Amherst Rheology Course

ARC 2004 "Merging Experiment with Theory in Rheology" June, 3-4 2004 University of Massachusetts, USA

The first Amherst Rheology Course (ARC2004), organized by H. Henning Winter of Chemical Engineering at the University of Massachusetts (UMass) Amherst, took place on June 3-4, 2004. Course participants were presented with new easy-to-use computer graphics tools and a new approach to rheology in which the "common" rheologist can access the most advanced data analysis and molecular theory. Short lectures on rheology were combined with hands-on tutorials. Our goal was that participants master rheology on a quantitative level and also understand the underlying concepts that lead to the quantitative results. Participants were encouraged to bring their own PC, install IRIS, and explore their own data.

Twenty-two participants from six countries were enrolled in ARC2004. Two-thirds of the participants came from industry (and from a hospital) and the other third were PhD students of other universities. An additional 12 students of UMass Amherst participated. The course was taught by a team consisting of Henning Winter, Jonathan Rothstein (UMass Amherst, MIE), Richard Blackwell (mathematician from Cambridge, UK), Marian Mours (UMass ChE alumnus, working in Germany), and Manfred Wagner (applied physicist and engineer from the Technical University of Berlin, Germany). Robert Huss of UMass Amherst (ChE) operated the computer laboratory.

Figure 1 (left): Jonathan Rothstein lecturing.

Figure 2 (right): Dinner after day one.

The course started on June 2nd with a welcome reception at the residence of H. H. Winter where the course participants could get acquainted with each other. On June 3rd, the participants learned to work with IRIS (Mours) and performed standard data analysis tasks such as data input, time-temperature superposition manually and computer optimized, spectrum calculation, expression of data in the wide range of linear viscoelastic material functions (Winter). Rothstein explained the fundamentals of extensional flow experiments and showed data on complex fluids. In the afternoon, Blackwell introduced the tube dilation theory and performed exercises in a practice session. The main topic was the relation between molecular architecture and rheology. Wagner concluded the day with a lecture on molecular stress function theory and a corresponding tutorial. Extensional flow data were compared to theoretical predictions for a wide range of polymers. In the evening, the entire group met for dinner at a restaurant near the Amherst town commons.

The tutorials continued on the second day. Mours introduced help and advanced graphics functions of IRIS. Winter modeled steady shear flow (time-temperature superposition and fitting to the most common functions) and yield stress functions in an interactive tutorial with the group. Rothstein explained optical methods for rheology. Winter practiced the second shift option (same as time temperature superposition but for parameters such as concentration, molecular weight, etc.). Winter and Mours presented time resolved mechanical spectroscopy and used gelation as example in a tutorial. Blackwell and Wagner, in a joint tutorial, analyzed experimen-

tal data of a model polymer melt and compared to predictions from theory.

The course participants discussed vigorously and curiously. The course evolved in a very positive atmosphere. The participants were able to merge experiment and theory graphically on the PC screen. The workshop allowed participants to explore their own materials in new ways, discover, and draw quantitative results.

The ARC will travel to Berlin/Germany in April 2005 and then return to Amherst in 2006.

Teaching Tools

ARC2004 built on the new teaching tools for rheology that became available with the IRIS rheology software. This user-friendly platform allows exploration of the newest developments in rheology.

Predictions from Theory: Theoretical predictions of linear viscoelastic material functions can be made directly in IRIS. Available are classical theories of polymer melts and solutions (Maxwell, Rouse, Doi-Edwards) and empirical models. Theory groups began to write modules for the IRIS platform. A common goal of these theories is to find a relation between molecular architecture (topology) and molecular dynamics as expressed in rheology. The theoretical part of IRIS also extends into non-linear rheology. The most common transient flows of polymer melts and solutions can be modeled with classical theories (Lodge rubberlike liquid, Doi-Edwards independent alignment), with empirical models, and with recent theory. The molecular stress function theory (Wagner and coworkers) has been fully implemented for predicting shear flow, uniaxial extension, planar extension and equi-biaxial extension of polymer melts. The tube-dilation theory (McLeish and coworkers) is established for linear viscoelastic predictions; it is in testing for non-linear flows. More theory modules are in progress.

Experimental Material Functions: For many complex materials, advances in the understanding of rheological behavior is driven by experimental observations. Careful experiments are followed by a detailed data analysis. The most commonly found rheological experiments are included in IRIS:

- Dynamic mechanical spectroscopy
- Steady shear
- Start-up of shear and extension
- Step strain
- Creep experiment

Data from a wide range of sources (various rheometers, literature data, e-mail, spreadsheet) merge into a standardized format. Steady shear data can be expressed in fit-functions that are commonly incorporated in models for polymer processing flows. Typically, time-temperature super position should be checked and used if applicable (Arrhenius and WLF function, density effects). The relaxation time spectrum and the retardation time spectrum is calculated from dynamic mechanical data (Baumgärtel et al., 1989). Time resolved rheological data get de-convoluted (Mours et al., 1994). This allows the study of evolving structure in a material (gelation, reverse gelation, crystallization, melting, degradation).

Seamless Communication: The high data volume in rheology has three main aspects: 1) the actual measurement and all its complications, 2) the analysis of the experimental data, and 3) the seamless communication of the results to larger user groups. The emphasis of ARC2004 was on the latter two. A more thorough understanding is gained by merging data analysis with molecular theory. Seamless communication is achieved with unified data structure and

Figure 3: Manfred Wagner and Marian Mours with two participants.

unified methods of applying these data. In the same way as participants of the course shared tutorial data and tutorial projects, members of a group (same laboratory, same company, or same international research team) can share data and communicate projects in which these data are applied. Predictions from theory are shared in the same way.

Figure 4: Relaxing after ARC2004.

Why Another Rheology Course?

It has been our impression that the most pressing problem in rheology is its lack of accessibility. The full use of rheology is limited to a small group of highly trained scientists. If there is widespread use of rheology today, it has been achieved partially by simplifications of rheological concepts, sometimes over-simplification. In spite of this, rheology has still proven to be useful to a certain extent, but simplified methods fall way short of revealing the full potential of the rheological information of a specific material of interest. The main objective of the course is to make rheology more accessible. Rheology will gain by the development of user-friendly methods that express rheology in its full complexity. This includes methods of freely communicating rheological data and theory as discussed here. To make rheology more accessible, we have started to develop a computer platform that allows a detailed analysis of experimental data and allows predictions from the newest theories in rheology (http://rheology.tripod.com/). The IRIS computer platform gives experts in specialized topics of rheology the opportunity to write modules that will seamlessly merge into a general code so that it can be used by a wide range of engineers and scientists.

User-friendly methods are essential not only for research and application, but also for the teaching of rheology. New teaching methods will potentially generate broad access to rheological concepts. This will lead to an appreciation of the significance that rheology has in technical applications. In-depth data analysis and evaluation of theory should become easy enough to be performed by non-rheologists after reasonable training (one week of training seems acceptable) and without relying on over-simplifications.

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