

Interactive Rheological Software (IRIS), a Dialog with Linear Viscoelasticity

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Impressive advances in the theory of polymer dynamics (Doi, Edwards, McLeish, Marrucci, Larson, Schieber, Oettinger, Rubinstein, and many others) call for similar advances in experimental observation of polymer dynamics. Comparison with experiments will serve in verifying or contradicting the wide range of theoretical predictions. Needed is a single platform that allows the direct comparison of experimental data with theoretical predictions.

Practical aspects are equally important. The understanding of a given polymer under applied conditions will allow optimization of processing, or it will allow definition of a meaningful window for the polymer's processing. Polymers need to be compared for specific applications. These are examples that require exploration of the viscoelasticity of the polymer as facilitated by IRIS.

For the experimentalist, the understanding of linear viscoelastic behavior has mostly advanced through the improvement of rheometer hardware and control. Detailed observations are now possible under well-controlled conditions. Experimental data are available in abundance. However, the analysis of the data has remained unsatisfactory. The main problems are the incompatibility of data from different instruments, the inconsistency between data, and the generation of artifacts during the analysis. Quite often the problem is the lack of time or the lack of trained personnel to perform the well-known (but tedious) procedures of data analysis. Answers need to be reached quickly. Data analysis is only effective if it provides comprehensive answers in a short time.

To overcome all these problems of unsatisfactory data analysis, we started to develop a computerized procedure that simplifies data input (based on a universal data

format in ASCII), and proceeds from there with interactive graphics. This sets the stage for the detailed rheological explorations of specific materials of interest.

We realize that advances are needed not only in the understanding of linear viscoelasticity but also in the large-strain non-linear behavior. However, for starters we had to limit ourselves to the linear response: the current IRIS is solely concerned with polymer dynamics in the linear range. The phenomenology of linear viscoelasticity is well established (Ferry, 1980) and most molecular dynamics theories make predictions of linear behavior even if their main emphasis is the large strain viscoelasticity. At this mature level of understanding, a comprehensive approach to data analysis can be assigned to a unifying algorithm on the computer.

On this basis we developed an all encompassing investigation of the viscoelastic properties of materials, an activity which we started to call 'dialog with viscoelasticity', a dialog between viscoelastic experiment and dynamics theory or the dialog of a researcher with the viscoelasticity of a specific material of interest. The data from mechanical spectroscopy are the starting position for this dialog. The language of this dialog is interactive graphics. Two rules guided us when designing the interactive graphics: We felt that it is essential (1) to create visual representation of rheological data in form of graphs for each step of the data analysis and (2) to give complete access to the original data as well as to the calculated number values. We adhered to these two rules very closely. This gives you the option of entering data from all kinds of sources and to export other media (spreadsheets, for instance). The result is an open forum of data exchange and comparison. It allows consistency checks between laboratories and within research groups thereby making rheology more interesting and reliable.

Effective use of the technical data, we felt, relies on two essential ingredients. These are a universal data format and a program which allows easy access to the data. Both are provided for by the IRIS program. It will be easy to communicate and exchange data throughout the rheology community, old data files and more recent ones. Data exchange is not only important for the rheological community but also for industry. Distributed branches within a large company, for instance, can use IRIS and communicate data very easily and, thus, make efficient use of the company's resources.

IRIS makes the rheologist's work more efficient by transforming laboratory results into a form that can also be communicated to the non-rheologist. A simple copy-and-paste action transfers the graphical results of IRIS to written reports and to audiovision. Graphs can be transferred, for example, to *MSWord* and *MSPowerpoint*. This presents the opportunity to broaden the public's understanding and appreciation of the value of the rheological research.

The main purpose of IRIS, obviously, is the rheological data analysis. A second, yet less developed function, is the viscoelastic modeling (comparison to rheological models; prediction of stress during start-up flows). The IRIS program provides convenience and rapid answers. We specifically looked for tools that could handle large amounts of rheological data from a variety of sources (various rheometers, plots in publications, e-mail communication, etc.) and then reach beyond the rheometry experiment, find patterns, compare data to the famous spectra of the literature, draw conclusions, predict the behavior of polymers in a range of kinematics, and communicate the results. Many of these tasks are covered with IRIS. However, the possibilities are endless and great potential exists for further expansion of the IRIS program which we need to explore to a larger extent.

New modules will be developed for entering polymer dynamics theory into IRIS. Theoretical predictions will be plotted side-by-side with the experimental observations.

The two main applications of IRIS are educational and professional. Iris is designed as interactive teaching tool for use in the class room and in teaching laboratories; however, it is equally well suited for the professional work of material scientists:

(1) *IRIS for Teaching* Using IRIS with a standard projector attached to the PC, the instructor enriches his/her teaching with interactive graphics in class. For example, the IRIS program allows you to perform time-temperature superposition in real time, to calculate the relaxation time spectrum immediately after that, and then to graph of all kinds of material functions. All of this is done within minutes so that teaching proceeds at normal pace. Predictions from analytical expressions (Rouse, Doi-Edwards, BSW) can be pulled in and graphed next to the data for comparison. In this way, the students directly

participate in the data processing and then can be asked to follow up with a reading assignment in the accompanying text. Teacher and student jointly explore the beauty and usefulness of linear viscoelasticity. Many variations are possible depending on topic and advancement of the class.

The program is designed so that students with minimal training are able shift and further evaluate experimental data by themselves. This 'hands-on' approach allows the student to get a feeling for rheological data, their analysis, and their application. The experiments become tangible and 'real'.

(2) *IRIS for the Professional* With IRIS, you can analyze and scrutinize rheological data from a wide range of rheometers, design effective experiments, determine the rheological parameters, and use these parameters for flow predictions of interest. The resulting data are the starting point for flow calculations (Polyflow modeling, for instance). The interactive graphics of IRIS visualize differences and common features of materials, detect systematic trends in the relaxation patterns (see for instance the study of Baumgärtel, Schausberger, and Winter, *Rheologica Acta* 29, 400, 1990), monitor phase transitions, or single out specific relaxation modes. Rheological data get scrutinized for inconsistencies (Winter, 1997). As inconsistencies in the data become apparent, methods can be devised to improve the rheometrical experiment. Large sections of IRIS are devoted to time-temperature superposition, conversion of dynamic data into relaxation time spectra, and linear viscoelastic modeling. Recent additions in IRIS compare these experimental findings with theoretical predictions for well defined classes of materials.

The main features of the IRIS dialog will be explored and discussed at the Faroe Island meeting.