

عنوان مقاله:

Development of a new Peng-Robinson Plus Association equation of state for water and alcohols

محل انتشار:

هفتمین کنگره ملی مهندسی شیمی (سال: 1390)

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نویسندگان:

Leila Eslami - *Thermodynamic Research Laboratory, School of Chemical Engineering, Iran University of Science and Technology, Tehran ۱۶۸۴۶-۱۳۷۱۱, Iran*

Farzaneh Feyzi - *Thermodynamic Research Laboratory, School of Chemical Engineering, Iran University of Science and Technology, Tehran ۱۶۸۴۶-۱۳۷۱۱, Iran*

Bahman Behzadi - *Thermodynamic Research Laboratory, School of Chemical Engineering, Iran University of Science and Technology, Tehran ۱۶۸۴۶-۱۳۷۱۱, Iran*

خلاصه مقاله:

Cubic plus association (CPA) equations of state (EoS) have found great interest for describing thermodynamic properties of associating fluids. In CPA EoSs, the association contribution proposed by Wertheim is added to a cubic EoSs such as Soave-Redlich-Kowng (SRK) and Peng-Robinson(PR). In different developments of CPA EoSs, it is common to adjust the pure component properties such as critical temperature and critical pressure in addition to the association parameters. In this work, the PR EoS has been extended to water, phenol and a number of alcohols (methanol up to dodecanol) by addition of the Wertheim association contribution. In contrast to other CPA-EoSs, the experimental values of critical properties are used. The energy and co-volume parameters of PR EoS are modified by introducing a correction factor that are correlated as a function of reduced temperature. The results show that this model is capable of reproducing experimental saturated liquid density and vapor pressure data accurately

کلمات کلیدی:

Cubic Plus Association; Equation of State; Water; Alcohols

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