Equation of State for Solid Benzene Valid for Temperatures up to 470 K and Pressures up to 1800 MPa

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The presence of BTEX compounds (benzene, toluene, ethylbenzene, and xylene) in natural gas can lead to solid freeze-out and blockages of the main cryogenic heat exchanger in a liquified natural gas (LNG) plant. In severe cases, this results in a plant shutdown and a severe cost penalty (e.g. $30 million). Among the BTEX compounds, benzene poses the highest freeze-out risk during LNG production due to its relatively high concentrations in natural gas (>1000 ppm) and its high pure-component triple-point temperature (278.7 K). Predicting the solubility of trace levels of benzene in LNG mixtures requires a reliable description of the solid phase at high pressures and cryogenic temperatures. However, there is currently no complete model that can predict the thermodynamic properties of solid benzene accurately.

In this work, we have developed an equation of state (EOS) for solid benzene following a methodology used previously for solid phase I of CO_2 [1]. The model was parameterised using available property data along the sublimation and melting curves and in the high-pressure region. The resulting EOS is able to predict all thermodynamic properties of solid benzene at temperatures up to 470 K and at pressures up to 1800 MPa. The estimated expanded relative uncertainties (k = 2) are 0.2% and 1.5% for molar volume on the sublimation curve and in the compressed solid, respectively; 8% to 1% for isobaric heat capacity on the sublimation curve between 4 K and 278 K; 4% for thermal expansivity; 1% for isentropic bulk modulus; 1% for enthalpy of sublimation and melting; 3% and 4% for the predicted sublimation and melting pressures, respectively. Through its improved representation of fugacity, this new solid EOS will enable improved predictions of solid benzene freeze out from multi-component LNG mixtures.

References

[1]. Trusler, J. P. M. Equation of State for Solid Phase I of Carbon Dioxide Valid for Temperatures up to 800 K and Pressures up to 12 GPa. *J. Phys. Chem. Ref. Data* **2011**, 40, 043105.