Workshop Report

Rheology Cyberinfrastructure for Integrated Research and Learning at ARC07

Technical University Berlin, Germany
March 20-21, 2007

The fourth Amherst Rheology Course (ARC07) met in Berlin/Germany at the Institute of Manfred Wagner at the Technical University Berlin. The theme of the course was "synergy between experiments and theory in rheology". ARC07 provided participants with a broad overview of experimental and theoretical rheology and then equipped them with the cyberinfrastructure (CI) tools to obtain quantitative answers in rheology. Lectures and practice sessions were combined to develop a deeper understanding for the underlying concepts that lead to quantitative results.

Rheology is an essential tool for solving complex problems at the frontiers of materials science. To be effective, materials scientists and engineers should be able to easily exchange rheological data and to merge data with theoretical viewpoints. We anticipate that, in the near future, companies will take advantage of CI and apply rheology more widely and efficiently. The company with the most effective CI tools and best CI-trained work force will be the most competitive.

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The CI tools of ARC07 consist of a single workspace ("rheology hub") that bundles expert codes on the PC. This system allows the world's leading rheology experts to easily share their expertise with a wide community of users. Implementation of such single workspace technology will introduce a new style of networking between individual researchers and/or between company sites. It allows for screening of materials, optimizing of processes, and evaluating hypothetical materials before even making them. Researchers and practitioners will routinely merge experimental data with modeling predictions and simulation (laboratory internal modeling tools, third party codes, free software). This merger will be further supported by the unified data standard that facilitates access anywhere-anytime. Global teleconferences and sales negotiations will be strengthened with rapid retrieval of material data and with 'on the spot' modeling calculations. Quantitative technical information will be retrieved or quickly generated (by modeling) for rapid decision-making. Practitioners of rheology in industry will evaluate their strengths locally by exploring their own ideas and hypotheses in the context of global rheology knowledge. Implementation of most of this CI technology is possible with today's tools [1].

This spring, ARC07 participants brought their own laptop computers and performed practice calculations with CI tools. Course participants used the "rheology hub" to compare experiments (dynamic mechanical, steady shear, startup of shear, startup various extensional flows, molecular weight distribution) with predictions from a range of theories, including classical theories (Maxwell, Rouse, Lodge, Doi-Edwards) and three recent polymer dynamics theories: the 'tube dilation' model of McLeish and coworkers [2 - 7], the hierarchical model of Larson and coworkers [8, 9] and the "molecular stress function" model of Wagner and coworkers [10]. The "NAPLES" code of Masubuchi and coworkers [11 - 13] was used to simulate molecular dynamics of homogeneous mixtures of molecules with different architecture. Furthermore, we practiced the new module for predicting the (monomodal, bimodal) molecular weight distribution of linear polymers from their dynamic mechanical data [14, 15]. Time-resolved rheometry tools [16] were applied to chemical gelation. Dynamic mechanical data were shifted into master curves and the (discrete and continuous) relaxation time spectra were calculated [17, 18]. In addition, Jonathan Rothstein expanded the scope by introducing into "Micro-Rheology" and "Rheology of Micellar Fluids". At the end of the 2-day course, participants were able to intuitively and seamlessly navigate the "rheology hub". Even course participants arriving at the course with minimal background in rheology efficiently navigated the rheology workspace.

The current group of rheology users worldwide is still fairly small and specialized, while the main workforce in materials science and engineering has little access to rheology. The Amherst Rheology Courses seek to broaden and diversify the population of individuals and institutions participating in rheological activities and to integrate rheology into wider areas of science and engineering. One reason for rheology's current insular state is the lack of intuitive tools for analyzing rheological experiments and for comparing experiments with theory. A second reason is the lack of a universally accepted data standard. These problems are being addressed by using the "rheology hub" and by teaching its use to a wider group of people.

Twenty-one rheologists participated in ARC07. The course was jointly directed and taught by H. Henning Winter (USA) and Manfred Wagner. Jonathan Rothstein (USA) joined the team as one of the instructors. The course started on March 19, 2007, with a welcome reception where the course participants got acquainted with one another. It ended with joint exercises and discussions on March 21. The Amherst Rheology Course (ARC08) will convene again in June 2008, in Amherst, Massachusetts, USA. New topics will be added concerning the rheology of emulsions. Information about the "rheology hub" and about future ARC can be found at http://rheology.tripod.com/ARC.htm.

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