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Course 565/665 Lecturer prof. Cavagnero

Day 4.6.04 Date 9:55 am

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free energy of mixing —

now combine expression for u and s

$$\frac{F(N_A, N_B)}{kT} = N_A \ln\left(\frac{N_A}{N}\right) + N_B \ln\left(\frac{N_B}{N}\right) + \left(\frac{z w_{AA}}{2kT}\right) N_A + \left(\frac{z w_{BB}}{2kT}\right) N_B + \chi_{AB} \frac{N_A N_B}{N}$$

$$\Delta F_{mix} = F(N_A, N_B) - F(N_A, 0) - F(0, N_B)$$

$$\frac{\Delta F_{mix}}{NkT} = x \ln x + (1-x)\ln(1-x) + \chi_{AB}\, x(1-x)$$

— the regular solution model (first given by JH Hildebrand)

(ex) oil and water don't mix.

$\chi_{AB} \approx 5$ for hydrocarbon / water interactions ; $x_{oil} = 0.3$, $T = 300K$.

$\frac{\Delta F_{mix}}{N} = 1.1 \frac{kJ}{mol} > 0$ ⇒ oil and water won't mix to form a random solution of this composition.

If $x_{oil} = 10^{-4}$, $\frac{\Delta F_{mix}}{N} = -1.3\ J\,mol^{-1} < 0$ ⇒ favorable mixing.

The chemical potentials

$$\frac{\mu_A}{kT} = \left[\frac{\partial}{\partial N_A}\left(\frac{F}{kT}\right)\right]_{N_B, T}$$

$$= \ln\frac{N_A}{N} + N_A \cdot \frac{N}{N_A} \cdot \frac{(N - N_A)}{(N_A + N_B)^2} + N_B \cdot \frac{N}{N_B} \cdot \frac{(-N_B)}{(N_A+N_B)^2} + \frac{z w_{AA}}{2kT} +$$

$$\chi_{AB} N_B \cdot \frac{N - N_A}{(N_A + N_B)^2}$$

$$= \ln x_A + \frac{z w_{AA}}{2kT} + \chi_{AB}(1 - x_A)^2$$

similarly

$$\frac{\mu_B}{kT} = \ln x_B + \frac{z w_{BB}}{2kT} + \chi_{AB}(1 - x_B)^2$$

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obtain $\mu = KT\ln x$ + other terms.

A small ambiguity from this lattice model: fully filled lattice. $N = N_A + N_B$.
so total V change with changing N_A (holding N_B constant).

more generally, $\mu = \mu^\circ + KT\ln \gamma x$

γ — activity coefficient

μ° — standard state chemical potential.

mixing entropy ($KT\ln x$) is always favorable for mixing process.

The exchange parameter χ_{AB} describes the energy change for the exchange process $\frac{1}{2}z(AA) + \frac{1}{2}z(BB) \longrightarrow z(AB)$.

according to Hildebrand's principle, for most systems, the AB affinity is weaker than the AA, BB affinities. So usually $\chi_{AB} > 0$

~~Interfacial Tension Describes the Free Energy of Creating Surface Area~~

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