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Supplementary material

SUPPLEMENTARY MATERIAL TO

A thermodynamic approach for correlating the solubility of drug compounds in supercritical CO_2 based on Peng–Robinson and Soave–Redlich–Kwong equations of state coupled with van der Waals mixing rules

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The constants of the PR and SRK equations of state are as below. For the SRK equation of state, c_1=0 and c_2=1.

$$a = a_c[1+m(1-\sqrt{T_r})]^2 \tag{S-1}$$

$$a_c = 0.42748\frac{R^2 T_c^{\ 2}}{P_c} \tag{S-2}$$

$$m = 0.48 + 1.574\omega - 0.176\omega^2 \tag{S-3}$$

$$b = 0.08664\frac{RT_c}{P_c} \tag{S-4}$$

where T_c, P_c and ω are indicative of critical temperature, critical pressure and acentric factor. T_r and R are reduced temperature and universal gas constant. Similarly, for the PR equation of state, c_1=1–$2^{1/2}$ and c_2=1+$2^{1/2}$.

$$a = a_c[1+m(1-\sqrt{T_r})]^2 \tag{S-5}$$

$$a_c = 0.42748\frac{R^2 T_c^{\ 2}}{P_c} \tag{S-6}$$

$$m = 0.37464 + 1.574226\omega - 0.26992\omega^2 \tag{S-7}$$

$$b = 0.007780\frac{RT_c}{P_c} \tag{S-8}$$

For a mixture of heavy component and SCF, the EOS parameters a and b are calculated by the following mixing rules:[1]

The vdW1 mixing rule:

$$a = \sum_i \sum_j y_i y_j a_{ij} \tag{S-8}$$

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$$b = \sum_{j} y_j b_j \tag{S-9}$$

$$a_{ij} = \sqrt{a_i a_j}(1 - k_{ij}) \tag{S-10}$$

The vdW2 mixing rule:

$$a = \sum_{i} \sum_{j} y_i y_j a_{ij} \tag{S-11}$$

$$b = \sum_{i} \sum_{j} y_i y_j \mathrm{b}_{ij} \tag{S-12}$$

$$a_{ij} = \sqrt{a_i a_j}(1 - k_{ij}) \tag{S-13}$$

$$b_{ij} = \frac{b_i + b_j}{2}(1 - l_{ij}) \tag{S-14}$$

where y_i and y_j are the mole fractions of components i and j and k_{ij} and l_{ij} are the binary interaction parameters and i and j refer to the ith and jth compounds in the mixture.
$\hat{a}_i$ and $\hat{b}_i$ in Eq. (6) of the manuscript are derivatives related to the attractive and repulsive parameters of EOS, which are calculated from the following equations:

For the vdW1 mixing rule:

$$\hat{a}_i = \left[\frac{\partial(na)}{\partial n_i}\right]_{T,P,n_{j\neq i}} = 2\sum_{i=1}^{N} y_i a_{ij} \tag{S-15}$$

$$\hat{b}_i = \left[\frac{\partial(nb)}{\partial n_i}\right]_{T,P,n_{j\neq i}} = b_i \tag{S-16}$$

For the vdW2 mixing rule:

$$\hat{a}_i = \left[\frac{\partial(na)}{\partial n_i}\right]_{T,P,n_{j\neq i}} = 2\sum_{i=1}^{N} y_i a_{ij} \tag{S-17}$$

$$\hat{b}_i = \left[\frac{\partial(nb)}{\partial n_i}\right]_{T,P,n_{j\neq i}} = 2\sum_{i=1}^{N} y_i b_{ij} \tag{S-18}$$