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(4) Quasichemical mass balances are:

$$\begin{cases} Z X_A = 2n_{AA} + n_{AB} \\ Z X_B = 2n_{BB} + n_{AB} \end{cases}$$

- When $Z=1$, these become identical to the associate model mass balances.
- The configurational entropy expression, however, is different from the associate model, so that $\Delta S = \Delta S^{ideal}$ when $\omega = 0$ (and $X_{AB} = 2X_A X_B$, $X_{AA} = X_A^2$, $X_{BB} = X_B^2$). The model will now also give more realistic results when $\omega > 0$.
- When $\omega = -\infty$, at $X_A = X_B = 1/2$, $X_{AA} = X_{AB} = 0$ and $X_{AB} = 1$

and

$$\Delta S^{config} = -R\left(\frac{Z}{2}\right)\left(X_{AA}\ln\frac{X_{AA}}{X_A^2} + X_{BB}\ln\frac{X_{BB}}{X_B^2} + X_{AB}\ln\frac{X_{AB}}{2X_A X_B}\right) - R(X_A\ln X_A + X_B\ln X_B)$$

$$= -\frac{RZ}{2}\left(0 + 0 + \ln 1/2\left(\tfrac{1}{2}\right)\left(\tfrac{1}{2}\right)\right) - R\left(\tfrac{1}{2}\ln\tfrac{1}{2} + \tfrac{1}{2}\ln\tfrac{1}{2}\right)$$

$$= -\frac{RZ}{2}(\ln 2) + R(\ln 2) = R\ln 2\left(1 - \frac{Z}{2}\right)$$

When $Z=1$, $\Delta S^{config} = \frac{1}{2}R\ln 2$

That is, it does not equal zero as it does in the associate model (and as it should).

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(4) $(A-A) + (B-B) = 2(A-B)$ $\quad \Delta g_{AB} = -10\,kJ/mol$

$$Y_A = X_A = (X_{AA} + X_{AB}/2) = 0.5 \quad (1)$$
$$Y_B = X_B = (X_{BB} + X_{AB}/2) = 0.5 \quad (2)$$

$$\frac{X_{AB}^2}{(X_{AA}X_{BB})} = 4\exp(-\Delta g_{AB}/RT) = 4\exp\left(\frac{+10000}{(8.315)(1000)}\right) = 13.31565 \quad (3)$$

By symmetry, $X_{AA} = X_{BB}$

From Eq. (1):

$$(X_{AB}/2) = (0.5 - X_{AA}) \qquad X_{AB} = 1.0 - 2X_{AA}$$

From Eq (3)

$$\frac{(1-2X_{AA})^2}{X_{AA}^2} = 13.31565$$

$$(1-2X_{AA}) = X_{AA}(13.31565)^{1/2}$$

$$\begin{cases} X_{AA} = 0.17702 \\ X_{BB} = 0.17702 \\ X_{AB} = 0.64596 \end{cases}$$

In an ideal mixture: $\begin{cases} X_{AA} = X_A^2 = (0.5)^2 = 0.25 \\ X_{BB} = X_B^2 = (0.5)^2 = 0.25 \\ X_{AB} = 2X_AX_B = 2(0.5)(0.5) = 0.50 \end{cases}$