

EFCE Spotlight Talks

Working Party on Thermodynamics
and Transport Properties

15 March
2024

13:00-15:30
CET



HOW INDUSTRY IS USING APPLIED THERMODYNAMICS

When the Working Party prepared the publications of the industrial survey in 2020 [1], and the follow-up opinion paper in 2022 [2], the need became clear of a sharper insight on the industrial common practice in applied thermodynamics. This insight would create a better understanding of the needs and requirements by industry, and the opportunities and options offered by academia, possibly enhanced through the interface of software suppliers. It would improve the dialogue between the parties involved: academia, software suppliers and industry. Hence, the working party decided to organize these spotlight talks on how industry is using applied thermodynamics.

[1] Georgios M. Kontogeorgis, Ralf Dohrn, Ioannis G. Economou, Jean-Charles de Hemptinne, Antoon ten Kate, Susanna Kuitunen, Miranda Mooijer, Ljudmila Fele Žilnik, and Velisa Vesovic, *Industrial Requirements for Thermodynamic and Transport Properties – 2020*, *Industrial & Engineering Chemistry Research* (2021), 60, 13, 4987–5013

[2] Jean-Charles de Hemptinne, Georgios M. Kontogeorgis, Ralf Dohrn, Ioannis G. Economou, Antoon ten Kate, Susanna Kuitunen, Ljudmila Fele Žilnik, Maria Grazia De Angelis, and Velisa Vesovic, *A View on the Future of Applied Thermodynamics*, *Industrial & Engineering Chemistry Research* (2022), 61, 39, 14664-14680

PROGRAM

- 13:00 **Welcome and introduction**
Prof. Maria-Grazia de Angelis, Chair Working Party on Thermodynamics, U. Edinburgh – UK
Dr. Antoon ten Kate, Nouryon RD&I, Deventer - Netherlands
Prof. Boelo Schuur, EFCE Scientific Vice-President
- 13:15 **How to develop accurate and reliable simulations of chemical processes**
Dr. Paul Mathias, Fluor
- 13:45 **Applied thermodynamics as part of simulations supporting activities ranging from research to investment at Neste**
Dr. Susanna Kuitunen, Neste
- 14:15 **Systematic development and benchmarking of electrolyte thermodynamic models for solvent-based CO₂ capture - and transportation**
Dr. Bjørn Maribo-Mogensen, Hafnium Labs ApS
- 14:45 **Advancing liquid formulation discovery and optimization through molecular modelling in applied thermodynamics**
Dr. Giuliana Giunta, BASF
- 15:15 **Discussion and conclusion**
Prof. Maria-Grazia de Angelis, Chair Working Party on Thermodynamics
Dr. Antoon ten Kate, Nouryon RD&I, Deventer - Netherlands
- 15:30 **Closure**

[REGISTRATION](#)

free of charge but mandatory

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