EFCE Spotlight Talks

Working Party on Thermodynamics and Transport Properties

5 June 2023

15:00 • 17:00 CEST

A VIEW ON THE FUTURE OF APPLIED THERMODYNAMICS

EFCE

The Working Party has published an opinion paper that discusses the challenges that the field of applied thermodynamics is facing in responding to the United Nations Sustainable Development Goals. This webinar aims at sharing with the community the priorities that we believe are important, both at the technical level (modelling and data) and at the non-technical level (education and development of collaborative projects). An open discussion with all panellists will aim to identify and promote new initiatives.

PROGRAM

15:00 **Welcome and introduction**
Prof. Maria-Grazia de Angelis, Chair Working party on Thermodynamics, U. Edinburgh - UK
Giorgio Veronesi, EFCE President

15:10 **Grand challenges of modern society, a pertinent role for applied thermodynamics**
Dr. Antoon ten Kate, Principal Scientist at Nouryon – The Netherlands
Modern society faces a multitude of grand challenges that need to be addressed appropriately and urgently. Hence, world-wide there is substantive attention paid to resolving thematic issues related to water, energy, climate and so on. As thermodynamics is the science of interaction between energy and matter, it is very well positioned to develop and judge the appropriate and timely action.

15:30 **Modeling and Simulation: tools and needs**
Richard Elliott, Professor Emeritus at the University of Akron - USA
Fundamental methods are beginning to supersede traditional methods in accuracy by factors of 3-5 for important properties like vapor pressure and formation energies. These trends will continue, encompassing properties that are essential to addressing issues like carbon capture, safe groundwater, and pharmaceutical production, to name a few.

15:50 **Data Challenges: Availability, Discoverability, Reporting, Quality**
Dr. Ala Bazyleva, Research Chemist at NIST - USA
When data users need experimental property data, they face a number of challenges: whether the required data exist, where/how to find the existing data, whether the found existing data useable (properly reported), and whether the obtained data are reliable. The situation, including identification of problems and potential solutions, will be briefly analyzed based on the author's experience.

16:10 **Education, training, networking: the "soft skills" needed to go forward**
Prof. Jean-Charles de Hemptinne, Research engineer at IFP Energies Nouvelles - France
Technical progress is not only a technical task. Many different stakeholders must be motivated to move in a common direction. Education is key for success, but this comes through many different channels, starting from general public all the way to decision-makers.

16:30 **Discussion and conclusion**

Registration

free of charge but mandatory

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