Lecture 8

Chapter 5

- Thermodynamic Web
- Departure Functions
- Review Equations of state (chapter 4, briefly)

Chapter 6

- Equilibrium (chemical potential)
  * Pure Component
  * Mixtures

Chapter 7

- Fugacity (chemical potential → fugacity → equilibrium calculations)
  * Vapor (overview), liquid, solids
- Activity Coefficients [Fugacity Coefficients (overview)]

Chapter 8

- Phase Equilibrium
  * Diagrams
  * Vapor – Liquid (VLE)
  * Liquid – Liquid (LLE)
  * Solid – Liquid (SLE)

Chapter 9

- Reaction Equilibria

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Fugacity Coefficient (methods to calculate)

$$\hat{\phi}_i^{\alpha}$$

1. **Data**
2. **Equations of State**
3. **Generalized correlations**

a. **Pure Fluid** ϕ_i^{α}

b. Multicomponent system: $\hat{\phi}_i^{\alpha}$

---

a. Pure Fluid

1. Data

$$\ln \phi_i^{\alpha} = \int_0^P (Z-1)\frac{dP}{P}$$

$$\ln \phi_i^{\alpha} = \int_0^P \left(\frac{P\upsilon}{RT} - 1\right)\frac{dP}{P}$$

$$\ln \phi_i^{\alpha} = \int_0^P \left(\frac{\upsilon}{RT} - \frac{1}{P}\right)dP$$

ϕ_{CO_2} at 38°C, 13.79 bar

P [bar]	Z
1	0.9964
5	0.9805
10	0.9607
20	0.9195

$$\phi_{CO_2}^{data} = 0.95$$

Fugacity Coefficient (methods to calculate)

ϕ_i^{α} a. Pure Fluid

   2. Equations of State

> See handout on website from Kyle
> for Peng-Robinson EOS

$$Z^3 + (B-1)Z^2 + (A - 3B^2 - 2B)Z + (B^3 + B^2 - AB) = 0$$

$$\ln \phi = Z - 1 - \ln(Z - B) - \frac{A}{2\sqrt{2}\,B} \ln \left[\frac{Z + \left(1 + \sqrt{2}\right)B}{Z + \left(1 - \sqrt{2}\right)B} \right]$$

ϕ_{CO_2} at 38ºC, 13.79 bar

$$\phi_{CO_2}^{PREOS} = 0.935$$

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Fugacity Coefficient (methods to calculate)

$\hat{\phi}_i^{\alpha}$ 1. Data

       2. Equations of State

       3. Generalized correlations

a.   Pure Fluid ϕ_i^{α}

b.   **Multicomponent system:** $\hat{\phi}_i^{\alpha}$

vdw EOS

$$\ln\left[\frac{\hat{f}_a^v}{y_a P}\right] = \ln\hat{\phi}_a^v = -\ln\frac{P(\upsilon - b_{mix})}{RT} + \frac{b_a}{(\upsilon - b_{mix})} - \frac{2\left(y_a a_a + y_b\sqrt{a_a a_b}\right)}{RT\upsilon}$$
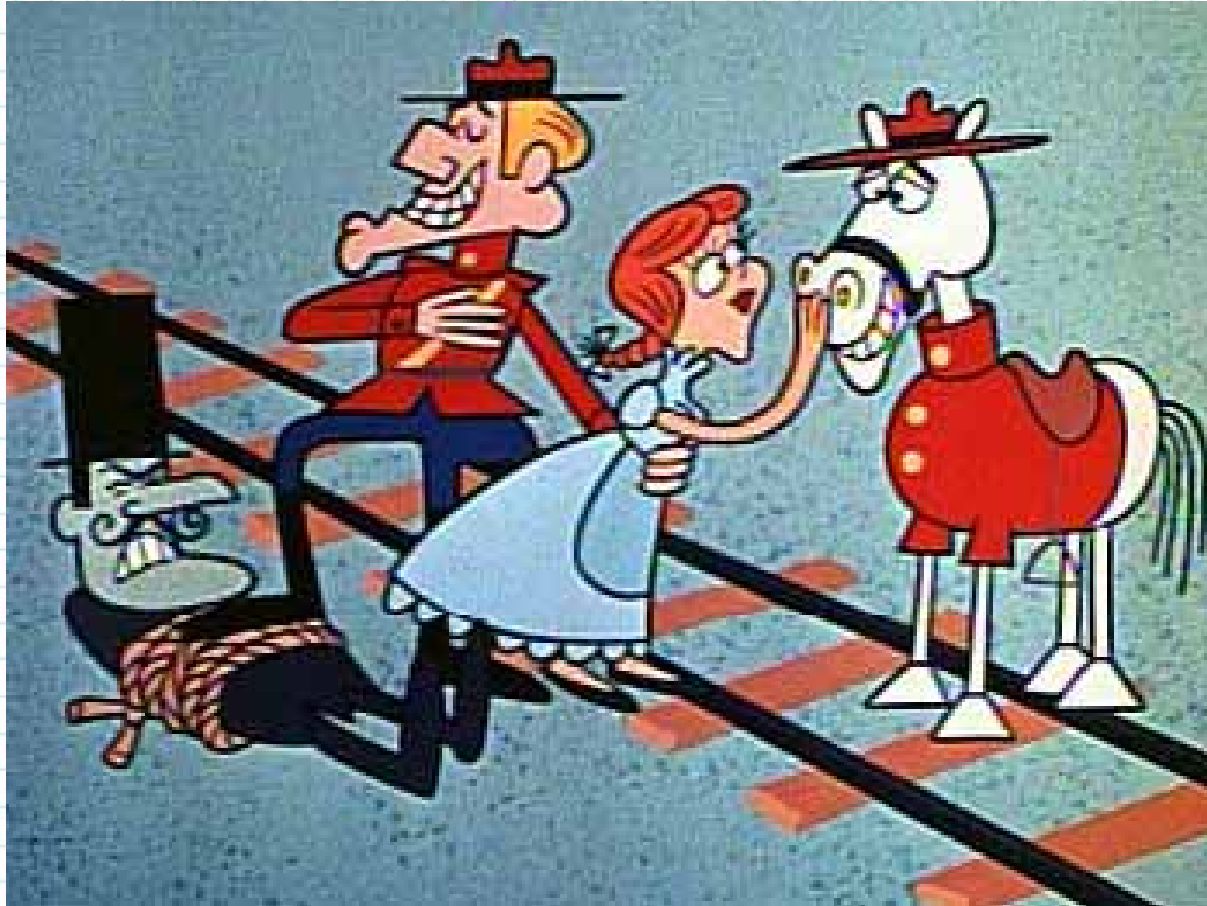
Peng Robinson EOS (see Kyle handout on web)

$$\ln\hat{\phi}_i = \frac{A}{2\sqrt{2}\,B}\left[\frac{B_i}{B} - \frac{2\sum_{j=1}^{c}\chi_j A_{ij}}{A}\right]\ln\left[\frac{Z + \left(1+\sqrt{2}\right)B}{Z + \left(1-\sqrt{2}\right)B}\right] + \frac{B_i}{B}(Z-1) \\ -\ln(Z-B)$$

Fugacity Coefficient (Continued)

Fugacity Coefficient (Continued)

Fugacity Coefficient (PREOS)

$$\ln \hat{\phi}_i^{\alpha} = \frac{A}{2\sqrt{2}\,B}\left[\frac{B_i}{B} - \frac{2\sum\limits_{j=1}^{c}\chi_j A_{ij}}{A}\right]\ln\left[\frac{Z+\left(1+\sqrt{2}\right)B}{Z+\left(1-\sqrt{2}\right)B}\right] + \frac{B_i}{B}\left(Z-1\right) - \ln\left(Z-B\right)$$

$$A_i = 0.45724\,\frac{P_{r_i}}{T_{r_i}^{\,2}}\left[1+\kappa_i\left(1-T_{r_i}^{\,1/2}\right)\right]^2 \qquad\qquad B_i = 0.07780\,\frac{P_{r_i}}{T_{r_i}}$$

$$A = \sum_{i=1}^{c}\sum_{j=1}^{c}\chi_i\chi_j A_{ij} \qquad\qquad B = \sum_{i=1}^{c}\chi_i B_i$$

$$A_{ij} = A_{ji} = \left(1-k_{ij}\right)\sqrt{A_i A_j}$$

$$Z^3 + (B-1)Z^2 + (A-3B^2-2B)Z + (B^3+B^2-AB) = 0$$

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Fugacity Coefficient (AspenPlus Examples)

1. ϕ_i^{α} for ethylene at 25°C and 40 bar

2. $\hat{\phi}_{CO_2}^{\alpha}$ for CO_2 in 50:50 (mole) mixture with toluene at 45°C and 40 bar

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Fugacity Coefficient (multicomponent approximation)

Lewis fugacity approximation (rule)

$$\hat{\phi}_i = \phi_i$$

Valid near ideal solution conditions,
i.e. y_i in excess (>0.9)

Fugacity / Equilibrium (SUMMARY)

$$\hat{f}_i^V = \hat{f}_i^L$$

1) $\quad y_i P \hat{\phi}_i^V = x_i P \hat{\phi}_i^L$

Vapor phase: good; liquid phase: good for HC or moderate – high pressures (compressible liquid phase)

2) $\quad y_i P \hat{\phi}_i^V = x_i \gamma_i P_i^{sat} \phi_i^{sat} P.C.$

Typically used for liquid phase fugacity calculations

3) $\quad y_i P \hat{\phi}_i^V = x_i H_i$

Used for special cases (like gases dissolving into liquid phase)

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Fugacity (Liquid Phase)

$\hat{f}_i^{\,L}$
1. Compressible liquids
2. Ideal and real solutions
3. Dissolved gases

1. Compressible liquids (mod – high P, and hydrocarbons)

$$\hat{f}_i^{\,L} = x_i P \hat{\phi}_i^{\,L} \qquad \text{Use EOS for: } \hat{\phi}_i^{\,L} \ \& \ Z^L \left(or \ \upsilon^L \right)$$

2. Ideal liquid solution

$$\hat{f}_i^{\,L} = \hat{f}_i^{\,ideal} = x_i f_i^{\,ideal} = x_i f_i^{\,o} \qquad f_i^{\,o} = \text{Pure species fugacity}$$

real solution

$$\hat{f}_i^{\,L} = \gamma_i \hat{f}_i^{\,ideal} = x_i \gamma_i f_i^{\,o} \qquad \text{Lewis/Randall basis}$$

$$\gamma_i = \text{Activity coefficient} \qquad \gamma_i \equiv \frac{\hat{f}_i^{\,L}}{\hat{f}_i^{\,ideal}} = \frac{\hat{f}_i^{\,L}}{x_i f_i^{\,o}}$$

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Fugacity (Liquid Phase)

real solution $\qquad \hat{f}_i^L = x_i \gamma_i f_i^o$ $\qquad\qquad$ Lewis/Randall basis

$$f_i^o = P_i^{sat} \phi_i^{sat} \exp\left[\int_{P_i^{sat}}^{P} \frac{\upsilon_i^L}{RT} dP\right] \qquad \text{at system T and P}$$

$\phi_i^{SAT}(P^{SAT}) \cong 1$

Poynting correction factor [P.C.]

$\upsilon_i^L \sim$ constant

$$P.C. = exp\left[\frac{\upsilon_i^L}{RT}(P - P_i^{SAT})\right]$$

$P < 100 \, bar \qquad P.C. \sim 1$

$$\boxed{\hat{f}_i^L = x_i \gamma_i P_i^{sat} \phi_i^{sat} \exp\left[\int_{P_i^{sat}}^{P} \frac{\upsilon_i^L}{RT} dP\right]}$$

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Fugacity (Typical Liquid Phase Models)

real solution

$$\hat{f}_i^{\,L} = x_i \gamma_i P_i^{sat} \phi_i^{sat} P.C.$$

Lewis/Randall basis

$$\gamma_i = ?$$

$1 \quad 1$

real solution – behaves ideally in the liquid phase then:

$$\hat{f}_i^{\,L} = x_i P_i^{sat}$$

$$\gamma_i = 1$$

real solution – behaves <u>non-ideally</u> in the liquid phase then:

$$\hat{f}_i^{\,L} = x_i \gamma_i P_i^{sat}$$

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Activity Coefficient (ways to calculate)

$$\overline{G}_i^E = \overline{G}_i - \overline{G}_i^{ideal} = u_i - u_i^{ideal} = RT \ln \frac{\hat{f}_i}{\hat{f}_i^{ideal}} \qquad but: \quad \gamma_i \equiv \frac{\hat{f}_i^L}{\hat{f}_i^{ideal}}$$
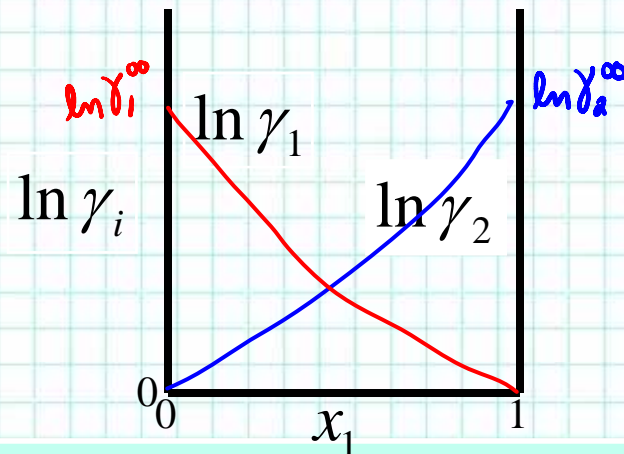
$$\boxed{\overline{G}_i^E = RT \ln \gamma_i} \qquad \overline{G}_i^E = \left(\frac{\partial n_T \overbrace{g^E}^{G^E}}{\partial n_i} \right)_{T,P,n_j} \qquad \boxed{RT \ln \gamma_i = \left(\frac{\partial n_T g^E}{\partial n_i} \right)_{T,P,n_j}}$$

Now, need models for calculating g^E and then can find γ_i

1. <u>2-suffix Margules (simple, symmetric) [binary]</u> $\quad g^E = A x_1 x_2$

$$\boxed{\begin{array}{l} RT \ln \gamma_1 = A x_2^2 \\ RT \ln \gamma_2 = A x_1^2 \end{array}}$$

$\ln \gamma_1^\infty$ $\ln \gamma_1$ $\ln \gamma_2^\infty$

$\ln \gamma_i$ $\ln \gamma_2$

0 at 0 x_1 1

$$\boxed{\gamma_1 = \exp\left(\frac{A}{RT}(1-x_1)^2 \right)}$$

$$\lim_{x_1 \to 0} \gamma_1 = \exp\left(\frac{A}{RT} \right) = \gamma_1^\infty$$

Activity Coefficient (2 suffix Margules model)

1. <u>2-suffix Margules (simple, symmetric) [binary]</u> $g^E = Ax_1x_2$

Find A: take data… $\quad y_iP = x_i\gamma_iP_i^{sat}$

EXP	T	P	X_1	Y_1	γ_1	γ_2 calc
1	const	$\sim$	—	—	=	—
2	"	$\sim$	—	—	=	—
3	"	$\sim$	—	—	=	—

$exp \; \gamma_1^\infty \longrightarrow \underline{\underline{A}}$

Example: binary mix of cyclohexane (a) and dodecane (b) at 39.33°C

$$\gamma^\infty \hat{=} 0.87 = e + p\left[\dfrac{A}{RT}\right]$$

$$A = -361.8 \; \dfrac{J}{mol}$$

$$\gamma_{cyclo-C6}^\infty = 0.88$$

$$\gamma_{C12}^\infty = 0.86$$

$$\lim_{x_1 \to 0} \gamma_1 = \exp\left(\dfrac{A}{RT}\right) = \gamma_1^\infty$$

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Activity Coefficient (Models)

1. 2-suffix Margules (simple, symmetric) [binary] $g^E = Ax_1x_2$

Asymmetric models:

2. Three-suffix Margules: (additional parameter)
3. Van Laar: (older model but still good and easy to work with)
4. Wilson: (not good for liquid-liquid-equilibria)
5. NRTL: (**N**on-**R**andom-**T**wo-**L**iquid; good first choice, usually)
6. UNIQUAC: (**UNI**versal **QUA**si-**C**hemical; also good)
7. UNIFAC: (only predictive model)

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Activity Coefficient (Binary Models)

TABLE 7.1 Common Binary Activity Coefficient Models

Model	g^E
Two-suffix Margules	$Ax_a x_b$
Three-suffix Margules	$x_a x_b[A + B(x_a - x_b)]$
or	$x_a x_b[A_{ba}x_a + A_{ab}x_b]$
Van Laar	$x_a x_b \left(\dfrac{AB}{Ax_a + Bx_b} \right)$
Wilson	$-RT \begin{bmatrix} x_a \ln(x_a + \Lambda_{ab}x_b)+ \\ x_b \ln(x_b + \Lambda_{ba}x_a) \end{bmatrix}$
NRTL*	$RTx_a x_b \left[\dfrac{\tau_{ba}\mathbf{G}_{ba}}{x_a + x_b\mathbf{G}_{ba}} + \dfrac{\tau_{nb}\mathbf{G}_{ab}}{x_b + x_a\mathbf{G}_{ab}} \right]$

*Nonrandom two-liquid.

Koretsky, 2004

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Activity Coefficient (Binary Models)

Model	$RT \ln\gamma_a$	$RT \ln\gamma_b$
Two-suffix Margules	Ax_b^2	Ax_a^2
Three-suffix Margules	$(A + 3B)x_b^2 - 4Bx_b^3$	$(A - 3B)x_a^2 + 4Bx_a^3$
or	$x_b^2[A_{ab} + 2(A_{ba} - A_{ab})x_a]$	$x_a^2[A_{ba} + 2(A_{ab} - A_{ba})x_b]$
Van Laar	$A\left(\dfrac{Bx_b}{Ax_a + Bx_b}\right)^2$	$B\left(\dfrac{Ax_a}{Ax_a + Bx_b}\right)^2$
Wilson	$-RT\left[\ln(x_a + \Lambda_{ab}x_b) + x_b\left(\dfrac{\Lambda_{ba}}{x_b + \Lambda_{ba}x_a} - \dfrac{\Lambda_{ab}}{x_a + \Lambda_{ab}x_b}\right)\right]$	$-RT\left[\ln(x_b + \Lambda_{ba}x_a) + x_a\left(\dfrac{\Lambda_{ab}}{x_a + \Lambda_{ab}x_b} - \dfrac{\Lambda_{ba}}{x_b + \Lambda_{ba}x_a}\right)\right]$
NRTL*	$RTx_b^2\left[\dfrac{\tau_{ba}G_{ba}^2}{(x_a + x_bG_{ba})^2} + \dfrac{\tau_{ab}G_{ab}}{(x_b + x_aG_{ab})^2}\right]$	$RTx_a^2\left[\dfrac{\tau_{ba}G_{ba}}{(x_a + x_bG_{ba})^2} + \dfrac{\tau_{ab}G_{ab}^2}{(x_b + x_aG_{ab})^2}\right]$

*Nonrandom two-liquid.

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Activity Coefficient (Binary Models)

Wilson Equation. Based on molecular considerations, Wilson (1964) presented the following expression for the excess Gibbs energy of a binary solution:

$$\frac{g^E}{RT} = -x_1 \ln(x_1 + \Lambda_{12}x_2) - x_2 \ln(x_2 + \Lambda_{21}x_1) \qquad (6\text{-}104)$$

The activity coefficients derived from this equation are

$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right) \qquad (6\text{-}105)$$

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) - x_1 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right) \qquad (6\text{-}106)$$

Prausnitz, et.al., 1999

Activity Coefficient (Binary Models)

Wilson's equation has two adjustable parameters, Λ_{12} and Λ_{21}. In Wilson's derivation, these are related to the pure-component molar volumes and to characteristic energy differences by

$$\Lambda_{12} \equiv \frac{v_2}{v_1} \exp\left(-\frac{\lambda_{12} - \lambda_{11}}{RT}\right) \qquad (6\text{-}107)$$

$$\Lambda_{21} \equiv \frac{v_1}{v_2} \exp\left(-\frac{\lambda_{21} - \lambda_{22}}{RT}\right) \qquad (6\text{-}108)$$

Wilson's equation has two disadvantages that are not serious for many applications. First, Eqs. (6-105) and (6-106) are not useful for systems where the logarithms of the activity coefficients, when plotted against x, exhibit maxima or minima. (Van Laar equations are also not useful for this case). Such systems, however, are not common. The second and more serious disadvantage of Wilson's equation lies in its inability to predict limited miscibility. When Wilson's equation is substituted into the equations of thermodynamic stability for a binary system (see next section), no parameters Λ_{12} and Λ_{21} can be found that indicate the existence of two stable liquid phases.[31] Wilson's equation, therefore, should be used only for liquid systems that are completely miscible or else for those limited regions of partially miscible systems where only one liquid phase is present.

Prausnitz, et.al., 1999

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Activity Coefficient (Binary Models)

NRTL Equation. The basic idea in Wilson's derivation of Eq. (6-104) follows from the concept of local composition that is discussed further in Sec. 7.7. This concept was also used by Renon (1968) in his derivation of the NRTL (*nonrandom, two-liquid*) equation; however, Renon's equation, unlike Wilson's, is applicable to partially miscible as well as completely miscible systems. The NRTL equation for the excess Gibbs energy is

$$\frac{g^E}{RT} = x_1 x_2 \left(\frac{\tau_{21} G_{21}}{x_1 + x_2 G_{21}} + \frac{\tau_{12} G_{12}}{x_2 + x_1 G_{12}} \right) \tag{6-109}$$

where

$$\tau_{12} = \frac{g_{12} - g_{22}}{RT} \qquad \tau_{21} = \frac{g_{21} - g_{11}}{RT} \tag{6-110}$$

$$G_{12} = \exp(-\alpha_{12}\tau_{12}) \qquad G_{21} = \exp(-\alpha_{12}\tau_{21}) \tag{6-111}$$

The significance of g_{ij} is similar to that of λ_{ij} in Wilson's equation; g_{ij} is an energy parameter characteristic of the *i-j* interaction. Parameter α_{12} is related to the nonrandomness in the mixture; when α_{12} is zero, the mixture is completely random and Eq. (6-109) reduces to the two-suffix Margules equation. The NRTL equation contains three parameters, but reduction of experimental data for a large number of binary systems indicates that α_{12} varies from about 0.20 to 0.47; when experimental data are scarce, the value of α_{12} can often be set arbitrarily; a typical choice is $\alpha_{12} = 0.3$. From Eq. (6-109), the activity coefficients are

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Activity Coefficient (Binary Models)

NRTL

$$\ln\gamma_1 = x_2^2\left[\tau_{21}\left(\frac{G_{21}}{x_1+x_2G_{21}}\right)^2 + \frac{\tau_{12}G_{12}}{(x_2+x_1G_{12})^2}\right] \qquad (6\text{-}112)$$

$$\ln\gamma_2 = x_1^2\left[\tau_{12}\left(\frac{G_{12}}{x_2+x_1G_{12}}\right)^2 + \frac{\tau_{21}G_{21}}{(x_1+x_2G_{21})^2}\right] \qquad (6\text{-}113)$$

For moderately nonideal systems, the NRTL equation offers no advantages over the simpler van Laar and three-suffix Margules equations. However, for strongly nonideal mixtures, and especially for partially immiscible systems,[32] the NRTL equation often provides a good representation of experimental data if care is exercised in data reduction to obtain the adjustable parameters. For example, consider the nitro-

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Activity Coefficient (Binary Models)

UNIQUAC

in a sense, extends the quasichemical theory of Guggenheim (see Sec. 7.6) for nonrandom mixtures to solutions containing molecules of different size. This extension was therefore called the *universal quasi-chemical* theory or, in short, UNIQUAC. As discussed in Sec. 7.7, the UNIQUAC equation for g^E consists of two parts, a *combinatorial part* that attempts to describe the dominant entropic contribution, and a *residual part* that is due primarily to intermolecular forces that are responsible for the enthalpy of mixing. The combinatorial part is determined only by the composition and by the sizes and shapes of the molecules; it requires only pure-component data. The residual part, however, depends also on intermolecular forces; the two adjustable binary parameters, therefore, appear only in the residual part. The UNIQUAC equation is

$$\frac{g^E}{RT} = \left(\frac{g^E}{RT} \right)_{combinatorial} + \left(\frac{g^E}{RT} \right)_{residual} \tag{6-114}$$

Prausnitz, et.al., 1999

Activity Coefficient (Binary Models)

(UNIQUAC)

For a binary mixture,

$$\left(\frac{g^E}{RT}\right)_{combinatorial} = x_1 \ln\frac{\Phi_1^*}{x_1} + x_2 \ln\frac{\Phi_2^*}{x_2} + \frac{z}{2}\left(x_1 q_1 \ln\frac{\theta_1}{\Phi_1^*} + x_2 q_2 \ln\frac{\theta_2}{\Phi_2^*}\right) \quad (6\text{-}115)$$

$$\left(\frac{g^E}{RT}\right)_{residual} = -x_1 q_1' \ln(\theta_1' + \theta_2'\tau_{21}) - x_2 q_2' \ln(\theta_2' + \theta_1'\tau_{12}) \quad (6\text{-}116)$$

where the coordination number z is set equal to 10. Segment fraction, Φ^*, and area fractions, θ and θ', are given by

$$\Phi_1^* = \frac{x_1 r_1}{x_1 r_1 + x_2 r_2} \qquad \Phi_2^* = \frac{x_2 r_2}{x_1 r_1 + x_2 r_2} \quad (6\text{-}117)$$

$$\theta_1 = \frac{x_1 q_1}{x_1 q_1 + x_2 q_2} \qquad \theta_2 = \frac{x_2 q_2}{x_1 q_1 + x_2 q_2} \quad (6\text{-}118)$$

Prausnitz, et.al., 1999

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Activity Coefficient (Binary Models)

Table 6-9 Some structural parameters for UNIQUAC equation.*

Component	r	q
Carbon tetrachloride	3.33	2.82
Chloroform	2.70	2.34
Formic acid	1.54	1.48
Methanol	1.43	1.43
Acetonitrile	1.87	1.72
Acetic acid	1.90	1.80
Nitroethane	2.68	2.41
Ethanol	2.11	1.97
Acetone	2.57	2.34
Ethyl acetate	3.48	3.12
Methyl ethyl ketone	3.25	2.88
Diethylamine	3.68	3.17
Benzene	3.19	2.40
Methylcyclopentane	3.97	3.01
Methyl isobutyl ketone	4.60	4.03
n-Hexane	4.50	3.86
Toluene	3.92	2.97
n-Heptane	5.17	4.40
n-Octane	5.85	4.94
Water	0.92	1.40

r and q depend on molecular size (volume) and external surface areas of pure components.

Prausnitz, et.al., 1999

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Activity Coefficient (Binary Models)

Table 6-10 Some binary parameters for UNIQUAC equation.*

System (1)/(2)	T (K)	Energy parameters (K)	
		a_{12}	a_{21}
Acetonitrile/benzene	318	-40.70	299.79
n-Hexane/nitromethane	318	230.64	-5.86
Acetone/chloroform	323	-171.71	93.93
Ethanol/n-octane	348	-123.57	1354.92
Formic acid/acetic acid	374-387	-144.58	241.64
Propionic acid/methyl isobutyl ketone	390-411	-78.49	136.46
Acetone/water	331-368	530.99	-100.71
Acetonitrile/water	350-364	294.10	61.92
Acetic acid/water	373-389	530.94	-299.90
Formic acid/water	374-380	924.01	-525.85
Methylcyclopentane/ethanol	333-349	1383.93	-118.27
Methylcyclopentane/benzene	344-352	56.47	-6.47
Ethanol/carbon tetrachloride	340-351	-138.90	947.20
Ethanol/benzene	350-369	-75.13	242.53
Methyl ethyl ketone/n-heptane	328	-29.64	1127.95
Methanol/benzene	528	-56.35	972.09
Chloroform/ethanol	323	934.23	-208.50
Chloroform/n-heptane	323	-19.26	88.40
Ethanol/n-heptane	323	-105.23	1380.30
Acetone/methanol	323	379.31	-108.42
Methanol/ethyl acetate	335-347	-107.54	579.61

* Data sources are given by Anderson (1978).

Prausnitz, et.al., 1999

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Activity Coefficient (Example)

Vapor

Liquid
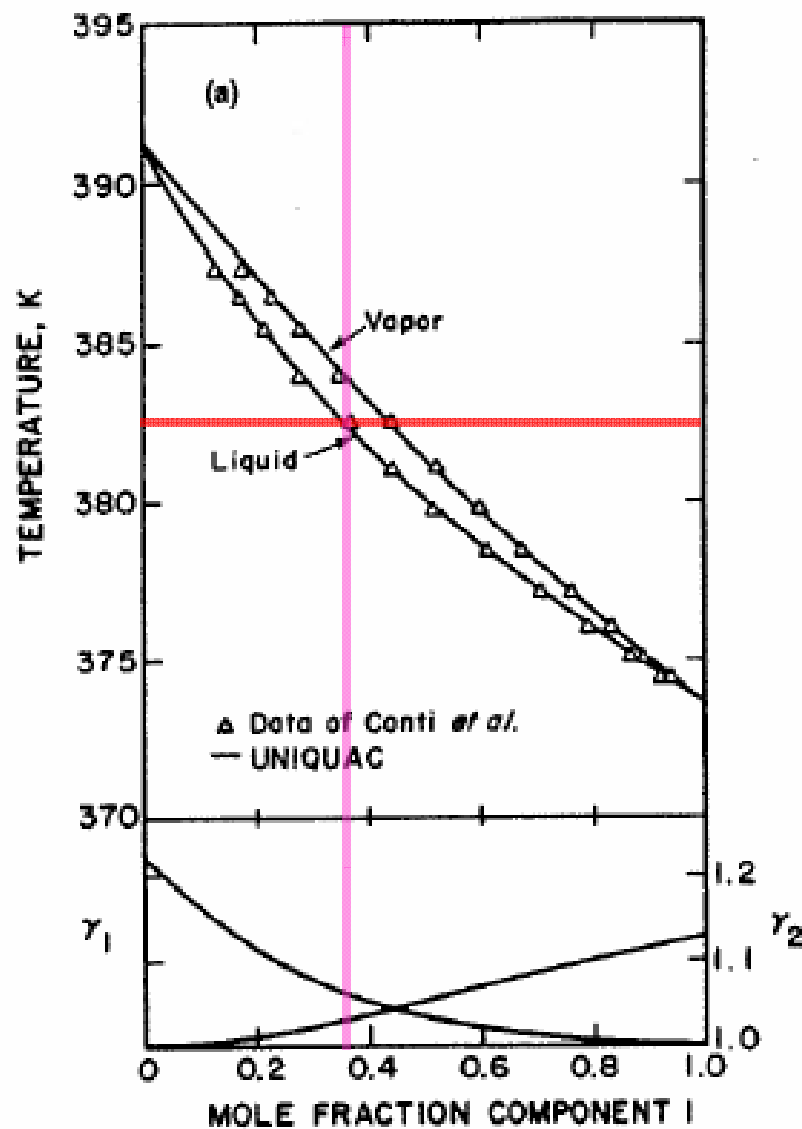
Temperature-composition diagram at 1.013 bar (1 atm) pressure for system: **formic acid (1)** and **acetic acid (2)**

Prausnitz, et.al., 1999

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Lecture 8

Chapter 5
- Thermodynamic Web
- Departure Functions
- Review Equations of state (chapter 4, briefly)

Chapter 6
- Equilibrium (chemical potential)
  * Pure Component
  * Mixtures

Chapter 7
- Fugacity (chemical potential → fugacity → equilibrium calculations)
  * Vapor (overview), liquid, solids
- Activity Coefficients [Fugacity Coefficients (overview)]

Chapter 8
- Phase Equilibrium
  * Diagrams
  * Vapor – Liquid (VLE)
  * Liquid – Liquid (LLE)
  * Solid – Liquid (SLE)

Chapter 9
- Reaction Equilibria

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