Sharing the World's Advanced Rheology Knowledge through Rheo-Hub

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Abstract. Recent advances in rheometer design and rheology theory have led to an abundance of rheological information, both experimental and theoretical. In response to this wonderful opportunity, many of the world's leading rheologists began to share their expert software codes with the wider community of materials researchers and practitioners. This became possible through "Rheo-Hub", a central computer platform from which the user interrogates rheological expert codes ("engines") and rheological data by comparing, merging, and funneling these into further interrogations and explorations. In this virtual environment, results are returned to the computer screen as visuals so that the visual intelligence of the user gets involved in the cognition process. Rheological explorations may be repeated in different ways (using different expert codes for answering the same research question) and viewed from different graphical viewpoints. This creates the multi-scale and multi-expertise workspace that is needed to support quantitative rheological explorations and to prepare for discovery. The virtual environment technology will be presented and examples will be shown. Rheo-Hub's strengths are data analysis, integration of experimental results with theoretically predicted rheology, visuals for communicating results, and introduction of a rheological data standard.

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BUNDLING OF GLOBAL EXPERTISE IN A VIRTUAL ENVIRONMENT

The objective of our project is to bundle globally distributed expertise into a virtual environment for rheology (VER). A personal computer of laptop size is sufficient for generating such VER (except for large simulation projects). Researchers in a laboratory, students and teachers in the class room, and by practitioners in industry can conveniently enter this virtual environment, perform calculations, and present results as visuals. The VER supports discussions, report writing, and teleconferences. The VER is known as Rheo-Hub and has been described in principle by Winter and Mours (1,2). The need for an easy-to-use VER came about because of several reasons:

- Rheology theory is known to be difficult to access for a wider user group since its application requires a challenging combination of knowledge in mathematics, physics, chemistry, biology, and engineering.
- Analysis of experiments has the reputation of being tedious and easy to miss. Quite often, single experts ("the house rheologist") or small expert groups supply larger user groups with rheological information but these groups remain uninvolved otherwise. For such service assignments, the rheology experts typically rely on their self-made software tool-box to perform repetitive data analysis tasks and to visualize results.
- Diverse rheology expertise is globally distributed.
- Incompatible data formats, as no two rheometer models use the same format.
- Rheological results are rarely integrated with other areas. As an example, the connection between polymer rheology and processing is mostly kept at an empirical level; quantitative relations are advanced with purely viscous models, but do not include the full rheological scenario.
- Few people have had formal rheological training and/or kept up with recent developments.

These problems are addressed by a bundling of globally distributed expertise into a single workspace that is easy to access and to use, see Figure 1. The user benefits from the rapid updating of results in visual form on the screen of the laptop. Based on these visuals, students, researchers, and practitioners can navigate intuitively and move seamlessly between rheology theory and data analysis, and between different theories or between different data sets.

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The VER allows users to analyze rheological data (3), search for patterns (4-7), and 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 (8-13), the "hierarchical model" of Larson and coworkers (14,15) and the "molecular stress function model" of Wagner and coworkers (16). The "NAPLES" code of Masubuchi and coworkers (17-19) simulates 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 (20, 21). Time-resolved rheometry tools (22) help with the analysis of physical and chemical gelation (23, 24). Dynamic mechanical data can be shifted into master curves and the (discrete and continuous) relaxation time spectra get calculated (25-27). Recently, the mode-coupling theory was implemented to model the yielding of colloidal dispersions (28).

As an essential part of the VER, literature references are provided for all calculations when 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. .

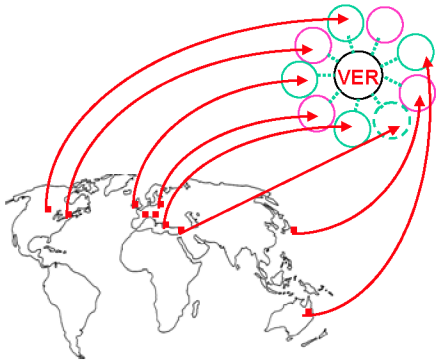

FIGURE 1. Creating the virtual environment fo rheology (VER) through global collaboration of the world's leading rheology experts

EDUCATION AND TRAINING

The VER technology has been integrated into classroom teaching of rheology. It also is the basis of the annual Amherst Rheology Course that alternates between Amherst/MA/USA and Berlin/Germany (2). With VER, 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.

INTEGRATION OF RHEOLOGY

Most recently we began to integrate Rheo-Hub with polymer process modeling. This occurred with an expert group that specializes in polymer processing. A rheological data standard had been introduced in 1992 and was kept ever since. The same data standard will now be used to connect into other topical areas that depend on rheological information.

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REFERENCES

1. Winter HH, Mours M (2006) The cyber infrastructure initiative for rheology. *Rheol Acta* 45:331-338
2. Winter HH (2007) Rheology Cyberinfrastructure for integrated research and learning at ARC07, *Applied Rheology* 17:302-304
3. Mours M, Winter HH (2000) Mechanical spectroscopy. Tanaka T, Ed, Experimental Methods in Polymer Science: *Modern Methods in Polymer Research and Technology*, Academic Press, San Diego CA. p. 495-546
4. Yasuda K, Armstrong RC, Cohen RE (1981) Shear-flow properties of concentrated solutions of linear and star branched polystyrenes. *Rheol Acta* 20:163-178
5. Baumgärtel M, Schausberger A, Winter HH (1990) The relaxation of polymers with linear flexible chains of uniform length. *Rheol Acta* 29:400-408
6. Stephens T, Winter HH, Gottlieb M (1988) The steady shear viscosity of filled polymeric liquids described by linear superposition of two relaxation mechanisms. *Rheol Acta* 27:263-272
7. Palde L,Verney V, Attane P (1996) A modified fractional model to describe the entire viscoelastic behavior of polybutadienes from the flow to the glassy regime. *Rheol Acta* 35:265-273
8. McLeish TCB, Larson RG (1998) Molecular constitutive equations for a class of branched polymers: the pom-pom polymer. *J Rheol* 42: 81-110
9. McLeish TCB, Allgaier J, Bick DK, Bishko G, Biswas P, Blackwell R, Blottiere B, Clarke N, Gibbs B, Groves DJ, Hakiki A, Hoenan RK, Johnson JM, Kant R, Read DJ, Young RN (1999) Dynamics of entangled H-polymers: theory, rheology, and neutron scattering. *Macromolecules* 32:6734-6758
10. Milner ST. McLeish TCB (1997) Parameter-free theory for stress relaxation in star polymer melts. Macromolecules 30:2159-2166
11. Milner ST; McLeish, TCB (1998) Reptation and contour-length fluctuations in melts of linear polymers. *Phys Rev Lett* 81:725-728.
12. Blackwell RJ, Harlen OG, McLeish TCB (2001) Theoretical linear and nonlinear rheology of symmetric treelike polymer melts. *Macromolecules* 34:2579-2596
13. Pryke A, Blackwell R J, McLeish TCB, Young RN (2002) Synthesis, hydrogenation, and rheology of 1,2-polybutadiene star polymers. *Macromolecules* 35:467-472
14. Larson RG (2001) Combinatorial rheology of branched polymer melts. Macromolecules 34:4556
15. Park SJ, Larson RG (2004) A Hierarchical Algorithm for Predicting the Linear Viscoelasitc Properties of Polymer Melts with Long-Chain Branching. *Rheol Acta* 44:319-330
16. Wagner MH, Yamaguchi M, Takahashi M (2003) Quantitative assessment of strain hardening of low-density polyethylene melts by the molecular stress function model. *J Rheol* 47:779-793
17. Masubuchi Y, Takimoto J, Koyama K, Ianniruberto G, Greco F, Marrucci G (2001) Brownian Simulations of a Network of Reptating Primitive Chains. *J Chem Phys* 115:4387-4394
18. Masubuchi Y, Ianniruberto G, Greco F, Marrucci G (2003) Entanglement molecular weight and frequency response of sliplink networks. *J Chem Phys* 119:6925-6930
19. Masubuchi Y, Ianniruberto G, Greco F, Marrucci G (2004) Molecular simulations of longtime behavior of entangled polymeric liquids by the primitive chain network model, modelling simulation. Mat Sci Eng 12:91-100
20. Nobile MR, Cocchini F (2001) Evaluation of molecular weight distribution from dynamic moduli. *Rheol Acta* 40:111-119
21. Cocchini F, Nobile MR (2003) Constrained inversion of rheological data to molecular weight distribution for polymer melts. *Rheol Acta* 42:232-242
22. Mours M, Winter HH (1994) Time resolved rheometry. *Rheol Acta* 33:385-397
23. De Rosa ME, Mours M, Winter HH (1997) The gel point as reference state: A simple kinetic model for crosslinking polybutadiene via hydrosilation. *Polym Gels Networks* 5:69-94
24. Winter HH, Mours M (1997) Rheology of polymers near their liquid-solid transitions. *Adv Polym Sci* 134:165-234
25. Baumgärtel M, Winter HH (1992) Interrelation between continuous and discrete relaxation time spectra. *J Non-Newtonian Fluid Mech* 44:15-36
26. Jackson JK, De Rosa ME, Winter HH (1994) Molecular weight dependence of relaxation time spectra for the entanglement and flow behavior of monodisperse linear flexible polymers. *Macromolecules* 27:2426-2431
27. Baumgärtel M, Winter HH (1989) Determination of the discrete relaxation and retardation time spectra from dynamic mechanical data. *Rheol Acta* 28:511519
28. Crassous JJ, Siebenbürger M, Ballauff M, Drechsler M, Henrich O, Fuchs M (2006) Thermosensitive core-shell particles as model systems for studying the flow behavior of concentrated colloidal dispersions. *J Chem Phys* 25:204906-10