

عنوان مقاله:

Simultaneous Prediction of Critical and Sub-critical Phase Behavior of Binary Mixtures Using Cubic Equations of State

محل انتشار:

پنجمین کنگره بین المللی مهندسی شیمی (سال: 1386)

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نویسندگان:

Nafise Reshadi - *Chemical Engineering Faculty, Iran University of Science and Technology Tehran ۱۶۸۴۶, Iran*

Farzaneh Feyzi - *Chemical Engineering Faculty, Iran University of Science and Technology Tehran ۱۶۸۴۶, Iran*

خلاصه مقاله:

Predicting critical behavior of mixtures is an important topic in thermodynamics, which has been studied by a few equations of state such as van der Waals, SRK, and SAFT. This work introduces a procedure to predict critical and sub-critical phase behavior of binary mixtures, using Elliott-Suresh-Donohue (ESD) [1, 2] and Peng- Robinson (PR) [3] equations of state. Different thermodynamic calculations are integrated into a general procedure that let us trace the critical lines, critical endpoints and three-phase lines with phase diagrams of type I to V [4, 5, 6]. The performance of the two EOSs is compared with available experimental data for illustrated systems. Phase calculation in critical region is strongly dependant on initial guess of mixture critical properties. We tried different methods for mixture critical point estimation and chose the method, which had the best agreement with experimental data. A software package is prepared which allows user to observe phase behavior of binary mixtures near to and far from critical region. Different types of critical phase diagrams have been constructed without adjusting any binary interaction coefficient. Very good results have been obtained in comparison with experimental data, which shows that the method .of calculations is reliable and predictive

کلمات کلیدی:

Critical Phase Behavior, Critical lines, LLE, VLLE, ESD EOS, Binary Mixtures

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