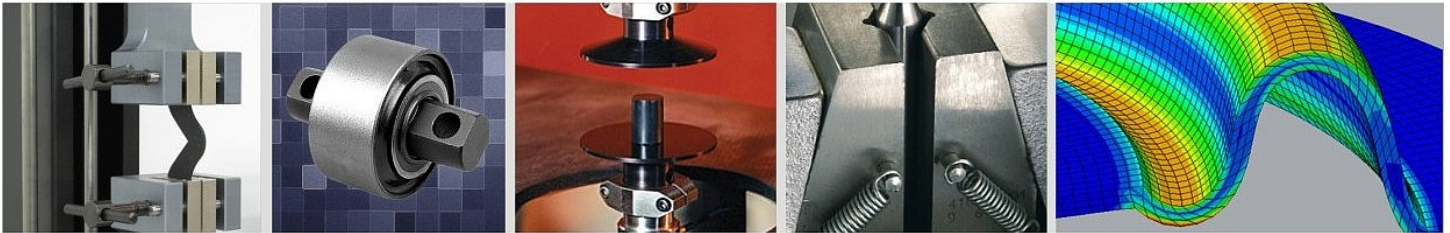


DESIGNING WITH POLYMERS: TOOLS AND PROCESS

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Finite element analysis (FEA) is a major CAE tool used for virtual product development in polymer engineering. The quality of the CAE carried out is directly related to the input material property and simulation technology.

Non-linear materials like polymers present a challenge to successfully obtain the required input data for FEA. In this paper we review the techniques and technology available to obtain the relevant data using existing methodologies for elastomeric materials and present information on how this can be improved for reliable simulations for rapid prototyping.

APPLICATION OF CAE TOOLS:

Predicting Stiffness: Establishing the correct stiffness for a component is an important specification requirement for the automotive and aerospace industry. It is preferred to “fine-tune” the stiffness of a part in all the three axes with the selected material before making the prototype.

Deformed Shapes: FEA and CFD can provide a deformed shape of the part with actual service conditions imposed on the part.

Durability Analysis: Based on the deformation and stress-strain distribution, relative durability analysis can be performed.

Life Prediction: With stress-strain information of a part from thermal aging, fatigue aging and unaged test data, one can develop an empirical estimate of service life of the part.

Identifying the “Hot Spots” of the Part:

Computational mechanics tools provide stress distribution of the part at various points. This information is helpful for identifying the stress “hot spots” in a particular design. This stress “hot spot” may be crack initiation point.

Mold Design: CFD and FEA can be used to design extruders, mixers, and other production equipment. Only low strain FEA is needed to optimize the mold design under the influence of a clamping force and internal pressures. By establishing the stress distribution throughout the mold, optimum design can be calculated for various zones in the mold.

Cure Simulation: CFD and FEA can be used to determine the temperatures in a molding process as a function to time. This transient thermal diffusion analysis needs input data such as thermal conductivity and thermal capacitance of the rubber as a function of temperature. Repeated FEA iterations can establish the optimum cure as a function of mold temperature and time.

Injection Molding: Similar to cure simulation, injection molding simulation by CFD and FEA is a transient process. The main purpose in examining injection molding is the characterization of apparent viscosity of the material with respect to shear rate and temperature. This type of analyses can check the positions of joint lines and accordingly adjust the position of the gates. CFD and FEA will allow the investigator to study the rates, temperatures, and compound formulations to avoid scorch and optimize the time for the injection cycle.

The application of computational mechanics analysis techniques to elastomers presents unique challenges in modeling the following characteristics:

1. The load-deflection behavior of an elastomer is markedly non-linear.
2. The recoverable strains can be as high 400 % making it imperative to use the large deflection theory.
3. The stress-strain characteristics are highly dependent on temperature and rate effects.
4. Elastomers are nearly incompressible.
5. Viscoelastic effects are significant.

FEA SUPPORT TESTING:

Most commercial FEA software packages use a curve-fitting procedure to generate the material constants for the selected material model. The input to the curve-fitting procedure is the stress-strain or stress-stretch data from the following physical tests:

1. Uniaxial tension test
2. Uniaxial compression test
3. Planar shear test
4. Equibiaxial tension test
5. Volumetric compression test

A minimum of one test data is necessary, however the greater the amount of test data, the better the quality of the material constants and the resulting simulation.

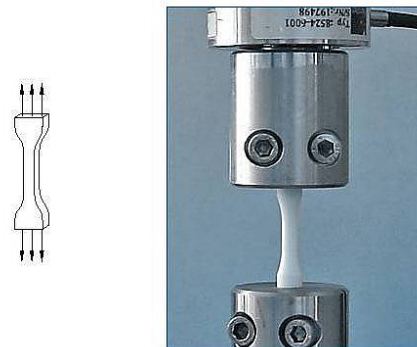


Figure 1

Testing should be carried out for the deformation modes the elastomer part may experience during its service life. The testing is carried out under a quasi-static process by carefully selecting the test parameters. The material can also be aged in a liquid or at elevated temperatures before testing and thus service conditions can be incorporated to generate the material constants and subsequent FE analysis. For applications involving very high strain rates a Hopkinson's bar can be used to test the materials and obtain the relevant stress-strain data.

A material model describing the elastomer as isotropic and hyperelastic is generally used and a strain energy density function (W) is used to describe the material behavior. The strain energy density functions are mainly derived using statistical mechanics, and continuum mechanics involving invariant and stretch based approaches.

Statistical Mechanics Approach:

The statistical mechanics approach is based on the assumption that the elastomeric material is made up of randomly oriented molecular chains.



Figure 2: Material Testing and FEA Examples

Invariant Based Continuum Mechanics Approach:

The Invariant based continuum mechanics approach is based on the assumption that for an isotropic, hyperelastic material the strain energy density function can be defined in terms of the invariants.

Stretch Based Continuum Mechanics Approach:

The Stretch based continuum mechanics approach is based on the assumption that the strain energy potential can be expressed as a function of the principal stretches rather than the invariants.

The choice of the material model depends heavily on the material and the stretch ratios (strains) to which it will be subjected during its service life. As a rule-of-thumb for small strains of approximately 100 %, simple models such as Mooney-Rivlin are sufficient.

For higher strains a higher order material model as the Ogden model may be required to successfully simulate the "upturn" or strengthening that can occur in some materials at higher strains.

THEORY OF VISCOMETRY:

The rheological analysis of samples is a fundamental part of developing rubber products. Whilst they still have their place, the use of melt flow indexers is being found to often give insufficient results. These simple devices do not match the versatility of modern rheometers, nor can they ensure that a new product will be suitable for use. A rheometer can actually measure sample properties at extremely low shear rates indicating the molecular weight, or the high shear rates seen in mixing, extrusion and molding. The rheometer can measure the viscosity of product at pre-programmed temperatures. This can also be used to evaluate the processability and degradation of materials at these temperatures.

Viscometry is probably the most common rheological technique and essentially defines the resistance of a fluid to flow. The equation for the coefficient of viscosity is:

$$\text{co-eff of viscosity} = \text{shear stress} / \text{shear rate}$$

The flow properties can be classified into two groups :

- Newtonian
- Non - Newtonian

Non-Newtonian materials such as non-drip paints have changing viscosities with different shear rates and should be characterized using controlled shear stress or controlled shear rate rheometers.

There are many types of non-Newtonian behavior but in broad terms they can be classified into one of the three following groups:

- Shear Thinning or Pseudoplastic
- Shear Thickening or Dilatant
- Plastic Shear Thinning (Yield Value)

Similar to material models used in FEA there are many mathematical models to describe the characteristic flow of a material including that described by the Bingham model;

$$\text{Shear stress} = \text{Yield stress} + K \times \text{Shear rate}$$

where, K is a constant.

Flowchart in Figure 3 shows the typical processes involved in a CFD simulation to model the extrusion process. The two major types of testing carried out is for testing the material viscosity vs. the shear rate and for material viscosity vs. temperature. Just as curve fitting of stress-strain data as a material model the viscosity vs. shear rate data is fitted to a material model and input into the software code.

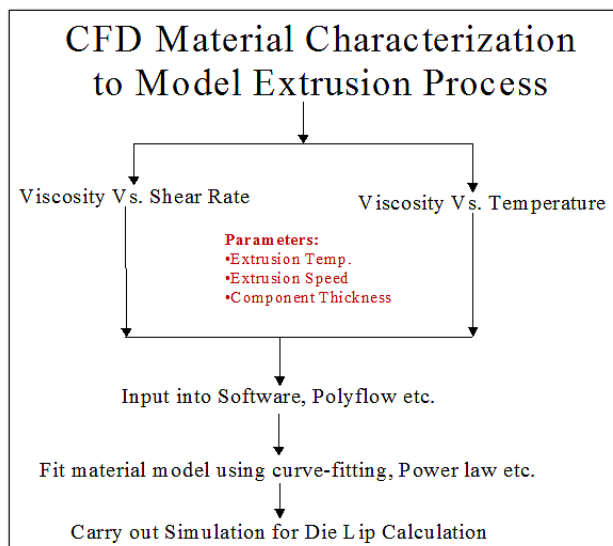


Figure 3: Flow Chart for Extrusion Simulation using CFD

The use of a particular type of rheometer is dictated by the type of test data needed for the simulation and different associated parameters. To model simulations at high extrusion speeds and temperature testing data is needed in the range of 20,000-30,000 sec⁻¹. Use of a capillary rheometer becomes necessary for such type of material characterization testing.

Summary: A brief review of material characterization testing methods for FEA and CFD simulation has been shown, limitations of the associated theory and instruments used in material characterization testing have been discussed. Studies have shown that CAE systems are not stand alone processes but require additional support procedures. Material characterization procedures for FEA and CFD have been presented and pitfalls reviewed. Input material properties are of prime importance for reliable CAE simulation. With better understanding of the testing procedure and associated theory, the quality of the simulation can be improved.

References:

1. ABAQUS Inc., ABAQUS: Theory and Reference Manuals, ABAQUS Inc., RI, 02
2. Attard, M.M., Finite Strain: Isotropic Hyperelasticity, International Journal of Solids and Structures, 2003
3. Bathe, K. J., Finite Element Procedures Prentice-Hall, NJ, 96
4. Bergstrom, J. S., and Boyce, M. C., Mechanical Behavior of Particle Filled Elastomers, Rubber Chemistry and Technology, Vol. 72, 2000
5. Bhowmick, A. K., Hall, M. M., and Benarey, H. A., Rubber Products Manufacturing Technology, Marcel Dekker, NY, 1994
6. Holden, G., Understanding Thermoplastic Elastomers, Hanser Gardner Publications, 1999
7. CD-Adapco, Star-CD Users Manual, CD-Adapco, 2004
8. Fluent, Fluent CFD users Manual, Fluent USA, 2004
9. Srinivas, K., Material And Rheological Characterization For Rapid Prototyping Of Elastomers Components, American Chemical Society, Rubber Division, 170th Technical Meeting, Cincinnati, October 2006