CERE
Center for Energy Resources Engineering

Online CERE-SEMINAR

Thursday 28 September 2023
09:15 to 10:30 a.m.
Building 229, Room 003
(Light breakfast from our own kitchen)
Online from link in calendar invitation

"Introducing the two-state theory of water in PC-SAFT EoS: PC-SAFT-TS

by

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Abstract
Water has more than 50 "anomalous" properties. At atmospheric pressure, water density and speed of sound have a maximum, heat capacity and isothermal compressibility have a minimum. Characteristic extrema also appear in mixtures, such as the solubility minimum of hydrocarbons in water. Currently, even the most well-known EoS that account for hydrogen bonding (SAFT-VR Mie, PC-SAFT, CPA) do not capture these anomalies, which might indicate a lack of fundamental understanding of the underlying phenomena.

One of the most promising theories for water that explains the anomalous properties, is the two-state theory. Experimental evidence that supports this theory have recently been published by Pettersson and Nilsson [1]. According to this theory, at low temperatures, water has two "states" or macroscopic phases, one with low-density (LD) and one with high-density (HD) and LDL and HDL are assumed to be different types of water clusters. At the range of conditions of interest to the chemical engineering community, water behaves as a homogeneous fluid, but the different types of water structures still exist in equilibrium, causing the anomalous behaviour.

In this work, we have introduced the two-state theory of water in the Statistical Associating Fluid Theory (SAFT). We have assumed that water is a mixture of two different types of water molecules, HDW and LDW, which are in chemical equilibrium and have different association schemes and association parameters. Using this approach, a generalized association term for SAFT is derived. This approach is applicable to all SAFT-type EoS, but in this work has been investigated in the framework of PC-SAFT EoS, called PC-SAFT-TS. The model captures several anomalous properties, including density and speed of sound maximum and isothermal compressibility minimum, as well as the minimum in hexane solubility in water-hexane LLE.

References
[1] L.G.M. Pettersson, R.H. Henchman, A. Nilsson, Water - The Most Anomalous Liquid, Chem Rev. 116 (2016) 7459–7462. https://doi.org/10.1021/acs.chemrev.6b00363.