SUPPLEMENTARY MATERIAL TO

A thermodynamic approach for correlating the solubility of drug compounds in supercritical CO2 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 $c_2=1$.

$$a = a_c[1 + m(1 - \sqrt{\frac{T}{T_c}})]^2$$  \hspace{1cm} (S-1)

$$a_c = 0.42748 \frac{R^2 T_c^2}{P_c}$$  \hspace{1cm} (S-2)

$$m = 0.48 + 1.574 \omega - 0.176 \omega^2$$  \hspace{1cm} (S-3)

$$b = 0.08664 \frac{R T_c}{P_c}$$  \hspace{1cm} (S-4)

where $T_c$, $P_c$ and $\omega$ 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 $c_2=1+2^{1/2}$.

$$a = a_c[1 + m(1 - \sqrt{\frac{T}{T_c}})]^2$$  \hspace{1cm} (S-5)

$$a_c = 0.42748 \frac{R^2 T_c^2}{P_c}$$  \hspace{1cm} (S-6)

$$m = 0.37464 + 1.574226 \omega - 0.26992 \omega^2$$  \hspace{1cm} (S-7)

$$b = 0.007780 \frac{R T_c}{P_c}$$  \hspace{1cm} (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:

$$a = \sum_i \sum_j y_i y_j a_{ij}$$  \hspace{1cm} (S-8)

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The vdW2 mixing rule:

\[ a = \sum_{i} \sum_{j} y_i y_j a_{ij} \]  
\[ b = \sum_{i} \sum_{j} y_i y_j b_{ij} \]  
\[ a_{ij} = \sqrt{a_i a_j (1 - k_{ij})} \]  
\[ b_{ij} = \frac{h_i + h_j}{2} (1 - l_{ij}) \]  

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 \( i^{th} \) and \( j^{th} \) 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:

\[ \hat{a}_i = \left[ \frac{\partial(na)}{\partial n_i} \right]_{n, p, \eta_{ji}} = 2 \sum_{i=1}^{N} y_i a_{ij} \]  
\[ \hat{b}_i = \left[ \frac{\partial(nb)}{\partial \eta_i} \right]_{n, p, \eta_{ji}} = b_i \]  

For the vdW2 mixing rule:

\[ \hat{a}_i = \left[ \frac{\partial(na)}{\partial n_i} \right]_{n, p, \eta_{ji}} = 2 \sum_{i=1}^{N} y_i a_{ij} \]  
\[ \hat{b}_i = \left[ \frac{\partial(nb)}{\partial \eta_i} \right]_{n, p, \eta_{ji}} = 2 \sum_{i=1}^{N} y_i b_{ij} \]