CERE
Center for Energy Resources Engineering

CERE - SEMINAR

Thursday 23 May 2024
09:15 to 10:30 a.m.
Building 229, Room 003
(Light breakfast is served from 9:00, please bring your own coffee/tea)
Online from link in calendar invitation

"A comprehensive approach to incorporating intermolecular dispersion into open COSMO-RS model"

By

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Abstract

Over the last two decades, advancements in computational chemistry have laid the foundation for a novel class of predictive thermodynamic models based on the COSMO (COnductor-like Screening Model) quantum chemical method. Among them, the COSMO-RS (COSMO for Real Solvents) was the first significant development in the field, while the COSMO-SAC (Segment Activity Coefficient) model is another widely adopted variant. At the core of their methodology lies the computation of screening charge density on each molecule's surface, followed by the calculation of thermodynamic properties based on the interactions between the surface patches with varying charge densities.

The original COSMO-RS only considered electrostatic interactions and hydrogen bonding, neglecting dispersion in fluid mixtures. However, recent versions of COSMO-based models, such as COSMO-SAC-dsp (COSMO-SAC with dispersion term) and the latest implementations of COSMO-RS in COSMOtherm, have integrated dispersive interactions. This seminar will introduce our latest work on incorporating dispersive interactions into openCOSMO-RS, an open-source implementation of COSMO-RS. We systematically evaluated the impact of various parametrization approaches and different combinatorial terms on the model performance. Our findings indicate that the modified model significantly improves the accuracy of phase equilibrium predictions for halocarbons and refrigerant mixtures.