Supporting Information:

Example calculation for determining solid solubility using the MOSCED model with the Wilson G^E equation

Solvent: 2-butanone
Solute: Benzimidazole
Temperature: 298 K

1. Obtain pure component data for solute and solvent

MOSCED Parameters	**2-butanone (1)**	**Benzimidazole(2)**
λ $(J/cm^3)^{0.5}$	14.74	16.21
τ $(J/cm^3)^{0.5}$	6.64	4.22
α $(J/cm^3)^{0.5}$	0	12.15
β $(J/cm^3)^{0.5}$	9.70	11.12
q	1	0.9
$\boldsymbol{v}$ (cm^3/mol)	90.2	92
$\boldsymbol{\Delta H^{fus}}$(kJ/mol)		22.7
$\boldsymbol{T^m}$(K)		444

2. Calculate infinite dilution activity coefficients using MOSCED

Calculation of γ_1^∞

$$R = 8.314 \frac{\mathrm{J}}{\mathrm{mol \cdot K}}$$

$$\alpha_1^T = \alpha_1 \left(293/T\right)^{0.8} = 0$$

$$\beta_1^T = \beta_1 \left(293/T\right)^{0.8} = 9.57$$

$$\tau_1^T = \tau_1 \left(293/T \right)^{0.4} = 6.6$$

$$POL_1 = q^4 \left(1.15 - 1.15 \exp\left(-0.002337 (\tau_1^T)^3\right)\right) + 1 = 1.56$$

$$\psi_1 = POL_1 + 0.002629 \alpha_1^T \beta_1^T = 1.56$$

$$\xi_1 = 0.68 (POL_1 - 1) + \left[3.24 - 2.4 \exp\left(-0.002687 \left(\alpha_1 \beta_1\right)^{1.5}\right)\right]^{\left(293/T\right)^2} = 1.23$$

$$aa_1 = 0.953 - 0.002314 \left((\tau_1^T)^2 + \alpha_1^T \beta_1^T\right) = 0.85$$

$$d_{21} = \ln \left(\frac{v_1}{v_2} \right)^{aa_1} + 1 - \left(\frac{v_1}{v_2} \right)^{aa_1} = -0.00014$$

$$\ln \gamma_1^\infty = \frac{v_1}{RT} \left[(\lambda_2 - \lambda_1)^2 + \frac{q_2^2 q_1^2 \left(\tau_2^T - \tau_1^T\right)^2}{\psi_2} + \frac{\left(\alpha_2^T - \alpha_1^T\right)\left(\beta_2^T - \beta_1^T\right)}{\xi_2} \right] + d_{21} = 0.36$$

$$\gamma_1^\infty = 1.43$$

Calculation of γ_2^∞

$$\alpha_2^T = \alpha_2 \left(293/T \right)^{0.8} = 11.99$$

$$\beta_2^T = \beta_2 \left(293/T \right)^{0.8} = 10.97$$

$$\tau_2^T = \tau_2 \left(293/T \right)^{0.4} = 4.19$$

$$POL_2 = q^4 \left(1.15 - 1.15 \exp\left(-0.002337 (\tau_2^T)^3\right)\right) + 1 = 1.12$$

$$\psi_2 = POL_2 + 0.002629 \alpha_2^T \beta_2^T = 1.47$$

$$\xi_2 = 0.68(POL_2 - 1) + \left[3.24 - 2.4\exp\left(-0.002687(\alpha_2\beta_2)^{1.5}\right)\right]^{\left(293/T\right)^2} = 3.16$$

$$aa_2 = 0.953 - 0.002314\left((\tau_2^T)^2 + \alpha_2^T\beta_2^T\right) = 0.62$$

$$d_{12} = \ln\left(\frac{v_2}{v_1}\right)^{aa_2} + 1 - \left(\frac{v_2}{v_1}\right)^{aa_2} = -7.4\cdot 10^{-5}$$

$$\ln\gamma_2^{\infty} = \frac{v_2}{RT}\left[(\lambda_1 - \lambda_2)^2 + \frac{q_1^2 q_2^2\left(\tau_1^T - \tau_2^T\right)^2}{\psi_1} + \frac{\left(\alpha_1^T - \alpha_2^T\right)\left(\beta_1^T - \beta_2^T\right)}{\xi_1}\right] + d_{12} = 0.65$$

$$\gamma_2^{\infty} = 1.91$$

3. Calculate Wilson parameters from predicted infinite dilution activity coefficients

Solve the Wilson equation for two unknown interaction parameters.

$$\ln\gamma_1^{\infty} = 1 - \ln\Lambda_{12} - \Lambda_{21} = 0.36$$

$$\ln\gamma_2^{\infty} = 1 - \ln\Lambda_{21} - \Lambda_{12} = 0.65$$

Solving for Λ_{12} and Λ_{21} yields

$$\Lambda_{12} = 1.28$$

$$\Lambda_{21} = 0.396$$

4. Calculate solubility using Wilson equation and ideal solubility

Solve for x_2 in

$$x_2\gamma_2 = x_2^{ideal}$$

where

$$\ln\gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) - x_1\left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2}\right)$$ and

$$x_2^{ideal} = \exp\left[\frac{-\Delta H_{fus}}{RT_m}\left(\frac{T_m}{T} - 1\right)\right]$$

$$x_2^{ideal} = 0.04854$$

Solution is x_2=0.027 and γ_2=1.79