Application of the PC-SAFT Equation of State Model to Solid-Liquid Equilibrium at High Pressures

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Pressure has an effect on the solid-liquid equilibrium (SLE) of pure materials and solutions. In this work, we have developed a rigorous, equation of state based approach to model the effect of pressure on SLE. The calculation based on a thermodynamic cycle approach due to Prausnitz et al. [1] yields equations involving quantities that can be easily calculated from an equation of state. We have used the PC-SAFT equation of state for example calculations. We have compared our approach with a more approximate method due to Pan and Radosz [2]. Our method requires information on heat capacity of crystalline solid and can be sensitive to it. The Pan and Radosz approach does not require heat capacity data. In terms of results, at low to moderate pressures, both approaches give similar results. However, at high pressures, our method gives much more reasonable results compared to the Pan and Radosz method. This is shown with the example of polyethylene melting point as a function of pressure. Our model accurately captures the melting point leveling off at high pressures whereas the Pan and Radosz approach gives a linear increase. A procedure for practical implementation of this approach will be outlined.

[1] J.M Prausnitz, N.L. Rüdiger, and E.G.D. Azevedo, *Molecular Thermodynamics of Fluid-Phase Equilibria*, Prentice Hall PTR (1999).
[2] C. Pan and M. Radosz, Modeling of solid-liquid equilibria in naphthalene, normal-alkane and polyethylene solutions. *Fluid Phase Equilibria*, **155** (1), 57-73 (1999).