Hydrate Dissociation Conditions of Associating Mixtures by Using Cubic – Plus –Association EoS (CPA)

Fatemeh Nikbakht, Amir Abaas Izadpanah* and Farshad Varaminian[2]
Department of chemical engineering, Engineering faculty, Persian Gulf University, Bushehr, Iran
Department of chemical engineering, Engineering faculty, Semnan University, Semnan, Iran
**aai27@hotmail.com*

Abstract

The classical cubic equations of state such as the SRK and PR EoS generally do not result in accurate prediction of the volumetric properties and phase equilibria of complex mixtures containing hydrogen bonding components. This is partly because of the strong hydrogen bonding forces, which cannot be well represented by the aforementioned EoSs. The Cubic plus Association (CPA) EoS has been proposed to combine a cubic EoS expression with an association term, derived from the Wertheim theory as applied in the Statistical Associating Fluid Theory (SAFT) for taking into account the hydrogen bond interactions. In this study the phase behavior of the water + hydrocarbons (methane and ethane) and aforementioned hydrocarbons + methanol aqueous solution systems is modeled. The van der Waals and Platteeuw solid solution theory is applied to deal with the hydrate phase and the CPA Eos is used for modeling the fluid phases.
The 4C and 2B association scheme for water and methanol is used, respectively. Acceptable agreements are found between the represented/predicted results by the applied thermodynamic model and the experimental phase equilibrium data of the pure methane or ethane + water systems and in the presence of methanol aqueous solution from the literature.

Keywords: Clathrate Hydrate, Inhibitor, CPA EoS

Research Highlights (Times New Roman 10 pt. Bold)

- **CPA EoS was used to model hydrate dissociation condition of methane and ethane**
- **Kihara parameters were found for methane and ethane based on CPA EoS.The first**
- **The optimized Kihara parameters were used to model hydrate formation conditions in the presense on methanol.**

1. Introduction

Gas hydrates are nonstoichiometric crystalline inclusion compounds formed by water and a number of small molecules at suitable temperature and pressure conditions [1]. Light hydrocarbons such as natural gas components and some refrigerants can form hydrate when come into contact with water under certain conditions of temperature and pressure.