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SUPPLEMENTARY MATERIAL TO

Modelling of pure components high pressures densities using CK-SAFT and PC-SAFT equations

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TABLE S-I. Equations for the dispersion term ($a^{\rm disp}$) used in different SAFT equations

Original SAFT
$a_0{}^{disp}=\frac{\varepsilon R}{k}(a_{01}^{disp}+\frac{a_{02}^{disp}}{T_R});T_{\rm R}=kT/\varepsilon;\rho_R=\left[6/(2^{0.5}\pi)\right]\eta$
$a_{01}^{disp}=\rho_R\left[-0.85959-4.5424\rho_R-2.1268\rho_R{}^2+10.285\rho_R{}^3\right]$
$a_{02}^{disp}=\rho_R\left[-1.9075+9.9724\rho_R-22.216\rho_R{}^2+15.904\rho_R{}^3\right]$
CK-SAFT
$\frac{a_0^{disp}}{RT}=\sum_i\sum_j D_{ij}\left[\frac{u}{kT}\right]^i\left[\frac{\eta}{\tau}\right]^j$
$u=u^0(1+e/kT);{\rm e/k}=10;\tau=0.74048$

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TABLE S-I. Continued

SAFT-VR
$a^{disp}=\frac{a_1}{kT}+\frac{a_2}{(kT)^2}$
$a_1=-\rho_s\sum_i\sum_j x_{s,i}x_{s,j}\alpha_{ij}^{VDW}g^{HS}\left[\sigma_x;\zeta_x^{eff}\right]$
$a_2=\sum_{i=1}^{n}\sum_{j=1}^{n}x_{s,i}x_{s,j}\frac{1}{2}K_{HS}\varepsilon_{ij}\rho_s\frac{\partial a_1}{\partial\rho_s}$
$\alpha_{ij}^{VDW}=2\pi\varepsilon_{ij}\sigma_{ij}^3(\lambda_{ij}^3-1)/3;\zeta_x^{eff}=c_1\zeta_x+c_2\zeta_x{}^2+c_3\zeta_x{}^3$
$\sigma_x^3=\sum_i\sum_j x_{s,i}x_{s,j}\sigma_{ij}^3;\zeta_x=\frac{\pi}{6}\rho_s\sigma_x^3$
$K_{HS}=\frac{\zeta_0(1-\zeta_3)^4}{\zeta_0(1-\zeta_3)^2+6\zeta_1\zeta_2(1-\zeta_3)+9\zeta_2{}^3}$
PC-SAFT
$\frac{a^{disp}}{kTN}=\frac{A_1}{kTN}+\frac{A_2}{kTN}$
$\frac{A_1}{kTN}=-2\pi\rho m^2(\frac{\varepsilon}{kT})\sigma^3\int_1^\infty\tilde{u}(x)g^{hc}(m;x\sigma/d)x^2dx$
$\frac{A_2}{kTN}=-\pi\rho m(1+Z^{hc}+\rho\frac{\partial Z^{hc}}{\partial\rho})^{-1}m^2(\frac{\varepsilon}{kT})^2\sigma^3\cdot$
$\cdot\frac{\partial}{\partial\rho}\left[\rho\int_1^\infty\tilde{u}(x)^2g^{hc}(m;x\sigma/d)x^2dx\right]$
$x=r/\sigma;\tilde{u}(x)=u(x)/\varepsilon$