Thermodynamics as a framework for technological transition

Industry members of the KT-Consortium:
Thermodynamic modelling needs to have a stronger position when it comes to renewable energy and sustainable use of resources.

Thermodynamics is the science of the interactions between energy and matter. While many of the pioneering works of thermodynamic modelling were done with a view to either upstream or downstream hydrocarbon applications, the field is equally relevant in many of the transitional technologies which currently sweep across society.

This is the main point of an opinion paper where Professor Georgios Kontogeorgis, leading the KT-Consortium, participates. The paper is an example of the KT-Consortium being a vehicle for industry-academia collaboration.

One consortium member company is Neste corporation headquartered in Finland. Coming from a history of crude oil refining, Neste has expanded its range of starting materials to include renewable feedstocks.

Dr. Susanna Kuitunen, Neste (FI)

"Crude oil refining is tricky in many respects. Still, introducing renewable feedstocks does add a new level of complexity. This highlights the importance of the thermodynamic models as well as their further development. If the quality of your model is poor, the results are not to be trusted, the business case is not met, and ultimately the risk of both safety hazards and environmental damage will increase," says Dr. Susanna Kuitunen, physical properties and thermodynamics expert in the process modeling team of Neste. She represents Neste in the KT-Consortium, and she is a co-author of the opinion paper.

The goal is predictive tools

The opinion paper is entitled "A view on the Future of Applied Thermodynamics "(submitted to Industrial & Engineering Chemistry Research). It builds on two surveys carried out in 2010 and 2020, both by the Working Party on Thermodynamics and Transport Properties of the European Federation of Chemical Engineering (EFCE).

Dr. Antoon ten Kate, Nouryon (NL)

"As thermodynamics specialists we do possess an expertise which is key to practically all the current trends be it transition to renewable energy, electrification, manufacturing through fermentation etc. Thermodynamics is just a very good framework for addressing these issues," says Dr. Antoon ten Kate, Principal Scientist at Nouryon, and co-author of the paper.

"We must face the fact that many – even some of our engineering colleagues in other fields – find thermodynamics very difficult. Therefore, we cannot assume that they automatically aspire our views. We need to be ready to actively pursue involvement, acknowledging that we are in a unique position to make statements about which are the key issues to address," Antoon ten Kate continues.

Nouryon is a leading producer of essential chemistry in the manufacture of everyday products such as paper, agrochemicals, building materials, and personal care items. Products are mainly sold business-to-business. The company is a long-standing member of the KT-Consortium, and Dr. Ten Kate has attended several Annual Meetings of the consortium, representing industry in its Advisory Board.

"Personally, I have always found collaboration between industry and academia important. Our role as industry will be so name the issues that are important, allowing researchers to work on solutions relevant to practice. We will also do our own research, obviously, building further on these developments."

"Further, I would say that in this context we need to maintain the triple collaboration with software providers being the third corner of the triangle besides academia and industry. Typically, the software providers make the methods available to industry that were originally developed at the university."

As for the commercial software products and the software developed in KT-Consortium, Antoon ten Kate is happy about the level of activity but still sees plenty of scope for further development:

"E.g., what we would really love in industry is predictive tools. In other words, that we can envision for instance a manufacturing process and simulate reliably what will happen even before we engage in experiments. Some progress has been made in that direction, but we are not there yet."

A learning process going both ways

Another opinion paper co-author is Dr. Jean-Charles de Hemptinne of IFP Energies Nouvelles (IFPEN), France:

Dr. Jean-Charles de Hemptinne, IFP Energies Nouvelles (FR)

"We see a trend in society towards renewable energy forms, recycling of materials etc. As chemical engineers we have a lot to offer, since thermodynamics is an essential element in the development of all these fields. Coming originally from oil and gas exploration and use, we are broadening our scope to encompass for example new energy sources (bioresources, wind or geothermal energy), carbon capture and storage technologies, energy storage technologies (hydrogen economy, gas storage in salt caverns or batteries) and increasingly the circular economy (recycling of polymers or metals). These applications require processes in sometimes extreme conditions, and therefore an advanced understanding of thermodynamic modelling tools."

"It is exciting to see how we as chemical engineers are able to contribute to energy transition and ecological transition," Jean-Charles de Hemptinne continues, mentioning geochemistry as an example:

"Traditionally, equations of state are not much applied to geochemistry, but to a chemical engineer it seems obvious that they should be. On the other hand, geochemists have a large body of data on equilibrium reactions with minerals, which lie beyond our expertise but are essential. So, this is a learning process which goes both ways."

Increasing responsibility for academia

Ioannis Economou is Professor of Chemical Engineering at Texas A&M University, USA, at Qatar. He too co-authored the opinion paper:

Prof. Ioannis Economou, Texas A&M University at Qatar (QA)

"To my mind, the most important thing is that we as thermodynamics researchers continue to work closely with industry. Recent years have seen a trend where the industry thermodynamics groups are shrinking. For instance, several of the large international energy corporations have reduced the sizes of their groups. Instead, companies are relying more on university collaborations. This is a nice thing for us on the academic side. You might even say that this is a natural division of work. But it also increases our responsibility when it comes to assuring that our projects are relevant to the industrial practice."

Assuring industrial relevance is not always straightforward, Professor Economou continues:

"In general industry tends to focus on achieving results within a short time horizon. This demand is not easy for us to meet. Research takes time and especially when it is done with students who also have other responsibilities with courses. Thus, we constantly need to balance considerations over academic versus industrial relevance."

Ioannis Economou has been associated with the thermodynamics group at DTU Chemical Engineering for more than two decades:

"Since Denmark is a small country, its implementation of new sustainable energy systems and industrial processes may not in itself have that much impact on a global scale. Still, by setting an example in these areas I believe the impact is actually very significant worldwide."

Keen on electrolyte systems modelling

To Dr. Susanna Kuitunen of Neste, the work in KT-Consortium on new software for property assessment and thermodynamics modelling is especially interesting.

"Neste was founded in the 1948, so before the emergence of computers. Thus, I cannot say that the company has always applied thermodynamic modelling, at least not with the help of software tools. I had a colleague, now retired, who remembers that distillation columns were sized with manual calculations before computers became available. However, those calculations were also based on the thermodynamic principles. But soon after relevant software was introduced, and developed in-house, Neste came onboard and ever since thermodynamic modelling has played a strong role," says Susanna Kuitunen.

She further notes the current research in KT-Consortium on software for thermodynamic modelling of electrolyte systems. This research is anchored in the project "New Paradigm in Electrolyte Thermodynamics," funded by the European Research Council (ERC) and headed by Professor Georgios Kontogeorgis, DTU Chemical Engineering.

"At this point the research is focusing on fundamentals and I do appreciate how much the involved scientists commit to sharing their results," Susanna Kuitunen comments.

"Qualitative understanding might help us immediately for example in the planning of experiments or interpretation of the observations from the laboratory and full-scale setups. But for the actual technology development and process design, we use simulators. Thus, I hope that among the developed or tested models the best ones are implemented into the commercial simulators or made available as plug-in solutions together with parameter databanks or parameterization guidelines."

Interviews for the article were made during the KT Consortium Annual Meeting 2022 held June 6-10 at the Comwell Borupgaard conference center in Snekkersten, Denmark.

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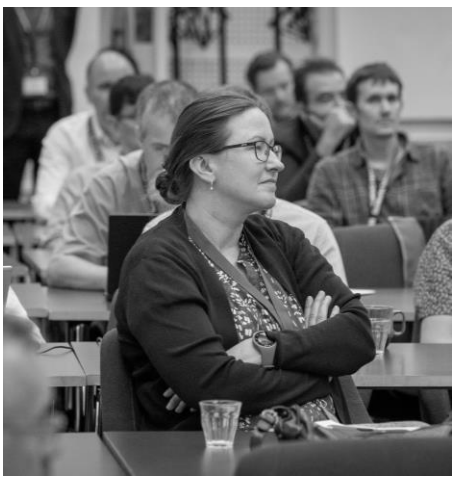

Prof. Georgios M. Kontogeorgis, Prof. Ioannis Economu, Dr. Jean-Charles de Hemptinne, Dr. Susana Kuitunen.