Experiencing Synergy Between Experiments and Theory in Rheology

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Abstract

Recent advances in rheometer design and rheology theory have led to an abundance of information, both experimental and theoretical. In response to this wonderful opportunity, many of the world's leading rheologists have begun to share expert software codes with a global community of materials researchers and practitioners. This has led to the creation of a virtual environment for rheology (called "Rheo-Hub") in which students, researchers and practitioners analyze experimental data comprehensively, compare experiments with theory, directly explore theories by varying parameters in a wide parameter space, and derive results in the form of graphs, which are ideal for conducting quantitative comparisons and searching for dominant patterns. Explorations may be repeated in different ways (different expert codes may lead to alternative answers for the same research question) and viewed from different graphical viewpoints. Such easy access to advanced rheology is important, as it allows us to efficiently harness the large, rapidly growing technical knowledge base in rheology for the purpose of research and industrial innovation. Currently, hub technology for rheology is used in over 70 laboratories throughout the world, both industrially and academically. The technology is described in recent papers on cyber infrastructure by Winter and Mours (2006) and Winter (2007).

Introduction

Imagine that you are working on a new materials formulation or a new materials processing method and someone suggests rheology as a major tool with which to proceed. How would you respond? You might say, "no way, it's too complicated" or "get me some quick data so that I can move on" or "let's find someone who knows rheology". The barriers that prevent understanding of rheology are indeed substantial and often prevent its use.

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.

So why aren't more people using rheology? What are the main barriers that prevent an efficient use of this important materials science, and how can we overcome these, possibly in a virtual rheology environment? This lecture will address these questions, provide examples and introduce recent advances of hub technology.

Overcoming Barriers

Lack of understanding is the most immediate of barriers, as few people have had formal rheological training and/or kept up with recent developments. Furthermore, a great hindrance is derived from incompatible data formats, as no two rheometer models use the same format. Insufficient data analysis tools raise even larger barriers and access to advanced modeling is tedious. And then there is the time issue: Many people simply do not have the time to deal with all this. Ideally, results should become available instantaneously (practically). Because of this compounded dilemma, rheology work typically gets assigned to a specialist ("the rheologist") within the company instead of involving a broad user group. Often, the use of rheology is avoided all together.

On the positive side, rheological data can be generated with high accuracy and speed (due to major advances in rheological instrumentation). Also, computer modeling of materials dynamics has advanced to a level that has made it extremely useful for technical work. Examples are modeling codes for polymerization reactions in production-size reactors (and connection to rheology) and codes that predict rheological properties for specific molecular architectures and molecular interactions. Rheology has to reinvent itself in a new approach that removes the barriers and takes advantage of abundant data and theories.

So, how does hub technology work? How does it address the difficulties listed above? Basically, it forges experiments and modeling codes into a single workspace ("hub") on your laptop. Attached to the "hub" are software modules ("engines") that represent individual modeling tasks. The single, standards-based workspace uses visuals for easy navigation and communication of results. Navigation through the rheology workspace is as easy as selecting a meal from a restaurant menu, having the meal cooked by a master chef in the kitchen, and then having the meal served without exactly knowing the culinary tricks of the chef. In continuation of this analogy, you initiate your rheological task by selecting the desired action from the hub-menu on the laptop PC and entering your specific parameter choices on the screen. This will invoke the action of some expert who may be on the other side of the world. However, you do not have to travel there since the expert code is on your laptop (due to hub technology), ready to perform the necessary calculations. The calculated rheology results will be presented in the form of easily digestible visuals, much like the festive meal served by the restaurant chef. Reaching this level of convenience is the objective of the new rheological workspace.

Main Features of Rheology Hub Technology

The new approach to rheology is guided by the following objectives:

- forging global partnerships between distributed expert groups: actively seeking out the world's leading expert groups in rheology and obtaining their most advanced modeling/simulation codes for sharing in a hub;
- enabling comprehensive data analysis;
- introducing a data standard for rheology. With such a standard, data from various rheometers can be superimposed and compared. Also, results from one modeling code can serve as input for another modeling code and results from various expert codes can be compared with each other and with experimental data;
- achieving a short response time and instantaneous graphics display through graphics tools that are installed on the client PC;
- achieving interscale results: a single software platform connects nanoscale engines with meter scale engines and length scales in between (molecular structure and conformations affect large-scale dynamics of rheology and vice versa);
- enabling interdisciplinary work involving synergy of mathematics, physics, chemistry, biology, and engineering;
- creating a participatory learning environment for students, researchers, and practitioners;
- creating a mechanism for expansion: adding more rheology topics and expert groups year by year.

With hub technology, users 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 (McLeish et al., 1998, 1999; Milner and McLeish 1997, 1998; Blackwell et al., 2001; Pryke et al., 2002), the hierarchical model of Larson and coworkers (2001, 2005) and the "molecular stress function" model of Wagner and coworkers (2003). The "NAPLES" code of Masubuchi and coworkers (2001, 2003, 2004) is used to simulate molecular dynamics of homogeneous mixtures of molecules with different architecture. One module is used for predicting the (monomodal, bimodal) molecular weight distribution of linear polymers from their dynamic mechanical data (Nobile and Cocchini, 2001, 2003). Time-resolved rheometry tools (Mours and Winter, 1994) help with the analysis of physical and chemical gelation. Dynamic mechanical data can be shifted into master curves and the (discrete and continuous) relaxation time spectra get calculated (Baumgaetel and Winter, 1992; Jackson et al., 1994). Recently, the mode-coupling theory was implemented for modeling of yielding dispersions (Crassous et al., 2006).

As an essential part of the hub technology, literature references are provided for all calculations invoked in the virtual environment. The user will be able to read these essential papers for her/his project, thereby learning the underlying physics or mathematics to understand the work in greater depth.

Education and Training

The hub technology has been integrated into classroom teaching of rheology. It also is the basis of the annual rheology course that alternates between Amherst/MA/USA and Berlin/Germany (Winter, 2007). With the hub technology approach, basic concepts of rheology can be taught to newcomers to rheology, while also making rheological work accessible to students earlier in their curriculum (as part of the undergraduate curriculum).

The virtual environment allows students to perform calculations with the most advanced theories and with widely diverse data sets. Imagine the following scenario: a student selects a polymer (star architecture mixed with a linear polymer, for instance), predicts the stresses when stretching the polymer into a fiber, and then compares the quantitative predictions to time-dependent stress measurements. The procedure gets repeated with molecules of different architecture, size, and/or size distribution, and at different stretching conditions. Comparison of the different predictions leads to an intuitive understanding of the effects of molecular architecture on the specific flow of interest.

Research

We envision rheology hub as a tool for developing new theories, for comparing theories to one another, and comparing theoretical predictions with experimental observations. Computer simulation will allow exploration of the fundamental principles that govern the dynamics of complex materials during deformation and, thus, will help to develop truly novel materials and thereby will suggest rational synthesis methods that are required for producing the respective material.

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 virtual rheology tools and apply rheology more widely and efficiently.

Industrial Application

After having implemented hub technology at a company, researchers and practitioners will routinely merge experimental data with modeling predictions and simulation. A unified data standard 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 technology is possible with today's tools (Winter and Mours, 2006).

Many applications can be envisioned. Imagine being able to use the Internet to instantly pursue a materials processing question from any location. You might want to compare new processing data from the most recent polymer formulation with observations on your favorite polymer of five years ago. Or imagine that you are in the middle of a conference call and need answers right then - or that your boss asks you to complete a technical report by tomorrow morning. No problem! You simply connect to your data source, plot the data, choose from several theories to predict rheological properties, relate the predictions of processing to the experimentally observed processing, explore variations in molecular architecture of formulation, connect into an application, and display the results graphically. Within a half hour, you compare processing experiments and theory and find critical answers. Short questions can be addressed directly within minutes. Does this scenario appear unrealistic? It isn't. For rheology, this sharing and accessing of knowledge has become real.

Broadening the Rheology Work Force

Most companies afford one or two experts who are in charge of generating rheological data and interpretation. Widespread use of rheology is rare. Typically, rheological data remain sequestered in the rheology laboratory, most likely on the computer next to rheometers. Hub technology can help with the basic training (see Winter, 2007) of a broader user group, and by creating synergy between the data and rheology theory.

Addressing Security Concerns

Security concerns have been raised since it is so easy now to use each other's data. However, security is completely addressed by distinguishing between data in the published literature and proprietary data. We are in the process of developing a reference library that contains data from the published literature. Even if hub technology finds widespread use, proprietary data and modeling results of individual companies will naturally remain in their private domain. Typical security methods include firewalls and passwords. The same security procedures that are currently commonplace for protecting proprietary text files can also be applied to research data.

Outlook

Our long-range goal reaches beyond the implementation of rheology hub technology. The major task before us is the integration of rheology into materials research in general. This will be achieved by generalization of hub technology and will be addressed in a new industry-supported initiative at UMass Amherst, the Amherst Center for Cyber Infrastructure for Engineering and Science Synergy (ACCESS). The approach will also be multiscale, since molecular details control the macroscopic flow and deformation behavior, and it must be interdisciplinary, since diverse topics of physics, chemistry, biology, mathematics, and engineering feed into one another. An example of such a complex problem of materials engineering is flow-induced crystallization of polymers in which molecular properties and the kinematics of a macroscopic flow determine the flow-induced molecular orientation, stretch, and entropy change. As a consequence of flow-induced molecular conformations, the crystal structure nucleates at increased rate and grows anisotropically. In turn, the growing crystal structure alters the flow since rheological properties get changed. This affects the nucleation and crystal growth even further. The complexity of such a process soon exceeds the technical capabilities of an individual or a single expert group. There are many such examples that require rheology knowledge but cannot be solved by rheology alone. Experience with the rheology hub technology will provide guidance along the path in this new territory.

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