

# At the heart of the advance

The Molecular Thermophysics and Fluid Technology group at the Centro de Química Estrutural are working to bridging the gap between scientific research and industrial utilisation

**T**hermophysics is the science and technology of thermophysical material properties. Thermophysical properties are all material properties affecting the transfer and storage of heat, which vary with the state variables temperature, pressure and composition (in mixtures), and of other relevant variables, without altering the material's chemical identity. These properties will include thermal conductivity and diffusivity, heat capacity, density, thermal expansion and thermal radiative properties, as well as viscosity and mass and thermal diffusion co-efficients, speed of sound, surface and interfacial tension in fluids.

The Molecular Thermophysics and Fluid Technology Group of Centro de Química Estrutural (at the University of Lisbon) is an internationally recognised group in Thermophysics of Fluids and Materials, with a strong experience of experimental measurement, modelling and correlation of thermophysical properties, and designing equipment and sensors for fundamental and industrial applications. As part of one of the leading research centres in the area of chemistry and chemical engineering in Portugal, now 40 years old, the group has made contributions of high quality research in the past, including early researchers' training and service procurement and supporting industrial research and development. The group's leader, Carlos A Nieto de Castro, has more than 40 years' experience in thermophysical properties, starting with simple gases and liquids such as Ar, N<sub>2</sub>, n-C<sub>1</sub> to C<sub>4</sub>, linear and branched hydrocarbons, refrigerants (low or zero ozone depletion potential), alcohols, water (including humid air) and water mixtures, salt solutions, molten salts and metals in a wide range of temperatures and pressures.



*High temperature oscillating-cup viscometer for new car engine molten alloys*

In recent years most of this research was directed at cutting-edge research, which include ionic liquids, nanomaterials and IoNanofluids, and new engineering fluids – but why? These fields are the object of very strong research, all with several problems, as applications need good values of properties and the existing/state-of-the-art/commercial equipment needs to be adapted/redesigned for such complex nanosystems. One of the main advantages of our knowhow is the possibility of implementing the cross-fertilisation of these research fields to resolve delicate problems, not only at a molecular level but for possible industrial applications.

Thermophysical properties play a significant role in the development of the Molecular Science of Fluids, both on the interpretation of the intermolecular forces and in the acquisition of the necessary experimental information to understand the dynamics of the gaseous and liquid states. They play an important role in several processes in the chemical, extraction and manufacturing industries, especially in those involving simultaneous heat and mass transfer. Most of the problems that affect our society need the values of these properties to control, design and characterise new products and processes, to replace unacceptable processes and compounds, and to optimise energy balances and efficiency.

## Our objectives

Our current research has the following objectives, with five main scientific streams, one technological, and one societal, complementary, and which overlap in some cases:

- Behaviour and structure of complex systems (including nanosystems): by measuring thermodynamic and transport properties, employing molecular models and developing molecular simulations and predictive methods. A wide range of temperatures will be covered in high temperature molten systems, normal temperatures and pressures as refrigerants, ionic liquids, aqueous mixtures and solutions of amphiphilic compounds, special gases (including corrosive mixtures), nanofluids, nanomaterials (carbon nanotubes, graphene, fullerenes, oxide ceramics), specially 'target designed' fluids (IoNanofluids, IoBiofluids), and fluid phase equilibria (water + alcohols);
- New sensors and instruments: developing new thin films sensors and ancillary equipment for the measurement of electrical and thermal conductivity and electrical permittivity, for several applications (including biological supports), with



*Transient hot-wire instrument for humid air thermal conductivity for advanced adiabatic compressed air energy storage (solving a problem open since 1928)*

single/dual functionality, and new instrumentation for selected properties/systems, namely for ionic liquids, nanomaterials/nanofluids and high temperature melts;

- Metrology: the establishment of standard reference values for the thermal conductivity and viscosity of liquids/molten materials/ionic liquids;
- Solution chemistry: this stream will conduct research aiming to improve the advanced understanding of interactions in amphiphilic solutions, ionic liquids and nanoparticles;
- Molecular simulation: ionic systems – molecular dynamics and free energy calculations of properties, phase diagrams and nucleation processes in bulk systems and ionic nanoclusters;
- Technological applications and technology transfer: creating added value to our scientific research, using top-down and bottom-up approaches, with national and European companies. It is our intention to promote technology transfer to ensure that scientific and technological developments can be available to society, by maintaining its affordability and at making advantageous use of existing equipment. Some examples, such as new spectrally selective coatings for solar

paints, will allow us to produce films at low cost. The development of new nano-based heat transfer fluids, and their performance enhancement, making a solar collector and heat exchangers more energy efficient without compromising the environmental goals set by the World Energy Council. Measuring the viscosity of new molten alloys for high-tech applications. Measuring thermal conductivity of humid air for high pressure turbines. Development of metal-film sensors for high temperature *in situ* measurements in incinerators; and

- History of chemistry and the chemical industry in Portugal: one of the main contributions of scientists to history is the understanding of the social/scientific/political environment of their discoveries and how they contributed to the development of the Portuguese society of their time. Deepen the co-operation of our former teachers to solve the problems of everyday life, research and development of new technologies, comparable to those of Europe at the time.

In summary, our experience paves the way for a strong collaboration with other research groups and industrial companies in the frame of Horizon 2020. The strength of the European economy and the welfare of our society depend heavily on this approach. We are prepared to make thermophysics contribute to this effort.

Finishing with one of my deepest thoughts:

To do or to do well is not enough! We must know how to do it well and how to use this knowledge to resolve new problems in society's emerging needs (energy, environment, materials, health and safety), and to transfer it to young generations of researchers.



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