Prediction of Thermodynamic Properties and Phase Behaviour of Nuclear Reactor Fluid Mixtures using the SAFT-γ-Mie equation of state: Modelling Heavy Water and Deuterium Mixture in Heavy Water Reactors

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Abstract

Accurate prediction of thermodynamic properties is an essential tool in any engineering setting. It is ever more valuable in settings where experimental data for the desired system is scarce – a repeating theme in mixtures found in novel nuclear reactors, notably in Molten Salt Reactors (MSRs) and CANDU reactors. SAFT equations of state promise to offer accurate estimates of a multitude of physical properties of interest including isobaric heat capacity, viscosity, and solubility under varying operating conditions. The objective of this research is to expand the database of modelled pure substances and mixtures by SAFT-γ-Mie to systems applicable to prominent nuclear reactors. Initial modelling studies on mixtures of Deuterium and heavy water in CANDU reactors will be presented, together with details of plans for expansion of the database to incorporate various Molten Salt Reactor mixtures. Statistical Associating Fluid Theory (SAFT) is a family of equations of state (EoS) that pride themselves in their theoretical approach, building EoS using perturbation theory and Wertheim's Thermodynamic Perturbation Theory (TPT1). The SAFT approach improves upon the prediction of crucial thermophysical properties of fluids that cubic EoS tended to struggle with, with non-spherical and associating fluids showing the greatest improvement. SAFT-γ-Mie is an EoS that uses a Group Contribution (GC) approach, allowing for the modelling of heterogenous chains unlike other variations of SAFT, which model all groups assuming an identical size. GC's main premise is the prediction of physical properties of a molecule based on the individual contribution from each functional group present. Hence, the aforementioned models present an effective tool to be used alongside available experimental data in the extreme conditions found in the nuclear industry.

Keywords: Group Contribution (GC), Equation of State, CANDU