EFCE Spotlight Talks

Working Party on Thermodynamics and Transport Properties

25 November 2022

09:30 am • 12:30 pm CET

MACHINE LEARNING and DATA MANAGEMENT for the ESTIMATION of FLUID PROPERTIES and PHASE EQUILIBRIA

The detailed knowledge of the thermophysical behaviour of fluids and complex molecules is essential in the design of chemical processes and in driving the transition to a low-carbon economy, as highlighted in the opinion paper recently published by the TTP WP "A view on the future of Applied Thermodynamics".
Machine Learning (ML) can play an important role in the management and prediction of data and in this session we will showcase the most recent examples of application of ML methods to the Thermodynamics and Transport Properties field. First, we will present a bench thermodynamics database for the training and validation of models. Then we will show how ML methods can be used in combination with physical models or in a purely data-driven mode for the prediction of mixture properties and flash calculations. Finally, we will explore how ML can assist thermodynamic models across different scales, such as in the parametrization of the PC-SAFT Equation of State or in the coarse grained molecular simulation of complex molecules.

PROGRAM

09:30	**Welcome and introduction** Maria Grazia De Angelis - Chair of the WP on Thermodynamics and Transport Properties Petr Kluson, EFCE Scientific Vice-President
09:40	**Benchmarking Equations of State using a Reference Database. A PC-SAFT Study** Ilias Nikolaidis, Demokritos Institute, Athens - Greece
10:05	**Hybridizing Machine Learning and Physical Modeling of Mixtures** Fabian Jirasek, TU Kaiserslauten – Germany
10:30	*Coffee break*
10:45	**PTFlash: A vectorized and parallel deep learning framework for two-phase flash calculation** Jingang Qu, IFP Energies Nouvelles - France
11:10	**Predicting PC-SAFT pure component Parameters by machine learning based on molecular fingerprints** Jonas Habicht, TU Dortmund - Germany
11:35	**Machine-Learning Methods to Facilitate Coarse-Grained Molecular Simulations** Eleonora Ricci, Demokritos Institute, Athens - Greece
12:00	**Conclusive remarks**

Moderators:
Maria Grazia De Angelis (University of Edinburgh, UK)
Christoph Held (TU Dortmund, Germany)
Antoon ten Kate (Nouryon, NL)

Registration

free of charge but mandatory

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