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Thermodynamic Modeling and Phase Prediction for Binary System Dinitrogen Monoxide and Propane

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ABSTRACT

One of the important activities in chemical engineering is designing and simulating different processes in order to optimize the unit economically and operationally. Thermodynamic and transmissivity properties of fluid in this process are required to be available carefully. In this article, thermodynamic equations operation in PR, SRK, LKP, UNIQUAC in expecting thermodynamic properties and phase operation of binary system of Dinitrogen monoxide and Propane have been studied in order to select the best equations of state (EOS) for simulation. According to the results it is obvious that equation of state PR in expecting Bubble point (P) have mean absolute error equals to 4.98 and mean absolute error in specifying the value of mole fraction of Dinitrogen monoxide in steam phase (Y_1) equals to 0.002338 . It is the minimum error among other models. As a result, alternatively PR, UNIQUAC equations are the best and the weakest models for expecting phase operation and simulating binary system of Dinitrogen monoxide and propane (among considered equations).

1. Introduction

In recent years, the modeling and simulation of physical, chemical and biological processes has received much attention due to its economic importance[1]. As a result, these operations will save a lot of money. But for successful modeling and simulation, the first basic step is adopting appropriate methods for calculating thermodynamic properties[2]. So that the mismatch of the thermodynamic properties calculated with the experimental data can cause modeling inaccuracy or reduce the accuracy of the results of simulation. Therefore, care must be taken in selecting methods and assumptions for predicting physical and thermodynamic properties in modeling and simulation operations. Due to the widespread use of vapor-liquid equilibrium data in various chemical industries, they have been widely studied. In general, the phase behavior of dihydrogen monoxide has been less studied. Physcher *et al.*, [3] conducted the studies under critical conditions for this system and for the nitrogen dioxide and ethane monoxide systems and compared these critical data with the Predictive Soave-Redlich-Kwong equation. In this paper, thermodynamic modeling and prediction of phase behavior of D-nitrogen and propane monoxide systems are performed using four thermodynamic models of Peng - Robinson, Soave - Redlich - Kwong, Lee – Kesler plocker and UNIQUAC. Experimental data equilibrium of vapor equilibrium data from Wagner *et al.*, [4] data were obtained at 10 degrees centigrade.

2. Thermodynamic Model

The polynomial equations, in which the molar volume is of the third degree, have a good relationship between simplicity and generalization, which is suitable for many purposes. In fact, third-degree equations are the simplest equations that can express liquid and vapor behavior [5-8]. Among the third-order mode equations, the Redlich Kwong mode equation will have three strands for volume, between which the two answers may be complex. Relation 1 shows the standard form of the RK mode equation. This equation provides very convincing

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