A Thermodynamics Calculation Package for the Prediction of Hydrate Formation Conditions

Ali Asghar Davoodi
Thermodynamics Research Laboratory, School of Chemical Engineering, Iran University of Science and Technology, Tehran, Iran

Mahtab Moghadam
CAPE Consultant Group, Tehran, Iran

Bahman Behzadi [C, S]
Thermodynamics Research Laboratory, School of Chemical Engineering, Iran University of Science and Technology, Tehran, Iran

An inherent problem with natural gas production or transmission is the formation of gas hydrates, which can lead to safety hazards and substantial economic risks. The correct prediction of hydrate formation conditions is therefore of great interest to the design engineer. In this work, a thermodynamic hydrate formation prediction package has been developed. It can predict incipient formation conditions required in process development and simulation. Several models concerning the general calculation procedures and property estimation methods which have been used in the software include: 1) hydrate formation models: the Parrish - Prausnitz model, and the Ng-Robinson model, 2) gas-phase models: Peng-Robinson and Soave-Redlich-Kwong equations of state, which are used in fugacity coefficient calculations, and 3) gas solubilities, which are estimated with the Krichevsky - Kasarnovsky equation. It should be noted that hydrate formation models generally highlight the necessary calculation frameworks. However, different combinations of calculation models and property methods lead to different results in each framework. Moreover, the proposed calculation trends often lead to convergence problems in actual calculations, especially at severe formation conditions. These pitfalls have been overcome by applying specific programming techniques and calculation procedures; a procedure has been proposed for the generation of new values of estimated pressure in the calculation loops. Gas hydrate dissociation conditions calculated with this package have been compared to available experimental results, and results obtained from other simulation software. CH_4, C_2H_6, C_3H_8, CO_2, and H_2S gas hydrate dissociation pressures were obtained, which result in relative errors of less than 3 % compared to available experimental data. Binary, ternary, and multi-component natural gas systems have been tested with the software. On the other hand, thermodynamic inhibitors are used for inhibiting gas hydrate formation problems in natural gas production and transportation facilities. Different inhibitors include methanol, ethanol, ethylene glycol (EG), diethylene glycol (DEG), and triethylene glycol (TEG) solutions. For treating systems containing inhibitors, the NRTL model has been used in the package. Acceptable predictions of hydrate-formation pressures in the presence of different inhibitors have been obtained, with results showing good agreement compared to reported experimental data.