

Invited Lecture IL 02
Methodology for Applying Equations of State to Phase Equilibrium Calculation for Mixtures
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Key Word (3 words)
Equations of state, Mixing rules, Phase Equilibria
Abstract (less than 300 words)
<p>Equations of state (EoS) are basically developed to represent the pressure-volume-temperature(PVT) behavior as well as the saturated properties of pure component. In applying such EoS to mixture property calculations, the effect of composition should be considered and several approaches have been proposed. Most popular approach is the mixing rules which defined the EoS parameters of mixtures by defining functional forms of the parameters in terms of composition. The mixing rules can provide very good performance for most cases, however the performance tends to decrease with asymmetric mixtures that consist of different size/polarity components. It would be noted that one possible reason is the difference in corresponding kinetic energy for asymmetric components even at same temperature. This indicates that, for a large asymmetric system, it is difficult to represent the PVT behaviors for both components by the same functional form of an EoS. It has been sometimes observed a singular PVT curve having multiple thermodynamic unstable regions in the case of virial type EoSs. The van der Waals mixing models, which combine the equation parameters as a function of composition, can be regarded as a mixing of the PVT curves of each pure component at the temperature. In other words, the model combines the stable and unstable PVT regions depending on the condition.</p> <p>The corresponding state principle is a good methodology to calculate the mixture properties from pure component information with pseudocritical values. We can adopt this method to mix the thermodynamic properties of each component with confirming the values in stable state. By extending the Lee-Kesler method, a kind of mixing rule can be derived to combine the different type EoSs for each component of the mixtures^[1]. In the presentation, I will show the deviation of methodology and its possible extensions for some examples.</p> <p>Reference</p> <p>[1]: K.Arai, H.Inomata, S.Saito, J. Chem. Eng. Japan, 15, 1-5(1982)</p>
MTMS '21