CERE
Center for Energy Resources Engineering

# CERE - SEMINAR

**Thursday 21 March 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**

# "Software Overview Recent developments of the tools from CERE & KT Consortium"

By

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**Abstract**
Several software tools have been developed at CERE and the KT Consortium since the founding of both centers, from simulations of thermodynamic properties of complex systems to models for process simulators. In this presentation, we will provide an overview of the different software available to consortium members. Moreover, we will showcase the tools that are under development in the centers, including application to selected systems and validation of results.

One of the major recent software developments was enabled with the funding obtained through DTU Skylab, allowing the creation of ElecThermo Beta. ElecThermo Beta is prototype software for simulating the density and mean ionic activity coefficient (MIAC) of single-salt electrolyte solutions with aqueous, non-aqueous, and mixed solvents using the eSAFT-VR-Mie equation of state (EoS) [1,2]. The software also contains a database with EoS model parameters for key compounds, as well as experimental data for aqueous solutions. With the help of the software, we carried out simulations for several aqueous and mixed solvent systems, allowing a thorough validation of the model. We also compared MIAC results with the leading model in process simulators, i.e. eNRTL [3].

In relation to the development of the tools from the KT Consortium, we are currently working on improvements for halogenated olefins. We have introduced in ICAS/ProPred new group contribution (GC) parameters from the work of Mondejar et al. [4]. Furthermore, we compared the results for selected halogenated olefins with the predictions of the MG model currently implemented in the software and experimental data taken from DIPPR.

References

[1] Novak, N.; Kontogeorgis, G. M.; Castier, M.; Economou, I. G., "Mixed Solvent Electrolyte Solutions: A Review and Calculations with the eSAFT-VR Mie Equation of State," *Ind. Eng. Chem. Res.*, vol. 62, pp. 13646-13665. https://doi.org/10.1021/acs.iecr.3c00717
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[4] Mondejar, M. E.; Cignitti, S.; Abildskov, J.; Woodley, J. M.; Haglind, F., "Prediction of properties of new halogenated olefins using two group contribution approaches," *Fluid Phase Equilib.*, vol. 433, pp. 79-96, 2017. https://doi.org/10.1016/j.fluid.2016.10.020