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Seamless Communication of Rheologica Data in a Mixed Research/Production Community

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Abstract

Seamless communication in rheology (SCR) is designed to integrate experiment, theory, and application in rheology. SCR is a quantitative tool that unites very diverse rheological tasks as they might arise in a company or in a research/development group, small or large. With SCR, it is not necessary for each member of the research/development group to own a rheometer as long as (s)he has direct access to rheological data (on a server, for instance). If access is established, data can easily put to use through the IRIS software (1-6). SCR also brings advantages to the experimentalist (‘owner’ of a rheometer) who wants to present his/her experimental results to a wide community of users. SCR, in combination with interactive graphics, is not only a research tool but also a means of producing ‘added value’ in industry. SCR supports the teaching of rheology in unprecedented ways. Instead of limiting rheology to a privileged group of researchers, seamless communication advances rheologists to a level where they can closely integrate with the entire community of materials scientists and application engineers.

For complex materials, the understanding of rheological behavior has greatly advanced through careful experiments that are followed by a detailed data analysis. Our initial focus was solely on the data analysis (2-6). There, we used and still use a comprehensive and efficient code that is designed to analyze data to the fullest extent and at high rate. Take mechanical spectroscopy data $G'(\omega),G''(\omega)$ as example, where a typical 5-to-10 minutes analysis provides time-temperature superposition, spectrum calculation, and plotting of the main material functions. Other topics are time-resolved mechanical spectroscopy, step-strain, creep, constant rate flow, and others.

In a new development, theory (7-13) has been merged with the visualization of the rheological experiments. Newest developments will be shown at PPS20.

Introduction

There is a need for establishing communication between the experts that generate material data and the wide group of users of material data with their diverse requirements. Such communication should be widely available and easy to use. Ideally, there should be no noticeable barriers (“seamless”) to this communication while, in reality, concerns of security, confidentiality, and documentation will establish barriers. However, within selected groups, which may be very large, free access to specific information may be considered advantageous. Here, the communication can be made seamless.

Rheology is agreeably the most important expression of molecular and supra-molecular dynamics. It profoundly affects the processing of complex materials, and also their end-use. Complex materials such as polymeric fluids, polymer emulsions, liquid crystals, and associative polymers are ubiquitous in today's economy, being used in everything from plastics, paints, and detergents to pharmaceuticals and liquid-crystal displays. An advanced understanding of the behaviour of these complex fluids in flows is crucial to their effective use and to the control of their ultimate properties. These complex materials are non-Newtonian in nature and have been shown to demonstrate shear-thinning in shear flows, strain-hardening in extensional flows, elasticity, yielding and/or a fading memory, for example. It is essential to understand the implications of their rheology since the material properties of these complex fluids are strongly affected by the deformation and alignment of their microstructure in addition to their molecular composition.

High Data Throughput Rheological instruments have matured to a level of high sophistication and, as a consequence, an abundance of quality rheological data became available for a wide variety of material classes. Data acquisition is further accelerated by combinatorial and high-throughput methods. These recent advances raise new questions such as: How can we cope with myriads of rheological data? How can we extract useful information in a reasonably short time? Are the data self-consistent? What are the dominating experimental parameters? The high data volume in rheology has three main aspects: (a) the actual measurement and all its complications, (b) the analysis of the experimental data, and (c) the seamless communication of results to larger user groups. The emphasis of SCR is on the latter two.

Greatest Problem at Current State of Rheology Rheology is still difficult to access. This is its biggest unsolved problem. 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 mostly 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. 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.

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. SCR will be an important tool for achieving that goal.

Integration The major advances in experimental and theoretical rheology of recent years can only be utilized if we succeed in merging application requirements with the results from the rheology laboratory and with predictions from molecular dynamics theory. These advances occurred separately from each other and have remained mostly separate. Typically, application engineers rely on rheological data given to them or measured for them in commission; experimentalists in rheometry laboratories are able to produce data but they are separate from their data's application; theoreticians understand underlying principles that govern the rheology of polymers, but they can not directly apply their theory or compare with experiments. Many attempts have been made to remove these barriers. A deeper understanding will be gained by merging data analysis with molecular theory and application. This is the topic of the following.

Seamless Communication in Rheology (SCR)

It still is common practice to sequester rheological data to the rheology laboratory. This has the advantage that experts are the 'guardians' of the data. However, it prevents rheology from been applied more widely. To overcome this problem, only two functions have to be implemented: (a) access to data for the entire technical staff, and (b) data analysis that is easy, fast, and informative. Both functions, access and analysis, are at the core of the proposed SCR technology. SCR integrates the resources of the rheology laboratory with applications company-wide or institute-wide. This maximizes the use of the laboratory resources. SCR allows members of an interdisciplinary group (same laboratory, same company, or same international research team) to share data and to communicate projects in which these data are applied. Predictions from theory are shared in the same way.

With the IRIS rheological software (1-6), we are developing a SCR approach for bringing the above three groups together (experiment, theory, application). The objective is to establish communication between the experts that generate the material data and a wide group of users with diverse rheological needs. The main features of SCR in rheology are

* user friendliness
* central data storage on server: security, documentation, data libraries.
* single data format: Thirteen years ago, we decided on a meaningful ASCII data standard and have used it ever since. Major advancements are expected from the new IUPAC data standard (IUPAC Working Party IV 2.1. Project 2003-009-1-400).
* worldwide access by users
* connectivity, simplicity, and flexibility
* communication of results (analyzed data, predictions from theory)
* fast response that allows utilizing large data volume
* leading experts from all three groups contribute to the project.

Analysis of Experimental Data A short demonstration will start with a typical data set of mechanical spectroscopy for a group of polymer melts. Time-temperature superposition will combine these data for each of the polymers, and time–molecular-weight superposition will combine the data into a single master curve. Data will then be shifted to new temperatures and/or to new molecular weights (if so desired). After spectrum calculations, the modulus and the creep compliance will be predicted. A wide range of viscoelastic material functions can be plotted and patterns may be discovered in this process. Viscosities will be predicted from the Cox-Merz relation and then fitted with the most common functions (Carreau, Cross, etc.). Steady shear viscosity data will be superimposed for comparison. Time-resolved rheometry will be shown for a sample during gelation.

Predictions from Theory The IRIS computer platform allows experts in specialized topics of rheology to write modules that will seamlessly merge into a general code that can be used by a wide range of engineers and scientists. Theory has advanced rapidly in recent years, but these advances have gone different ways for different research groups. In contrast to the well established analysis of rheometry data, theory is far from being consolidated. Because of this exciting diversity and novelty of ideas, we invited two experts in the field of theoretical rheology to write modules inside the IRIS program The module for 'tube dilation' (theory of McLeish and coworkers) (7-12) was written by Richard Blackwell, Cambridge, UK, and the modulus for the molecular stress function (MSF) theory (13) was written by Manfred Wagner, Berlin, Germany. The new IRIS extends the current molecular theory calculations to non-linear viscoelasticity (large strain behavior). Again, the language is interactive graphics. Predictions of one theory will be plotted against predictions of the other theory. This will allow critical evaluation of theory. Beyond this practical aspect, theory describes the underlying molecular dynamics to a level that exceeds the realm of current experimentation. The gained insight in molecular details produces new challenges for experimentalists and for the practice of rheology.

Implementation of SCR

One single computer graphics approach on a common SCR platform allows comprehensive analysis of rheometry experiments together with quantitative exploration of molecular theory.

SCR Stage 1: The process begins with the generation of rheological data and their filing on a dedicated server. In industry, the rheology laboratory (and its experimentalist in charge) will perform this task of data generation and documentation. If a theory group is working on the same group of materials, its rheological predictions will be stored on the same dedicated server, see left side of figure 1. Data files are typically divided in a documentation part and a section with the actual data columns. Data files are written in ASCII (American Standard Code for Information Interchange) and in a standardized format that is uniform for a research group (small group) or for an entire industry (general data standard). The server typically is programmed such that data are accessible and protected as well (documentation, back-up, systematic labeling, and controlled access). This completes the first requirement of the communication process. Data are available for their use.

SCR Stage 2: The second requirement is the user's access to the data. The diverse needs of the wide group of users is best served by giving direct access to the data and by allowing individual users to combine, rearrange, and analyze these data as required for specific applications, see right side of figure 1. This is achieved with a support program (IRIS code) that can read data from the central server and can combine, rearrange, and analyze these data in efficient ways as described above. Depending on the rheological knowledge of the specific user, the analysis may be rather simple or highly sophisticated. Both options have their justification.

SCR Stage 3: Having both components in place, the communication process will lead us to the next level. Users will work with the data and have the option of storing entire sets of analyzed data ("projects") on the server. The IRIS platform supports communication through projects. For communication within a research group, such projects get freely exchanged. Collaborators (or plain users) may access these projects on the server, explore them further, and generate new or revised projects. Experimentalists, theoreticians, and practitioners participate in this dialog and express entire data sets in form of projects. Written internal reports will include server addresses for importing support material in form of original data or entire projects. The result of such activity will be a deeper understanding of the rheological data; this will generate new questions and will result in requests for more experiments and more theories. New applications for materials can be found and new processes get developed. Seamless communication in rheology is at work.

Applications

Current Status A SCR rheology system is in operation at UMass since 1996. It has allowed interaction within the rheology research group and with a wide range of researchers worldwide. Integration of theory is a recent development. This sets the framework for connecting into polymer processing applications in the future.

Research and Innovation SCR and the associated tools generate a research environment that focuses on rheological concepts and their application while minimizing the time that is spent with repetitive tasks. SCR helps to validate data, explore their limits, search for patterns, and connect into theory.

Added Value in Industry SCR can add value to the service a company gives to its customers. A sales engineer, for instance, will be able to address specific questions of a customer by providing quantitative rheological information without delay. Consider a sales engineer with a customer that requests creep data of a specific polymer ABC at 150^{o}C. However, the only data available for ABC are omega, *G*', *G*" at 120^{o}C, 140^{o}C, 160^{o}C, 180^{o}C, and the sales engineer is far away from her/his office. A meaningful response to the customer will require additional work and will cause delay. This is where SCR can add value. Instead of promising the delivery of 150^{o}C creep data in a week or two, (s)he accesses the central server, downloads the data (omega, *G*', *G*" at 120^{o}C, 140^{o}C, 160^{o}C, 180^{o}C), applies time-temperature superposition to merge these data into a master curve, calculates the retardation time spectrum, calculates the creep function, transfers the resulting plot to a word processor, and prints the 150 ^{o}C creep graph for the customer. All of these actions can be performed while continuing the interactions with the customer. The sales engineer has to be trained for the interactive SCR work, but the training is not extensive.

Education The meaningful use of rheology requires a deeper understanding of the underlying principles. Such understanding is critically needed both in industry and in academia. The interactive graphics approach to rheology, as proposed here, makes it a great teaching tool for introducing rheology to a wide audience. Graphics has the advantage that it can explain complex concepts to students at an early state of their education. The interactive graphics also helps non-rheologists (post graduates or the sales engineer of the above example) to develop rheological skills that are necessary for understanding experiments or applications. At the same time, they will explore the molecular origin of their observed flow phenomena. Predictive tools allow calculating flow induced molecular stretch and orientation in polymer melts as function of molecular topology (linear, short-chain branched, stars, pom-pom; size).

Conclusions

The basic framework for seamless communication in rheology (SCR) is now defined. Experimental data can be shared and explored by large groups of experimentalists, theoreticians, and applied engineers. The necessary tools are established and tested. Several theories are implemented, and more will come. SCR adds value to rheological research, education, and industrial application. Further applications should be added. This is planned for the near future.

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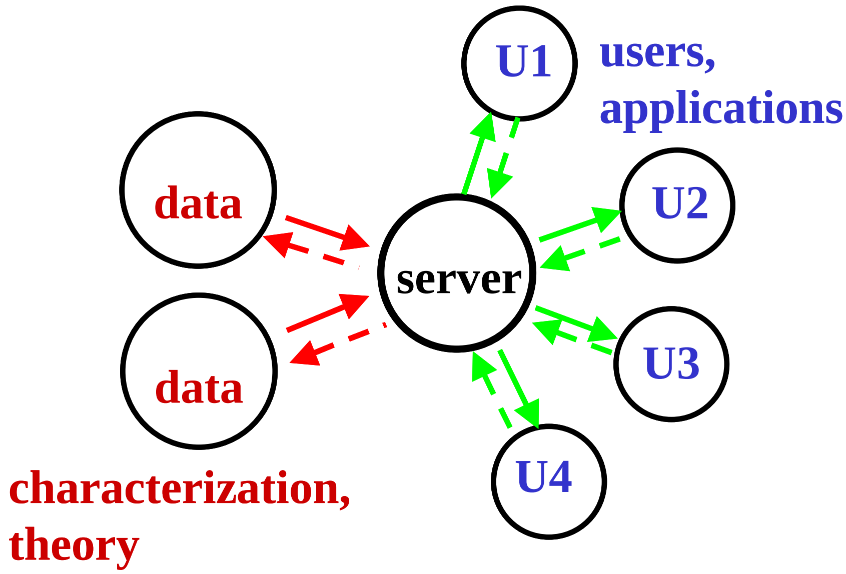

Figure 1: Schematics of SCR: in stage 1 (arrows with solid lines, left side of figure), rheological data get generated and transferred to a central server. In stage 2, users access the data (arrows with solid lines, right side of figure), work with the data, return information to the server (arrows with dashed lines), and possibly request further data. In stage 3 (solid lines and dashed lines), rheological information is freely exchanged either as data files or as entire projects. Seamless communication is facilitated by a code that is equally used by all participants.