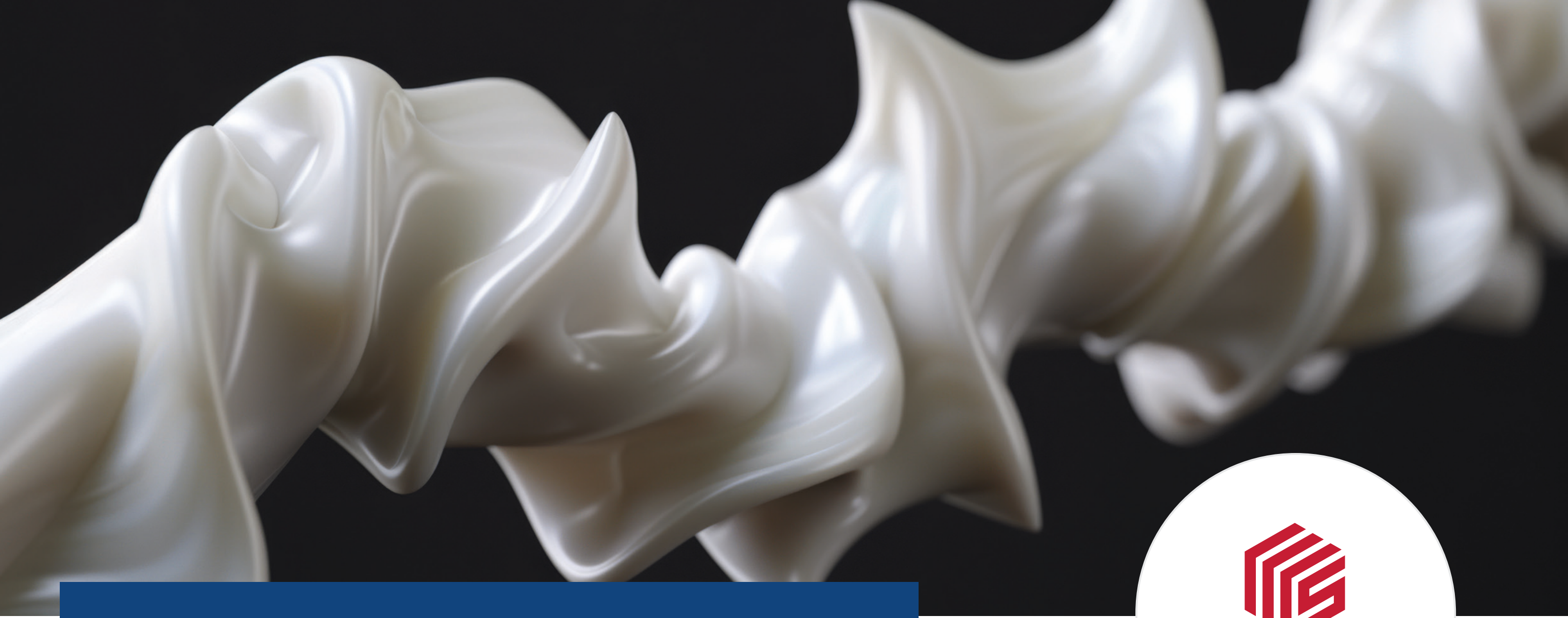

Innovative curve-fitting tool for viscoelastic materials introduced: Contributes to sustainability from a materials perspective

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Have you ever grappled with the non-linearity of materials? CYBERNET Multiscale.Sim is an analysis system that easily predicts the behaviour and physical properties of materials without needing to rely on actual tests. In past issues of Futurities, we introduced its ability to predict material behaviour using virtual material testing; this article introduces Multiscale.Sim's curve-fitting feature for predicting material constants for viscoelastic problems.

Introduction

Materials with a low environmental impact are increasingly being used. While there are clearly significant benefits in terms of sustainability, changing materials and maintaining product reliability is never easy. To make matters worse, these new materials are often highly non-linear and therefore difficult to manage in analysis. For example the thermosetting resins used traditionally generate microplastics that cause water pollution, so now reusable thermoplastics are favoured. However, their low melting temperature compared to other structural materials makes it impossible to design with them without considering the material's viscous behaviour.

In many generic CAE tools, a material's viscoelastic behaviour is represented by a material model that combines the generalized Maxwell model with a shift function, as shown in Fig. 1.

Since there are so many material constants, it is impractical to manually fit the material test data onto the material model. This article describes CYBERNET's new viscoelastic curve-fitting tool, that has recently been released as a feature of Multiscale.Sim, an Ansys Workbench add-on for multiscale analysis (see Fig. 2).

What is a curve fitting tool and why use one?

To account for non-linear material behaviour in an analysis, a material model is needed to represent the material behaviour. Material models in structural problems mainly express the relationship between stress and

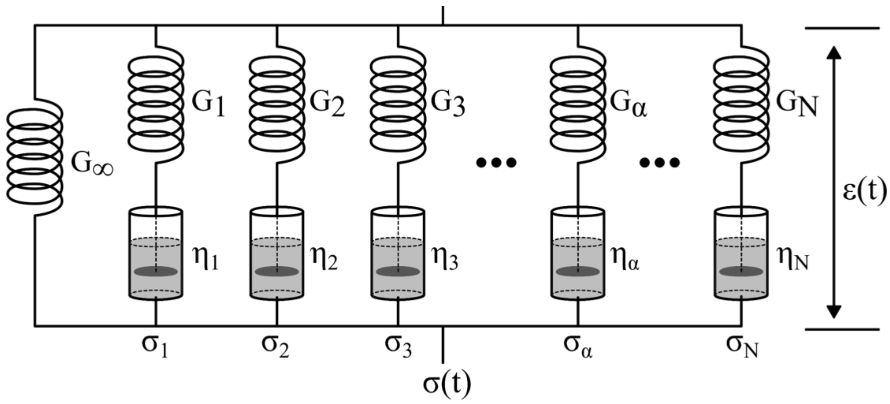

Fig. 1. Generalized Maxwell model to express viscoelastic material behaviour.

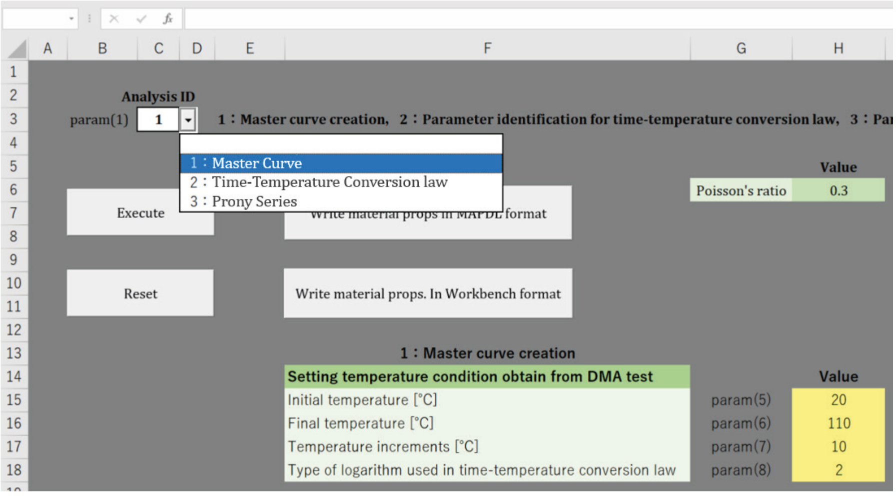

Fig. 2. Overview of curve-fitting tool for viscoelasticity, provided as an option in Multiscale.Sim.

strain in the form of a function with different coefficients (called material constants). These constants express the actual material-dependent behaviour.

In other words, to reflect the material behaviour in the analysis, it is necessary to observe the actual non-linear behaviour experimentally and then adjust the material constants to better fit the data. The curve fitting operation refers to the adjustment of this material constant.
CYBERNET developed the curve-fitting tool because many generic CAE tools do not have sufficient fitting capabilities for viscoelastic material models. The following three issues, specifically, affect both for accuracy and ease of use:

a. Raw data from the dynamic material analysis (DMA) study cannot be used

Existing viscoelastic curve-fitting functionalities, for instance in Ansys software, require experimental data on stress relaxation properties. This may seem natural since viscoelastic material models are formulated as a function of time. However, it is unrealistic to directly determine long-term stress relaxation behaviour through actual experiments because it requires accelerated testing at varying temperatures. Furthermore, frequency rather than time should be used as the arbitrability condition for quasi-static observations of a particular strain rate state. Tests conducted under these conditions are called dynamic mechanical analysis (DMA) tests. It should be possible to perform viscoelastic curve fitting based on raw DMA test data (details below).

b. Shift functions to express temperature dependence are not supported

The temperature dependence of viscoelastic material behaviour is represented by a shift function. Many tools do not provide a curve-fitting function to identify the constants that constitute this function. As a result, users have to deal with this manually or develop their own programs.

c. There is an upper limit on the number of Maxwell elements

Although stress relaxation properties can be obtained with some effort, the number of Maxwell elements can be limited when fitting properties to a curve. This can significantly reduce the expressive power of the material model.

The overall fitting process consists of three steps, as shown in Fig. 3. The next section introduces the functionality of the curve-fitting tool we developed to resolve these problems.

Step 1: Master curve creation

As previously mentioned, it is difficult to directly measure the long-term relaxation behaviour of viscoelastic materials, so their behaviour is typically measured with DMA tests that periodically vary the loads. Images of this test are shown in Fig. 4.

For materials with viscous behaviour, the phase difference between stress and strain is expressed by decomposing the stress into in-phase and out-of-phase components. These are called storage modulus E' and loss modulus E", respectively, and are defined as follows:

$$E' = \frac{|\sigma|}{|\varepsilon|}\cos\theta, \qquad E'' = \frac{|\sigma|}{|\varepsilon|}\sin\theta$$

The applicable frequency bands for DMA tests are also limited. Accelerated tests at varying temperatures are necessary to obtain characteristics over a wide frequency range. For thermorheologically simple

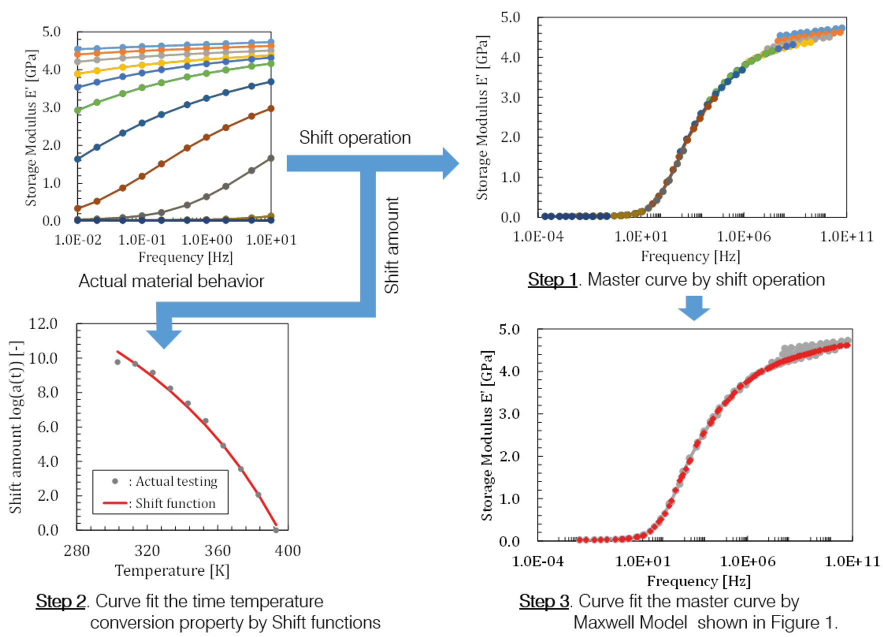

Fig. 3. Operational flow of the curve-fitting analysis to identify material constants.

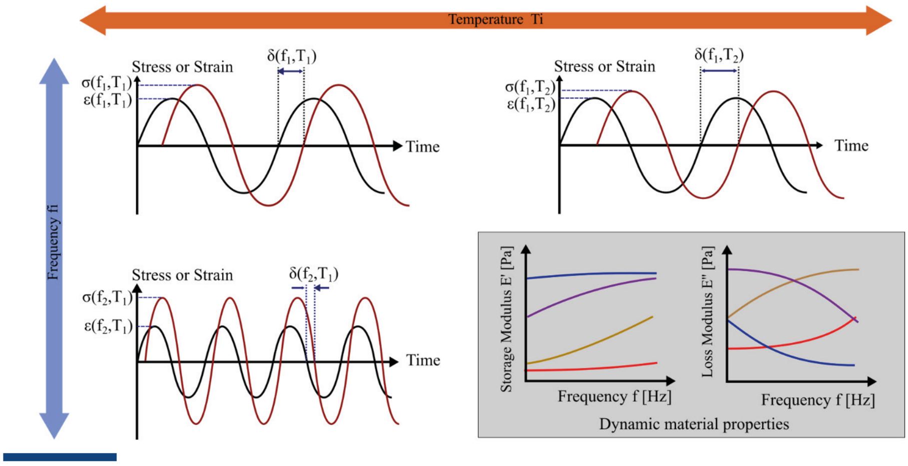

Fig. 4. Images of material testing by Dynamic Mechanical Analysis (DMA).

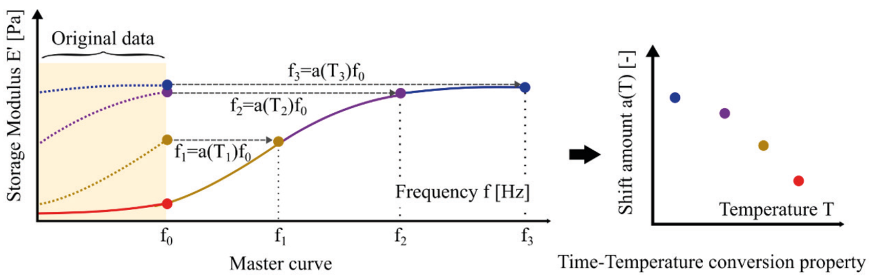

Fig. 5. Creating the master curve by performing a horizontal shift operation.

viscoelastic materials, temperature changes can be matched to changes in frequency (or time). This characteristic relates to the time-temperature conversion law and allows users to virtually obtain the behaviour of a material over a wide frequency range at a specific temperature by taking multiple temperature levels, even for limited frequency range tests. In Step 1 we obtain this characteristic.

The task of converting temperature to frequency corresponds to the operation of converting the frequency-dependent elasticity modulus along the horizontal axis, as shown in Fig. 5. This operation is performed for each temperature to generate a single connected, or master, curve (see Fig. 5). The curve-fitting tool automatically adjusts the amount of shift for each thermal elastic modulus to minimize deviation from the master curve.

Step 2: Master curve creation

The shift amount obtained in Step 1 must also be expressed as some kind of material model. This is called the shift function.

Ansys offers the Tool-Narayanaswamy and Williams-Landel-Ferry (WLF) equations. The former can only be used for analysis in the temperature range below or above the glass transition temperature (hereafter abbreviated as Tg). While WLF can represent the shift behaviour over a wide temperature range across Tg, it is a simple functional form and does not necessarily provide a good curve fit.

CYBERNET has developed Arrhenius- and polynomial-type shift functions in which the shift behaviour changes discontinuously after Tg. Fig. 6 shows examples of time-temperature conversion characteristics for epoxy and PMMA (polymethyl methacrylate) resins using three shift functions for curve fitting.

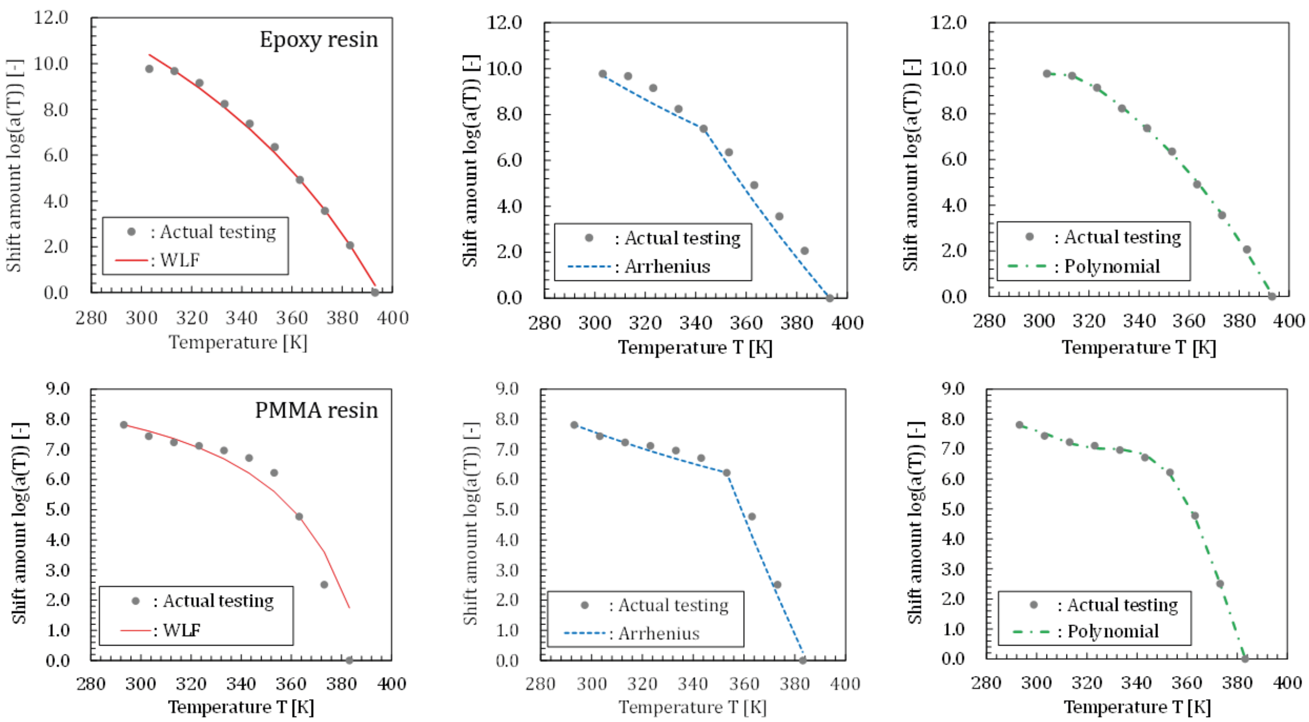

Fig. 6. Time-temperature conversion characteristics of epoxy and PMMA resins fitted using three different shift functions. Of these, Ansys only provides the WLF shift function.

If the properties change discontinuously after Tg, as with PMMA, reproducibility by WLF becomes poor especially near Tg. The polynomial form provides the most rigorous fitting of experimental data, but also allows overfitting for small experimental errors. The optimal shift function to use therefore depends on the type of resin.

Multiscale.Sim provides a rich set of shift functions and robust curve-fitting capabilities, allowing users to account for the temperature-dependent behaviour of different resins in their analyses in a simple and versatile way.

Step 3: Prony series identification

Finally, the master curve obtained by the shift function of the time-temperature conversion law is fitted according to a material model called the Prony series.

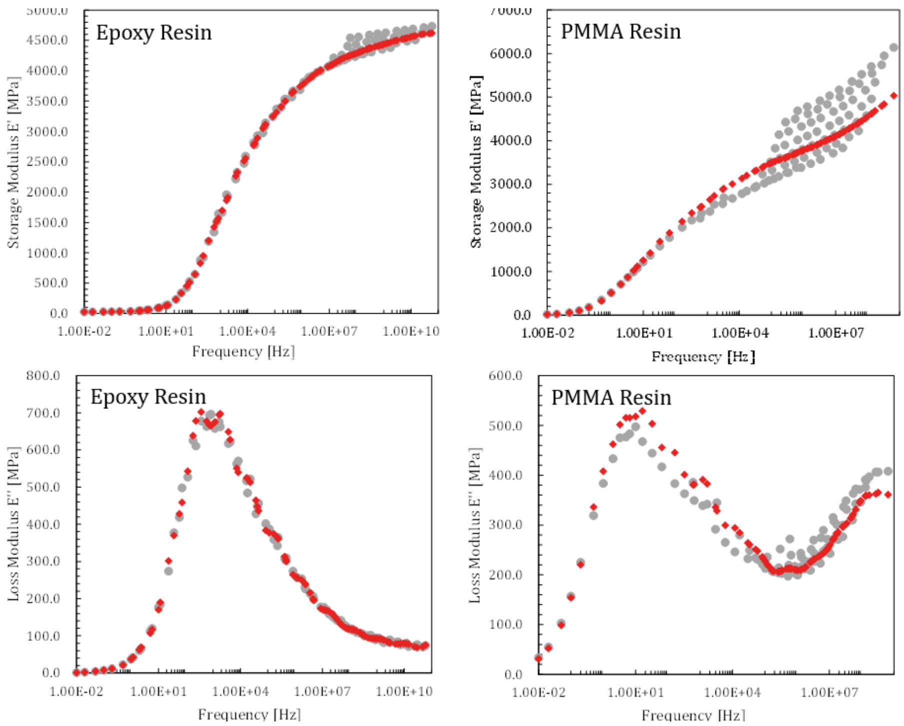

Fig. 7. Master curve-fitting results of the dynamic viscoelastic properties of epoxy and PMMA resins using the Prony series. Maxwell elements were set to 22.

Multiscale.Sim's tool allows the storage and loss modules obtained from DMA tests to be directly fitted rather than using the relaxation modules, with no limit on the number of Maxwell elements. This feature is very important because generic CAE tools incorporate errors associated with the conversion of dynamic viscoelastic properties into relaxation coefficients, and their limited number of Maxwell elements result in poor fitting capabilities.

Fig. 7 shows the master curve-fitting results for the epoxy and PMMA resins mentioned in the previous section. The PMMA resin is on the low temperature (high frequency) side; the test data for each temperature is not listed on the master curve.

This is because PMMA resin has a strong temperature dependency not only in viscous terms of the material properties, but also in elastic terms that shift toward the elastic modulus axis.

To accurately describe this phenomenon, we think it is necessary to introduce a new time-temperature conversion law. We have already built a material model for this purpose and plan to release it in a future version.

Conclusion

This article presented the curve-fitting tool for viscoelastic properties created by CYBERNET for its Multiscale.Sim tool. Compared to the same functionality offered by generic CAE tools such as Ansys, it has the following unique features:

- The master curve of temperature-dependent viscoelastic properties can be obtained automatically by applying the time-temperature conversion law.
- Three types of shift functions are provided to represent time-temperature conversion characteristics, allowing for a general adaptation of different shift behaviours for different materials.
- Fitting with the Prony series can be performed directly using the dynamic viscoelastic properties instead of the relaxation modulus. In this case, there is no upper limit to the number of Maxwell elements, so good fitting results can be obtained universally for resins with various characteristics.

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About CYBERNET

CYBERNET SYSTEMS CO. LTD. is a leading CAE company established in 1985, headquartered in Tokyo, Japan. Its corporate vision is "Creating a sustainable society and inspiring the world through technology and ideas". The company's goal is to solve the problems of its customers, who face increasingly diverse and complex technological issues every day, with technology and ideas that exceed their expectations, and to lead them to the next level of innovation.
CYBERNET is an Apex Channel Partner and a Technology Partner (Software) of Ansys. The company has been developing Multiscale.Sim since 2007 and it is being used by many customers in Japan and in other countries.
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