Hydrate Model for CCS Relevant Gases Compatible with Highly Accurate Equations of State- II. Results and Implementation in TREND 2.0

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The fitted hydrate models presented in detail in part I of this contribution are in good agreement with the available experimental three phase equilibrium data up to about 100 MPa. Two phase data and hydrate composition data are represented well by the established models, too. The model results for enthalpies of formation for the gas hydrates along the three phase lines are in good agreement with experimental literature data. The developed hydrate models have been implemented in a software for the calculation of thermophysical properties, which was developed at Ruhr-Universitaet Bochum. This software is called TREND (Thermophysical Reference & Engineering Data). The most accurate equations of state available for fluid phases of pure substances and mixtures have been implemented in TREND 2.0 [1], e.g., the mixture model for CCS-relevant components by Gernert [2]. Furthermore, equations for pure solid phases [3,4] and the proposed gas hydrate models have been implemented. The phase equilibrium algorithms for fluid phases discussed in [5] have been extended to all solid phases considered in this work. Thus, up to three fluid and solid phases in equilibrium can be predicted at given temperature and pressure, pressure and enthalpy, or pressure and entropy.

References

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