Plenary Lecture PL 01

How can molecular concepts help in the development of more predictive advanced equations of state?

Authors and affiliation

Georgios M. Kontogeorgis* and Xiaodong Liang

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering

Technical University of Denmark

Key Word (3 words)

Association models (SAFT, CPA), molecular simulation, electrolytes

Abstract (less than 300 words)

Since about 1990's, advanced equations of state which incorporate the concept of association have brought a new dimension in engineering thermodynamics [1]. 30 years after these models are not just theoretical curiosity but are being implemented in simulators and also otherwise used in practice. These models perform in many cases superior over classical models and for a wider range of systems and conditions but they do require many parameters and extension to mixtures e.g. uncertainties of mixing and combining rules make their use cumbersome. On the other hand, the theoretical origin of these association theories is a strong positive feature and could imply that molecular concepts e.g. from statistical thermodynamics, quantum chemistry, spectroscopy and molecular simulation may provide valuable input in some cases.

In this presentation, we will illustrate examples from recent research in our group [2-5] of how some of these molecular concepts can contribute to the development of predictive approaches, which can enhance the range of applicability of these modern approaches. But also cases where limitations exist and further studies are needed [6-11].

References

[1] Kontogeorgis, G.M., Liang, X.D., Arya, A., Tsivintzelis, I., 2020. Equations of state in three centuries. Are we closer to arriving to a single model for all applications? Chem. Eng. Science X, vol. 7, May 2020 (100060).

[2] Velho, P., Liang, X.D., Macedo, E.A., Gomez, E., Kontogeorgis, G.M., 2021. Towards a predictive Cubic-Plus-Association equation of state, Fluid Phase Equilibria, 540, article 113045.

[3] Town, J. Liang, X., Kontogeorgis, G.M., 2021. Application of quantum chemistry insights to the prediction of phase equilibria in associating systems. Ind. Eng. Chem. Res. (in press)

[4] Ten Kate, A.J.B., Gerretzen, J., Van Manen, H.J., Kontogeorgis, G.M., Bargeman, G., 2020. Methodology to predict thermodynamic data from spectroscopic analysis. *Ind. Eng. Chem. Res.,* 59(49): 21548-21566.

[5] Muthachikavil, A.V., Peng, B., Kontogeorgis, G.M., Liang, X., 2021. Distinguishing Weak and Strong Hydrogen Bonds in Liquid Water – A potential of the mean force-based approach. J. Phys. Chem. B. (in press).

[6]Tsochantaris, E., Liang, X.D., Kontogeorgis, G.M., 2020. Evaluating the performance of the PC-SAFT and CPA Equations of State on Anomalous properties of water. *J. Chem. Eng. Data,* 65 (12): 5718-5734.

[7]Kontogeorgis, G.M., Maribo-Mogensen, B., Thomsen, K., 2018. The Debye-Huckel theory and its importance in modelling electrolyte solutions. Fluid Phase Equilibria, 462: 130-152.

[8]Sun, L., Lian, X.D., von Solms, N., Kontogeorgis, G.M., 2020. Analysis of some electrolyte models including their ability to predict the activity coefficients of individual ions. Ind. Eng. Chem. Res., 59(25): 11790-11809.

[9]Lei, Q, Peng, B.L., Sun, L., Luo, J.H., Chen, Y., Kontogeorgis, G.M., Liang, X.D., 2020. Predicting activity coefficients

with the Debye-Hückel theory using concentration dependent static permittivity. AIChE J., 66(11), Article number e16651.
[10] Zhu, C.Y., He, M., Liu, X.Y., Kontogeorgis, G.M., Liang, X.D., 2021. Quantification of dipolar contribution and modeling of green polar fluids with the polar Cubic-Plus-Association equation of state. ACS Sustainable Chem. Eng., 9(22): 7602-7619.
[11] Walker, P.J., Liang, X., Kontogeorgis, G.M., 2021. Importance of the Relative Static Permittivity in electrolyte SAFT-VR Mie Equations of State. Fluid Phase Equilibria (submitted)