Secrets of Cubic Equations of State and beyond

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Classical thermodynamic models, both excess Gibbs energy (GE) ones and cubic equations of state (EoS), have many secrets, previously not fully appreciated. These secrets indicate that their capabilities are, in many cases, greater than originally believed. This has been demonstrated in some of our studies [1-3].

The most powerful use of these classical models is when we use cubic EoS combined with GE models in the so-called EoS/GE mixing rules. These models are now widely used in many industrial applications, and they are available in many forms e.g. Huron-Vidal, MHV2, Wong-Sandler, LCVM, PSRK and VTPR. Professor Michael L. Michelsen had once said about these models: "A technology whose time has passed" – he possibly thought all questions have been answered.

We believe that an ultimate secret of cubic EoS, see [4], comes from the careful analysis of these EoS/GE mixing rules which demonstrates how the best cubic EoS should be modified towards the development of future even more powerful models.

Despite their enormous success, some of the limitations of cubic equations of state can be addressed by combining them with the association term of the SAFT approach, which led to the development of the CPA approach [5-7].

This presentation will start with the success and secrets of cubic EoS and conclude with some highlights of the CPA development over the last 30 years.

References

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