INVERSE PROBLEMS AND EMERGING TECHNIQUES IN MATERIALS CHARACTERIZATION

UNIVERSITY OF WALES – INSTITUTE OF NON-NEWTONIAN FLUID MECHANICS LAKE VYRNWY HOTEL, U.K. APRIL 10TH - 12TH, 2000

"A representation [model, experiment] is a formal system for making explicit certain entities or types of information, ... there is a trade-off; any particular representation makes certain information explicit at the expense of information that is pushed into the background and may be quite hard to recover"

DAVID MARR (1980)

Rheological experiments are routinely and successfully applied in the characterization of a wide range of materials. The measurements thereby performed see the macroscopic ramifications of the molecular dynamics within the flows which the experiments induce. Theoretical rheology has allowed dynamical and static molecular encapsulations of the underlying dynamics, such as various reptation models and mixing rules, to be formulated to explain, model and interpret such indirect measurements. But, the successful formulation of theoretical models depends heavily on the choice of the indirect measurements chosen to monitor the properties of the material being examined. Though various forms of indirect measurements have been utilized in the past, there is a need, as is implied by the above comment of Marr (1980), to seek new forms of indirect measurement, especially if they allow one to recover new information which had previously been "pushed into the background".

Traditional forms of indirect measurements have proved invaluable in understanding the processes occurring during the mixing of wheat-flour doughs and the drying of pasta as well as industrial processing of synthetic polymers. Now, using such technologies as atomic force microscopy and nuclear magnetic resonance, one can complement and supplement this information with images which see the molecular structure of materials in even finer detail. Consequently, from the joint inversion perspective of inverse problems, it is the simultaneous use of all the available forms of measurements on all possible scales which is required to recover a comprehensive and representative picture of the material being examined.

For rheologists, one of the key challenges of this new century is the extension of traditional rheology to the study of more exotic materials such as biopolymers and, in particular, foods. But such materials are far more complex than synthetic polymers and, therefore, generate the need to have stronger constraints available when modelling and interpreting their flow and deformation behaviour. This again generates the need for new forms of indirect measurements which allow one to bring in from the cold information which traditional measurements have pushed into the background.

In many ways, the meeting in Lake Vyrnwy represented a meeting between rheology and various emerging technologies including atomic force microscopy, nuclear magnetic resonance and ultrasound. An overriding goal was an examination of how rheology and such emerging technologies could be of mutual benefit.

A key and pleasing feature of the presentations and discussions was the explicit acknowledgement of the various

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inverse problems with the modelling and interpretation of the indirect measurements being made. There was implicit recognition of the trade-off that is involved when using indirect measurements and the need to be aware of the information that is being pushed into the background at the expense of that which is being recovered. The various emerging technologies examined at the workshop were:

- Atomic Force Microscopy: W. R. Bowen (Swansea) showed atomic force pictures of the internal structure of biofilms, while A. Badía (Zaragoza) illustrated the potential for this emerging technology in the study of superconductors.
- Magnetic Resonance Imaging (MRI): W. J. Frith (Unilever Research Colworth) illustrated how MRI had been successfully applied in the study of the structure of microgels, while L. Sun (Cambridge) explained the basic science of MRI and discussed how to recover molecular movement using MRI measurements.
- Rheo-Optical Techniques: J Mewis (Leuven) gave a lucid talk about the physics behind rheo-optical techniques along with a discussion of its application to the alignment in latex particle suspensions.
- Ultrasound: M. J. W. Povey (Leeds) discussed the challenges posed in the modelling of (low energy) ultrasound measurement and explained how the ultrasonic stimulation of an oil drop in water heats the oil which in turn becomes a sound source. C. Verdier (Grenoble) explained how ultrasonic measurements, in conjunction with optical microscopy, had allowed results to be obtained about phase inversion in polymer blends.
- Molecular Weight Distribution and Relaxation Spectrum Recovery: The individual talks by C. Friedrich (Freiburg), C. Bailly (Louvain-la-Neuve), A. R. Davies (Aberystwyth) and I. Emri (Ljubljana) illustrated, in various ways, how new mathematical models and techniques have a role to play as emerging technologies.
- The Continuing Role of Traditional Techniques: The individual talks by G. J. A. Sevink (Amsterdam), J. Maia (Minho), L. Yeow (Melbourne), D. R. Oliver (Birmingham) and R. S. Anderssen (Canberra) discussed, from various points of view, how the more traditional techniques of rheology will have a continuing role to play in the future study of exotic materials, and, therefore, should also be seen as emerging technologies when applied in new and innovative ways.
- Physical and Statistical Insight: The talks by G. N. Greaves (Aberystwyth) and M. B. Hansen (Aalborg), respectively, examined how future insight will follow from the physics of zeolite collapse and Bayesian inversion.

One of the highlights of the workshop was the decision to benchmark relaxation spectrum and molecular weight distribution recovery and to hold another workshop on this topic soon (contact R. Keunings, Louvain-la-Neuve).

The organizers, Dr. Gareth Roberts ably assisted by members of the Institute of Non-Newtonian Fluid Mechanics of the University of Wales, are congratulated on and thanked for the success of their efforts.

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