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Guest Editorial

Joint European Thermodynamics Conference 10

From 22 to 24 June 2009 the Joint European Thermodynamics Conference (JETC 10) took place at the Niels Bohr Institute, University of Copenhagen. This was the decennial conference of what started out in 1989 as Journées Européennes de Thermodynamique Contemporaine and which is now a truly international conference covering all aspects of thermodynamics.

JETC 10 focused on four rapidly developing areas:

- Thermodynamics at the meso- and microscopic level (e.g., nano structures, elemental electronic components, individual macromolecules)
- Thermodynamics of agglomerated systems (e.g., entire organelles like mitochondria and muscle fibers, extremely complex systems like entire animals or plants or an ecosystem, building on the ability of thermodynamics to extract a few crucial parameters from a huge chemical soup)
- Advanced uses of thermodynamics in engineering (e.g., the entire chain from designing a molecule with particular properties, suggesting a practical path of synthesis, through designing the process equipment, to analysis of stability and control of the process, as well as generating reliable property data)
- Conceptual thermodynamics (e.g., foundations of thermodynamics, new definitions of old quantities, connections to statistical mechanics, generalized entropy, chaos, complex systems, teaching of thermodynamics)

These areas were introduced in a few keynote talks and invited talks, and further elaborated and intensely discussed in topical sessions. In addition, almost all participants contributed abstracts and posters of their ongoing work. These represent the layer of growth in the field and therefore proba-

bly the most lasting contributions. All those abstracts as well as other material related to the conference may still be found at the conference website (`www.jetc10.fys.ku.dk`).

Let me highlight a couple of very active and promising new developments reported at the conference. Thermodynamics was originally developed in a macroscopic continuous universe where quantities like temperature and pressure are defined at every point, and time evolution follows normal differential equations. As we began to observe individual molecules, this picture was still useful at the mesoscopic level, i.e., for small volumes but not too small. Today many systems of interest are of such a small size that the discreteness of individual molecules or the size of the container has an important influence on the behavior. Maybe the most obvious case is the thermal behavior of a few electrons trapped in a potential well in an electronic memory element or in a single molecule bridge between larger components. However, the discreteness also shows up, e.g., in strong shearing, in strong electric fields, in molecular sieves, and often in connection with interfaces. Thermodynamics, in particular non-equilibrium thermodynamics, is in the process of reformulation these years.

At the opposite extreme of very large and complex systems, thermodynamics is also enjoying novel development. The idea is to apply thermodynamic concepts and thinking to much larger entities than molecules, e.g., bacteria, ecological communities, or evolution in general. The important ability of thermodynamics to describe the overall macroscopic behavior of a reacting system without detailed knowledge of the motion and reactions of individual molecules only relies on a large ensemble and on the many interactions between members of the ensemble. The rest is statistical mechanics. This way of thinking is beginning to make its way into descriptions of bacterial and macroscopic ecological communities as well as into the description of overall evolution. Naturally, the concepts of temperature, chemical potential, entropy, etc., take on new meanings, but relations are the same and can be derived without detailed knowledge of predatory chains and more.

A very important predictive power of thermodynamics is setting limits on performance. The ultimate limit of the Carnot efficiency is quite unrealistic for practical processes proceeding at non-vanishing rates. More realistic limits have been developed for a number of years now, but only recently has optimal control theory taught us not only these improved limits but also the process path to follow in order to achieve them. These limits not only tell us how efficiently we can operate traditional chemical processes but also how low a temperature a quantum system can reach and the most rapid control

sequence needed to approach that temperature. This has implications for computing speeds as well. These limits to control go much further than traditional adiabatic inaccessibility.

A new marriage of fluid dynamics and thermodynamics is underway. Finite-time thermodynamics is being applied to the elemental volumes of flows. A new thermodynamic "phase" of turbulent flow has been used to describe the degradation of kinetic energy to thermal energy. And still further in abstraction, Niven has applied thermodynamic thinking to the flow elements rather than the individual fluid molecules and thus arrived at a maximum entropy formulation of the steady state rather than an equilibrium state. In particular, the latter is a very important extension of thermodynamics.

During JETC 10 the *Ilya Prigogine Prize in Thermodynamics* was bestowed on David Andrieux from the Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles for his thesis "Nonequilibrium statistical thermodynamics at the nanoscale."

Finally, all participants were given the chance to publish full-length papers of their work in a dedicated issue of Journal of Non-Equilibrium Thermodynamics, the one you have in your hands now. The first focus area of the conference is represented by the paper by Cimmelli, Jou, and Sellito on thermal conduction in nanowires where the very small-scale boundary conditions severely limit propagation and suggest a new definition of a non-equilibrium temperature. In particular, the speed of propagation depends on the difference in properties between the core and the shell of the nanowire.

In the same mesoscopic world, Herman and Engelbrecht formulate a continuum theory for liquid crystals, treating the microstructure of the fluid on par with, e.g., the spatial coordinates. This results in a more compact formulation and in a more natural description of the particle spins.

At the other end of the size spectrum, the paper by Annila and Salthe suggests the application of entropic thinking to describe evolution. It is not sufficient for an organism to be very efficient, it must also possess considerable variability (entropy) in order not to be evolutionarily fragile.

A couple of papers treat strongly forced systems. Formulations of non-equilibrium situations frequently run into trouble with non-monotonically increasing entropy. The papers by Pérez-Madrid, Rubí, and Lapas and by Serdyukov and Voskresenskii analyze such situations for radiation and heat conduction, respectively, and suggest ways to resolve the problem in a fashion which maintains the traditional approach to thermodynamics.

In the same category, some systems with long-range interactions or driven at high speed are non-local in nature. Thus the usual set of thermo-

dynamic variables is insufficient to yield a coherent description satisfying, e.g., energy conservation and entropy flow. One way of handling this is to use extended irreversible thermodynamics which includes rates of change in an additional set of constitutive equations. Cimmelli, Sellito, and Triani follow a different route, modifying the energy and entropy equations, and apply their procedure to Korteweg fluids.

Turning to applications of thermodynamics, the Russian group around Tsirlin very cleverly applies strong theorems in optimal control theory to set limits on the performance of thermodynamic processes. In the paper by Tsirlin and Grigorevsky they derive limits to the separation performance of a diabatic distillation column as well as specifications of the precise processes which achieve these limits, depending of course on the material properties of the mixture and its components.

Heffer and Lewins solve the Arrhenius rate equation for auto-ignition of a fuel-air mixture using an exact series expansion in order to arrive at a more precise timing of the onset of ignition than what is possible with the traditional Taylor expansion. Application to both Diesel and Otto (constant pressure and constant volume) paths are presented.

It is very important to know the physical properties of organic solvents in connection with production syntheses. Shukla, Dwivedi, Kumar, and Srivastava combine Prigogine and Flory theories to calculate very realistic values of surface tension and excess molar volumes for six mixtures of frequently used organic solvents over the entire mixing range.

Calculating properties of liquid metals is often done with a simple hard-core model plus a square-well attraction in order to keep the problem manageable. Dubinin, Yuryev, and Vatolin extract the best possible such interaction potential from experimental data for liquid Na to obtain a lower upper bound for the Helmholtz free energy of the system.

Happy reading!

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