOU WANT TO PRINT RESULTS? [Y/N] ');
        READLN(ANS);
      UNTIL (ANS = 'Y') OR (ANS = 'Y') OR (ANS = 'N') OR (ANS = 'N');
      IF (ANS = 'Y') OR (ANS = 'Y') THEN
        BEGIN
```

```
          WRITELN(LST,' HE_EXP       HE_CAL   (J/MOL)');
          FOR I:= 1 TO N DO
            WRITELN(LST,HE[I]:8:4,'      ',HEC[I]:8:4);
          WRITELN(LST);
          WRITELN(LST,' %AAD = ',AAD:12:7 );
         END;
        REPEAT
         WRITE('DO YOU WANT OUTPUT FILE? (Y/N) ');
         READLN(ANS);
        UNTIL (ANS = 'Y') OR (ANS = 'Y') OR (ANS = 'N') OR (ANS = 'N');
        IF (ANS = 'Y') OR (ANS = 'Y') THEN OUTPUT;
       END;
  UNTIL SELECT = '0';
END.
```

F.3 Calculate saturation pressure

```
PROGRAM ERRP;
USES CRT;
CONST RC = 8.314;
TYPE A1 = ARRAY[1..40,1..2] OF REAL;
   A2 = ARRAY[1..40] OF REAL;
   A3 = ARRAY[1..2,1..2] OF REAL;
VAR  I,J,K,N : INTEGER;
   X,LNG,GW,Y,GM,GU : A1;
   BETA,P,PW,PU,DEP,DEG,DEPU : A2;
   AADG,AADP,AADPU,DP,DU:REAL;
   SL,U,UU : A3;
   V,PSAT,R,Q,QP : ARRAY[1..2] OF REAL;
   TEMP,LAM12,LAM21,LAM12R,LAM21R,L12,L21 : REAL;
   NAME : ARRAY[1..5] OF STRING;
   KEY:CHAR;
   FILETEXT : TEXT; FREC:STRING;
FUNCTION ERROR(E:REAL):REAL;  (***)
BEGIN
   ERROR := E/100;
END;
PROCEDURE OUTP;    (***)
BEGIN
  WRITE('INPUT NAME FILE = ');
  READLN(FREC);
  FREC := FREC + 'P.DAT';
  ASSIGN(FILETEXT,FREC);
  REWRITE(FILETEXT);
  WRITELN(FILETEXT,NAME[1],'[1] + ',NAME[2],'[2] AT ',TEMP:7:3,' K');
  WRITELN(FILETEXT,'LAMDA12   LAMDA21   %AAD(P)_WILSON');
  WRITELN(FILETEXT,LAM12:11:8,'  ',LAM21:11:8,'  ',AADP:13:8);
  WRITELN(FILETEXT,'U12   U21   %AAD(P)_UNIQUAC');
  WRITELN(FILETEXT,U[1,2]*RC:9:7,'  ',U[2,1]*RC:9:7,'  ',AADPU:13:8);
```

```
  WRITELN(FILETEXT,'WILSON    UNIQUAC         DEVW   DEVU ');
  WRITELN(FILETEXT,' ',AADP:10:4,' ',AADPU:10:4,' ',DP:10:4,' ',DU:10:4);
  CLOSE(FILETEXT);
END;
PROCEDURE CALGU;
TYPE A1 = ARRAY[1..40] OF REAL;
   A2 = ARRAY[1..40,1..2] OF REAL;
   A3 = ARRAY[1..5] OF REAL;
   A4 = ARRAY[1..5,1..5] OF REAL;
VAR PHI,THI,THIPR,WL : A3;  E : REAL;
  TA : A4;  IT,IS : INTEGER;
  SPHI,STHI,STHIPR,SXL,STHTJI,GC,FS,STHT,GR : REAL;
BEGIN
   WRITELN('********** UNIQUAC EQUATION **********');
 WRITELN;
 WRITE('SELECT %ERROR TO CALCULATE [-20 -10 -5 0 5 10 20] : ');
  READLN(E);
  WRITELN;
 U[1,2] := UU[1,2] + UU[1,2]*ERROR(E);
 U[2,1] := UU[2,1] + UU[2,1]*ERROR(E);
 U[1,2] := U[1,2]/RC;
  U[2,1] := U[2,1]/RC;
IS := 2;
FOR IT:= 1 TO N DO
     X[IT,2]:= 1.0-X[IT,1];
FOR IT:= 1 TO N DO
     BEGIN
  SPHI := 0.0; STHI := 0.0; STHIPR := 0.0;
    FOR J:= 1 TO IS DO
     BEGIN
       SPHI := SPHI + X[IT,J]*R[J];
       STHI := STHI + X[IT,J]*Q[J];
       STHIPR := STHIPR + X[IT,J]*QP[J];
     END;
    FOR J:= 1 TO IS DO
     BEGIN
       PHI[J] := X[IT,J]*R[J]/SPHI;
       THI[J] := X[IT,J]*Q[J]/STHI;
       THIPR[J] := X[IT,J]*QP[J]/STHIPR;
       WL[J] := 5.*(R[J]-Q[J])-(R[J]-1.0);
     END;
    FOR I:= 1 TO IS DO
     FOR J:= 1 TO IS DO
       TA[I,J] := EXP(-U[I,J]/TEMP);
(*--- COMBINATOTIAL PART ---*)
   FOR I:= 1 TO IS DO
    BEGIN
      SXL := 0.0; STHTJI := 0.0;
      FOR J:= 1 TO IS DO
       BEGIN
```

```
            SXL := SXL + X[IT,J]*WL[J];
            STHTJI := STHTJI + TA[J,I]*THIPR[J];
          END;
        GC := LN(PHI[I]/X[IT,I]) + 5.*Q[I]*LN(THI[I]/PHI[I]);
        GC := GC + WL[I] - PHI[I]*SXL/X[IT,I];
(*— RESIDUAL PART —*)
        FS := 0.0;
        FOR J:= 1 TO IS DO
          BEGIN
            STHT := 0.0;
            FOR K:= 1 TO IS DO
              STHT := STHT + THIPR[K]*TA[K,J];
            FS := FS + THIPR[J]*TA[I,J]/STHT;
          END;
        GR := QP[I]*(1.0-LN(STHTJI)-FS);
(*— ACTIVITY COEFFICIENT —*)
        GU[IT,I] := EXP(GC+GR);
      END;
    END;
END;
PROCEDURE CALGW;
VAR E : REAL;
BEGIN
    WRITELN(' ********** WILSON EQUATION **********');
    WRITELN;
    WRITE('SELECT %ERROR TO CALCULATE [-20  -10  -5  0  5  10  20] : ');
    READLN(E);
   WRITELN;
    LAM12 := L12 + L12*ERROR(E);
    LAM21 := L21 + L21*ERROR(E);
    WRITELN('  LAM12 = ',LAM12:10:5,'  LAM21 = ',LAM21:10:5);
    SL[1,2] := (V[2]/V[1])*EXP(-LAM12/(RC*TEMP));
    SL[2,1] := (V[1]/V[2])*EXP(-LAM21/(RC*TEMP));
  FOR I:= 1 TO N DO
   BETA[I] := (SL[1,2]/(X[I,1] + X[I,2]*SL[1,2])) - (SL[2,1]/(X[I,2] + X[I,1]*SL[2,1]));
  FOR I:= 1 TO N DO
   BEGIN
     LNG[I,1]:= -LN(X[I,1]+X[I,2]*SL[1,2]) + X[I,2]*BETA[I];
     LNG[I,2]:= -LN(X[I,2]+X[I,1]*SL[2,1]) - X[I,1]*BETA[I];
   END;
  FOR I:= 1 TO N DO
   FOR J:= 1 TO 2 DO
     GW[I,J] := EXP(LNG[I,J]);
  FOR I:= 1 TO N DO
  BEGIN
   DEG[I]:= ABS((GW[I,1]-GM[I,1])/GM[I,1]) + ABS((GW[I,2]-GM[I,2])/GM[I,2]);
  END;
  AADG:= 0.0;
  FOR I:= 1 TO N DO
   AADG := AADG + DEG[I];
```

```
   AADG := AADG*100/N;
END;
PROCEDURE CALP;
BEGIN
 FOR I:= 1 TO N DO
      BEGIN
          PW[I]:= 0.0;
          PU[I]:= 0.0;
      END;
 FOR I:= 1 TO N DO
  BEGIN
   PW[I]  := GW[I,1]*X[I,1]*PSAT[1] + GW[I,2]*X[I,2]*PSAT[2];
   PU[I]  := GU[I,1]*X[I,1]*PSAT[1] + GU[I,2]*X[I,2]*PSAT[2];
  END;
 FOR I:= 1 TO N DO
   WRITELN('PW[',I:2,']  = ',PW[I]:11:4,'    PU[',I:2,'] = ',PU[I]:11:4);
 READLN;
 FOR I:= 1 TO N DO
  BEGIN
  DEP[I]:= ((PW[I]-P[I])/P[I]);
  DEPU[I]:= ((PU[I]-P[I])/P[I]);
  END;
 AADP:= 0.0; AADPU:= 0.0;     DP:= 0.0; DU:= 0.0;
  FOR I:= 1 TO N DO
   BEGIN
    DP := DP + DEP[I];
    DU := DU + DEPU[I];
    AADP := AADP + ABS(DEP[I]);
    AADPU:= AADPU + ABS(DEPU[I]);
   END;
  AADP := AADP*100/N;
  AADPU:= AADPU*100/N;
  WRITELN(' WILSON  : AADP  = ',AADP:10:7,'    DEV = ',DP:10:7);
  WRITELN(' UNIQUAC : AADPU = ',AADPU:10:7,'   DEVU = ',DU:10:7);
  READLN;
END;
BEGIN                    {MAIN PROGRAM}
   CLRSCR;
   WRITELN('*************************************************');
   WRITELN('                INPUT DATA');
   WRITELN('*************************************************');
   WRITE('NAME OF COMPONENT 1 : ');          READLN(NAME[1]);
   WRITE('NAME OF COMPONENT 2 : ');          READLN(NAME[2]);
   WRITE('NO. OF DATA : ');                  READLN(N);
   WRITE('TEMPERATURE [K] : ');              READLN(TEMP);
   WRITE('PSAT[1] : ');                      READLN(PSAT[1]);
   WRITE('PSAT[2] : ');                      READLN(PSAT[2]);
   WRITELN('MOLAR VOLUME ');
   WRITE('V[1] : ');                         READLN(V[1]);
   WRITE('V[2] : ');                         READLN(V[2]);
```

```
    WRITELN('VOLUME PARAMETERS ');
    WRITE('R[1] : ');                          READLN(R[1]);
    WRITE('R[2] : ');                          READLN(R[2]);
    WRITELN('SURFACE AREA PARAMETERS ');
    WRITE('Q[1] : ');                          READLN(Q[1]);
    WRITE('Q[2] : ');                          READLN(Q[2]);
    QP[1] := Q[1];
    QP[2] := Q[2];
    WRITELN;
    WRITELN('PRESSURE, MOLE FRACTION OF COMPONENT 1, GAMMA1 AND GAMMA2 ');
    FOR I:= 1 TO N DO
      BEGIN
        WRITE('   P[',I:2,']  [KPA] : ');      READLN(P[I]);
        WRITE('   X1[',I:2,'] : ');            READLN(X[I,1]);
        WRITE('   GAMMA1[',I:2,'] : ');        READLN(GM[I,1]);
        WRITE('   GAMMA2[',I:2,'] : ');        READLN(GM[I,2]);
        WRITELN;
      END;
  FOR I:= 1 TO N DO BEGIN DEG[I]:= 0.0; DEP[I]:= 0.0; END;
  FOR I:= 1 TO N DO
    BEGIN
    X[I,2]:= 1.0-X[I,1]; Y[I,2]:= 1.0-Y[I,1];
    END;
(*--------------------*)
WRITELN('ENTER BINARY PARAMETERS ');
  WRITELN('   LAM12 : ');                      READLN(L12);
  WRITELN('   LAM21 : ');                      READLN(L21);
  WRITELN('   U12   : ');                      READLN(UU[1,2]);
  WRITELN('   U21   : ');                      READLN(UU[2,1]);
(*--------------------*)
 REPEAT
    BEGIN
      WRITELN;
      CALGW;
      CALGU;
      CALP;
      WRITELN;
      REPEAT
        WRITE('DO YOU WANT TO SAVE DATA (Y/N) '); READLN(KEY);
      UNTIL (KEY = 'Y') OR (KEY = 'y') OR (KEY = 'N') OR (KEY = 'n');
      IF (KEY = 'Y') OR (KEY = 'y') THEN OUTP;
    END;
    WRITELN;
    WRITE('DO YOU WANT TO ANOTHER CAL (Y/N) '); READLN(KEY);
UNTIL (KEY = 'N') OR (KEY = 'n');
END.
```

F.4 Calculate excess enthalpy

```
PROGRAM ERRH;
USES CRT;
CONST RC = 8.314;
TYPE A1 = ARRAY[1..40] OF REAL;
   A2 = ARRAY[1..40,1..2] OF REAL;
   A3 = ARRAY[1..2,1..2] OF REAL;
   A4 = ARRAY[1..3] OF REAL;
VAR  I,J,K,N : INTEGER;
   TEMP, LAM12, LAM21 ,AADW,AADU,L12,L21: REAL;
   KEY:CHAR;
   SL,U,A,TOR,UU : A3;
  X : A2;
  HCAL,HEU, HW,HEW,HEEXP,HE,DEW,DEU : A1;
  V,R,Q,QP,PSAT : A4;
  NAME : ARRAY[1..3] OF STRING;
  FILETEXT : TEXT; FREC:STRING;
PROCEDURE OUTH;   (***)
VAR E:REAL;
BEGIN
  WRITE('INPUT NAME FILE = ');
  READLN(FREC);
  FREC := FREC + 'H.DAT';
  ASSIGN(FILETEXT,FREC);
  REWRITE(FILETEXT);
  WRITELN(FILETEXT,NAME[1],'[1] + ',NAME[2],'[2] AT ',TEMP:7:3,' K');
  WRITELN(FILETEXT,'LAM12   LAM21    AADHW');
  WRITELN(FILETEXT,LAM12:14:8,'  ',LAM21:14:8,'   ',AADW:11:8);
  WRITELN(FILETEXT,'U12    U21    AADHU');
  WRITELN(FILETEXT,U[1,2]:11:8,'  ',U[2,1]:11:8,'   ',AADU:11:8);
  WRITELN(FILETEXT,'AADW     AADU');
  WRITELN(FILETEXT,AADW:11:8,'  ',AADU:11:8);
  WRITELN(FILETEXT,' ');
  CLOSE(FILETEXT);
END;
FUNCTION ERROR(E:REAL):REAL;  (***)
BEGIN
   ERROR := E/100;
END;
PROCEDURE CALHU;   (***)
LABEL 20,30;
VAR SXR,SXQ,SXQP,SFAC : A1;
     E:REAL;
     PHI,TETA,TETAP,XR,XQ,XQP,TTETAP,STTETAP,PART,FAC : A2;
BEGIN
WRITELN('************ UNIQUAC EQUATION ********************');
WRITELN;
WRITE('SELECT %ERROR TO CALCULATE [-20  -10  -5  0  5  10  20] : ');
```

```
 READLN(E);
 WRITELN;
U[1,2] := UU[1,2] + UU[1,2]*ERROR(E);
U[2,1] := UU[2,1] + UU[2,1]*ERROR(E);
A[1,2]  := U[1,2]/RC;
A[2,1]  := U[2,1]/RC;
FOR K:= 1 TO N DO
 BEGIN
  SXR[K]:= 0.0;  SXQ[K]:= 0.0;  SXQP[K]:= 0.0;
   FOR I:= 1 TO 2 DO
    BEGIN
     PHI[K,I]:= 0.0;   TETA[K,I]:= 0.0; TETAP[K,I]:= 0.0;
     XR[K,I]:= 0.0;    XQ[K,I]:= 0.0;   XQP[K,I]:= 0.0;
    END;
 END;
  FOR K:= 1 TO N DO
 FOR I:= 1 TO 2 DO
  BEGIN
    XR[K,I] := X[K,I]*R[I];
    XQ[K,I] := X[K,I]*Q[I];
    XQP[K,I]:= X[K,I]*QP[I];
    SXR[K]  := SXR[K] + XR[K,I];
    SXQ[K]  := SXQ[K] + XQ[K,I];
    SXQP[K] := SXQP[K] + XQP[K,I];
  END;
FOR K:= 1 TO N DO
 FOR I:= 1 TO 2 DO
    BEGIN
      PHI[K,I]   := XR[K,I]/SXR[K];
      TETA[K,I]  := XQ[K,I]/SXQ[K];
      TETAP[K,I] := XQP[K,I]/SXQP[K];
    END;
FOR I:= 1 TO 2 DO
 FOR J:= 1 TO 2 DO
  TOR[I,J] := EXP(-A[I,J]/TEMP);
FOR K:= 1 TO N DO
 FOR I:= 1 TO 2 DO
  BEGIN
    TTETAP[K,I]:= 0.0; STTETAP[K,I] := 0.0;
  END;
FOR K:= 1 TO N DO
 FOR I:= 1 TO 2 DO
  FOR J:= 1 TO 2 DO
   IF I = J THEN GOTO 20 ELSE
     BEGIN
       TTETAP[K,I]:= TETAP[K,J]*TOR[J,I];
20:    END;
 FOR K:= 1 TO N DO
  FOR I:= 1 TO 2 DO
   FOR J:= 1 TO 2 DO
```

```
        STTETAP[K,I] := STTETAP[K,I] + TETAP[K,J]*TOR[J,I];
   FOR K:= 1 TO N DO
    FOR I:= 1 TO 2 DO
     FOR J:= 1 TO 2 DO
      IF I = J THEN GOTO 30 ELSE
        BEGIN
         PART[K,I] := (XQP[K,I]/STTETAP[K,I])*TTETAP[K,I];
         FAC[K,I] := PART[K,I]*A[J,I];
30:      END;
   FOR K:= 1 TO N DO
    BEGIN
     SFAC[K] := 0.0; HCAL[K]:= 0.0;
    END;
   FOR K:= 1 TO N DO
    FOR I:=1 TO 2 DO
     SFAC[K]:= SFAC[K] +  FAC[K,I];
   FOR I := 1 TO N DO
    HCAL[I] := RC*SFAC[I];
  FOR I:= 1 TO N DO
   WRITELN('HCALU[',I:2,'] = ',HCAL[I]:10:4);
  READLN;
  AADU := 0.0;
  FOR I:= 1 TO N DO
   DEU[I] := ABS((HCAL[I]-HE[I])/HE[I]);
  FOR I:= 1 TO N DO
   AADU := AADU + DEU[I]*100/N;
  WRITELN('AADU = ',AADU:10:3);
  READLN;
 END;
 PROCEDURE CALHW;  (***)
 VAR E : REAL;
 BEGIN
    WRITELN(' ********** WILSON EQUATION **************');
    WRITELN;
    WRITE('SELECT %ERROR TO CALCULATE [-20  -10  -5  0  5  10  20] : ');
    READLN(E);
   WRITELN;
    LAM12 := L12 + L12*ERROR(E);
    LAM21 := L21 + L21*ERROR(E);
     WRITELN('  LAM12 = ',LAM12:10:5,'  LAM21 = ',LAM21:10:5);
  WRITELN;{ READLN;}
   SL[1,2] := (V[2]/V[1])*EXP(-LAM12/(RC*TEMP));
   SL[2,1] := (V[1]/V[2])*EXP(-LAM21/(RC*TEMP));
 FOR I:= 1 TO N DO
      HW[I]:= 0.0;
 FOR I:= 1 TO N DO
  BEGIN
   HW[I]  := (LAM12*SL[1,2]/(X[I,1]+SL[1,2]*X[I,2])) + (LAM21*SL[2,1]/(X[I,2]+SL[2,1]*X[I,1]));
   HEW[I] := X[I,1]*X[I,2]*HW[I];
  END;
```

```
FOR I:= 1 TO N DO
 WRITELN('HEW[',I:2,'] = ',HEW[I]:10:4);
READLN;
AADW := 0.0;
FOR I:= 1 TO N DO
 DEW[I] := ABS((HEW[I]-HE[I])/HE[I]);
FOR I:= 1 TO N DO
  AADW := AADW + DEW[I]*100/N;
WRITELN('AADW = ',AADW:10:3);
READLN;
END;
BEGIN                    {MAIN PROGRAM}
   CLRSCR;
   WRITELN('**************************************************');
   WRITELN('              INPUT DATA');
   WRITELN('**************************************************');
   WRITELN;
   WRITE('NAME OF COMPONENT 1 : ');                    READLN(NAME[1]);
   WRITE('NAME OF COMPONENT 2 : ');                    READLN(NAME[2]);
   WRITE('NO. OF DATA : ');                            READLN(N);
   WRITE('TEMPERATURE [K] : ');                        READLN(TEMP);
   WRITE('PSAT[1] : ');                                READLN(PSAT[1]);
   WRITE('PSAT[2] : ');                                READLN(PSAT[2]);
   WRITELN('MOLAR VOLUME ');
   WRITE('V[1] : ');                                   READLN(V[1]);
   WRITE('V[2] : ');                                   READLN(V[2]);
   WRITELN('VOLUME PARAMETERS ');
   WRITE('R[1] : ');                                   READLN(R[1]);
   WRITE('R[2] : ');                                   READLN(R[2]);
   WRITELN('SURFACE AREA PARAMETERS ');
   WRITE('Q[1] : ');                                   READLN(Q[1]);
   WRITE('Q[2] : ');                                   READLN(Q[2]);
   QP[1] := Q[1];
   QP[2] := Q[2];
   WRITELN;
   WRITELN('EXPERIMENTAL EXCESS ENTHALPY AND MOLE FRACTION OF COMPONENT 1');
   FOR I:= 1 TO N DO
     BEGIN
      WRITE('   HEXP[',I:2,']  [J/MOL] : ');          READLN(HEEXP[I]);
      WRITE('   X1[',I:2,'] : ');                     READLN(X[I,1]);
      WRITELN;
     END;
(* - - - - - - - - - - - - - - - - - - - - - - - - - *)
  WRITELN('ENTER BINARY PARAMETERS ');
  WRITELN('    LAM12 : '); READLN(L12);
  WRITELN('    LAM21 : '); READLN(L21);
  WRITELN('    U12   : '); READLN(UU[1,2]);
  WRITELN('    U21   : '); READLN(UU[2,1]);
(* - - - - - - - - - - - - - - - - - - - - - - - - - - - - *)
 FOR I:= 1 TO N DO
```

```
 BEGIN
   X[I,2]:= 1.0-X[I,1];
  HE[I]:= HEEXP[I];
  DEW[I]:= 0.0;
  DEU[I]:= 0.0;
 END;
FOR I:= 1 TO 2 DO
  FOR J:= 1 TO 2 DO
      A[I,J]:=0.0;
REPEAT
   BEGIN
    WRITELN;
    CALHW;
    CALHU;
    WRITELN;
    REPEAT
      WRITE('DO YOU WANT TO SAVE DATA (Y/N) '); READLN(KEY);
    UNTIL (KEY = 'Y') OR (KEY = 'Y') OR (KEY = 'N') OR (KEY = 'N');
    IF (KEY = 'Y') OR (KEY = 'Y') THEN OUTH;
   END;
   WRITELN;
  WRITE('DO YOU WANT TO ANOTHER CAL HEAT (Y/N) '); READLN(KEY);
UNTIL (KEY = 'N') OR (KEY = 'N');
END.
```

VITA

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