Implementation of a material model with shear rate and temperature dependent viscosity

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ABSTRACT:

A material model with shear rate and, optionally, temperature dependent viscosity was implemented. Shear rate dependence is expressed with a Yasuda function and temperature dependence with an Arrhenius function. The functions were fitted to viscosity data from oscillatory rheometry of polystyrene. Validation of the viscosity function in the material model was done with a single element with prescribed shear rate and temperature. Steady state results from a Newtonian simulation of plane Poiseuille flow with the implemented user material model were found to be identical to results from a simulation with LS-DYNA's MAT_NULL. Flow through a 4:1 contraction with shear rate dependent viscosity was simulated explicit and compressible as well as implicit and incompressible. Reasonable agreement was found for pressure loss, inlet force and outflow velocity.

Keywords:

Key words: Viscosity, shear rate, temperature, Cross, Carreau, Yasuda, Arrhenius, polymer melt

INTRODUCTION

The implementation of the user material model with variable viscosity, was carried out with the purpose of simulating polymer flow in LS-DYNA. In polymer flow, the viscosity often shows large variations due to shear thinning, cooling or heat dissipation. In LS-DYNA 971, the material models MAT_ELASTIC_WITH_VISCOSITY and MAT_ALE_VISCOUS are available, and they include temperature dependent and shear rate dependent viscosity, respectively. The ambition with the user material model was to take both shear and temperature dependency of a viscosity tensor into account. Simulations in LS-DYNA were compared to simulations in the computational fluid dynamics programme, FIDAP.

SHEAR RATE AND TEMPERATURE DEPENDENT VISCOSITY

In the user material model, the equations 1 to 8 are applied in the order of numbering. The user material model can only handle simulations with solid elements. The normal strain rates are calculated as:

$$\dot{\varepsilon}_{ii} = \frac{\Delta\varepsilon_{ii}}{\Delta t} \qquad \text{(Eq. 1)}$$

The stored shear strains, γ, are halved to deviatoric strains, ε, in calculation of deviatoric strain rate [1]:

$$\dot{\varepsilon}_{ij} = \frac{1}{2}\dot{\gamma}_{ij} = \frac{\Delta\gamma_{ij}}{2\Delta t} \qquad \text{(Eq. 2)}$$

The viscosity tensor is dependent on the shear rate, and on the temperature if it is specified, i.e. the absolute temperature is above 273K. Shear rate dependency of the viscosity is expressed with a *Yasuda* function, also known as a *generalised Cross/Carreau* function [2,3]:

$$\mu_{ij}(\dot{\gamma}_{ij}) = \mu_{\infty} + (\mu_0 - \mu_{\infty})(1 + (k\dot{\gamma}_{ij})^a)^{(n-1)/a} \qquad \text{(Eq. 3)}$$

μ_{∞} = lower limit for viscosity at infinite shear rate,

μ_0 = upper limit for viscosity at zero shear rate,

k = characteristic time,

a = material constant,

n = material constant.

The *Carreau* model is a special case of equation 3, where the parameter, *a,* is fixed at the value of 2 rather than fitted to the current material. Other special cases of the Yasuda function is *Cross*, where a=1-n, and *modified Carreau*, where a=1. If temperature dependence is included, it is expressed through the zero shear viscosity which is calculated from an Arrhenius expression, specifically known as the Arrhenius-Frenkel-Eyring formula [4]:

$$\mu_0(T) = A\exp\left(\frac{E_a}{RT}\right) \qquad \text{(Eq. 4)}$$

where

A = material constant,

E_a = activation energy,

R = universal gas constant,

T = temperature.

The function for temperature dependence of viscosity has some theoretical justification and is described as semi-empirical, where the functions for shear rate dependence must be considered empirical [4,5]. Bulk viscosity depends on the viscosity, here average normal viscosity, according to Stokes hypothesis:

$$\mu_B = -\frac{2}{3}\frac{\mu_{kk}}{3} \qquad \text{(Eq. 5)}$$

Bulk viscosity can often be neglected, and in the user material model the value of it can be held within specified limits or set to zero. The viscous stress tensor is determined as:

$$\tau_{ij} = 2\mu_{ij}\dot{\varepsilon}_{ij} - \mu_B\dot{\varepsilon}_{kk}\delta_{ij} \qquad \text{(Eq. 6)}$$

Pressure is calculated from the hydrostatic stress from the previous time step and the volume strain increment from the current time step:

$$p = \frac{-\sigma_{kk}}{3} - B\varepsilon_{kk} \qquad \text{(Eq. 7)}$$

Total stress tensor:

$$\sigma_{ij} = \tau_{ij} - p\delta_{ij} \qquad \text{(Eq. 8)}$$

where

δ_{ij} = Kronecker delta,

Δt = time step,

B = bulk modulus.

MATERIAL DATA

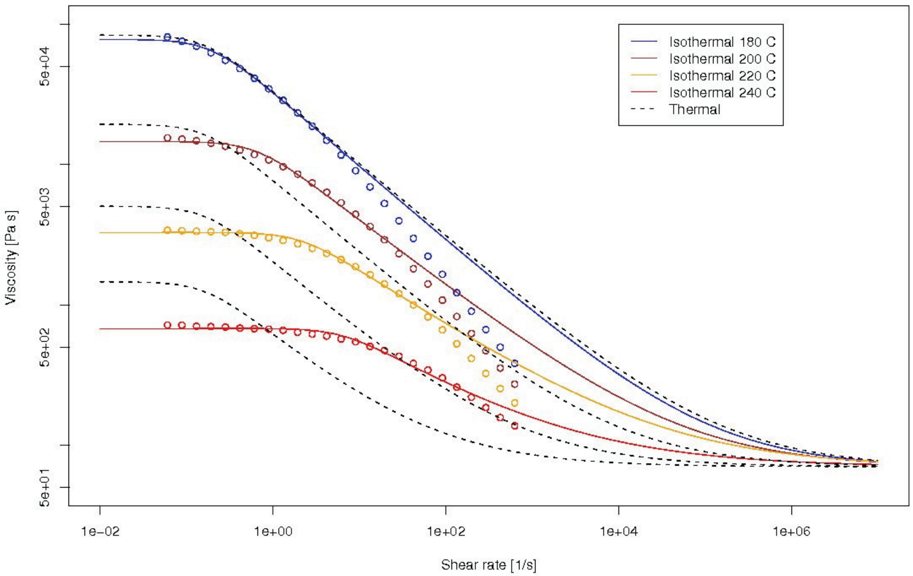

Figure 1: Measured viscosities and fitted functions.

Complex viscosity as a function of angular frequency was measured at four temperatures with a cone and plate viscometer, where the empirical Cox-Merz rule states that this can be assumed to be equal to viscosity as function of shear rate [2,4].

Simulations with the user material model in LS-DYNA were compared to simulations in FIDAP, which holds the material parameter, *a*, from equation 3 fixed at 2. To allow these comparisons, the parameter was fixed at 2 in LS-DYNA simulations as well. An isothermal function was fitted to the measurements at each of the four temperatures, and one function with thermal dependency was fitted to the complete data set, as it is shown in figure 1. For all functions, the lower viscosity limit at infinite shear rate was preset at 70 Pa s. The shear rate interval of the measurements covered the shear rates experienced in the simulations.

Table 1: Parameters for viscosity functions for polystyrene; Polystyrol 158 K from BASF.

	Thermal	180°C	200°C	220°C	240°C
μ_0 [Pa s]	-	7.82E+4	1.46E+4	3.28E+3	679
A [Pa s]	7.56E-11	-	-	-	-
k [s]	5.96	5.18	1.55	0.480	-0.160
n [-]	0.482	0.471	0.526	0.594	0.617
Ea [J/mole]	1.30E+05	-	-	-	-

The characteristic time for the material, *k*, assumes a negative and non-physical value for the isothermal function at 240°C, but the fitted value serves the purpose in this case.

VALIDATION OF THE MATERIAL MODEL

Plane Poiseuille flow, with the mesh shown in figure 2, driven by a parabolic velocity profile, was simulated with a constant viscosity in order to validate the Newtonian part of the material model.

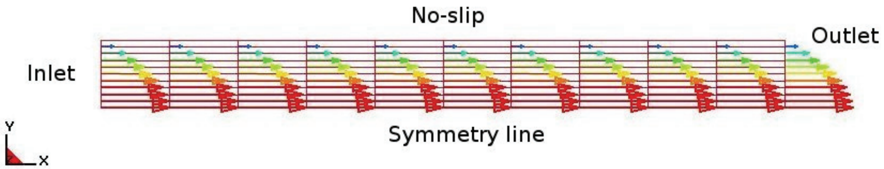

Figure 2: Mesh for simulation of plane Poiseuille flow.

When simulated with a Newtonian user material model and with MAT_NULL, where equal viscosities and equal bulk modules were given, the steady state pressure and the node velocities were equal to four significant digits.

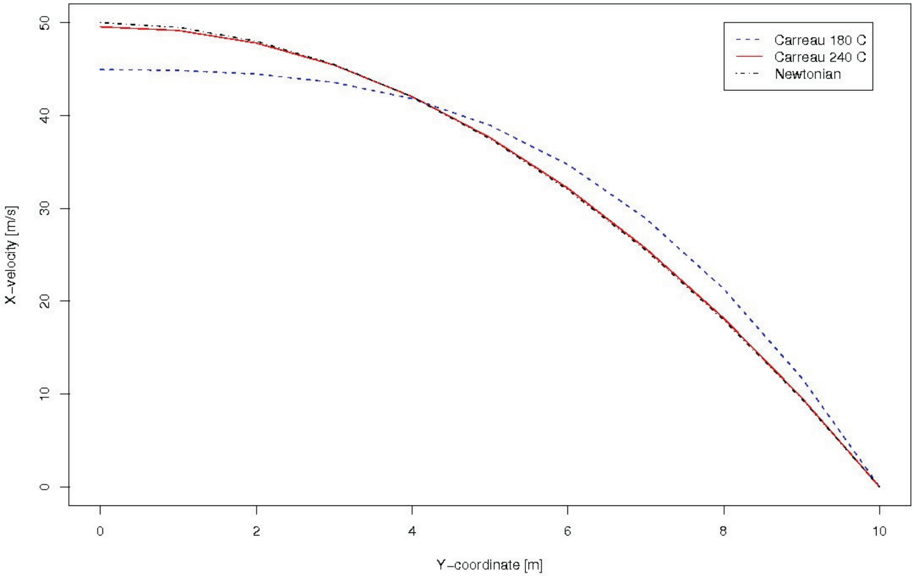

Figure 3: X-velocity at the mesh outlet as function of y-coordinate.

Figure 3 serves as an illustration of shear thinning occurring in simulations with the thermal Carreau function at different prescribed temperatures. The x-velocities at the outlet are plotted as function of y-coordinate, i.e. distance from the symmetry line. The velocity profile for 240°C is close to the Newtonian parabola. At 180°C, the effect of shear thinning is visible on the velocity profile; approaching the no-slip wall at y = 10, the velocity is larger than the Newtonian due to shear thinning. This agrees with the thermal function in figure 1, where the shear thinning decreases with temperature.

The shear thinning and temperature dependence of the viscosity was validated by simulation of plane Couette flow in a single element model with a known shear rate and temperature development.

COMPRESSIBLE AND INCOMPRESSIBLE SIMULATION OF A 4:1 CONTRACTION WITH CARREAU-VISCOSITY

A plane 4:1 contraction was simulated as explicit and compressible in LS-DYNA 971 and as steady state, implicit and incompressible in the computational fluid dynamics programme FIDAP 8.7.0 from Fluent Inc. These two different programmes were employed in order to validate the material model in more complex flows. Simulations in FIDAP were done with incompressible material to reduce computation times. The FIDAP mesh was 2 dimensional and the LS-DYNA mesh had solid elements, as specified by the user material model, with plane strain prescribed to emulate a 2-dimensional simulation. But in the xy-plane the meshes were identical.

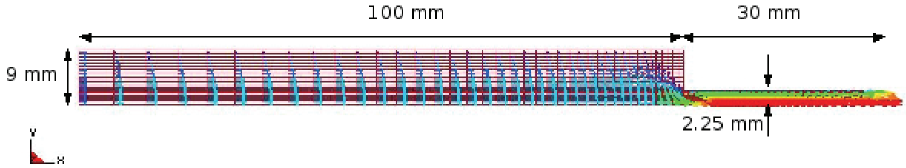

Figure 4: The mesh for 4:1 contraction.

The mesh with steady state velocity vectors is shown in figure 4. No-slip conditions were specified at the three upper edges. The left side edge is the inlet where the flow was driven by a velocity of 1.67 mm/s. Y-velocity is set to zero at the symmetry line at the lower edge. The outlet is the right edge of the nozzle. In both simulations, the viscosity was modelled by isothermal Carreau functions. Bulk viscosity in LS-DYNA had no effect on time to steady state flow, but it significantly increased computation times, wherefore it was set to zero. To reduce computation time further, 10 times mass scaling was applied. Quantitative comparison of the simulations were done through the steady state values of pressure drop over the nozzle, maximum outflow velocity and inlet force. The differences between these values for a scaled and an unscaled simulation were below 1%.

The pressure drop over the nozzle along the symmetry line is plotted in figure 5, where there is a decrease with temperature because of the lower viscosity. Deviations between pressure drops from simulations in FIDAP and LS-DYNA are all below 10%. The total forces at the inlet decrease with temperature as well, and in LS-DYNA they were, for the lowest temperatures first: 15 N, 6.2 N, 2.5 N and 0.72 N. The total forces from FIDAP deviated no more than 10%. The agreement between the results for both pressure drop and inlet force is considered satisfactory.

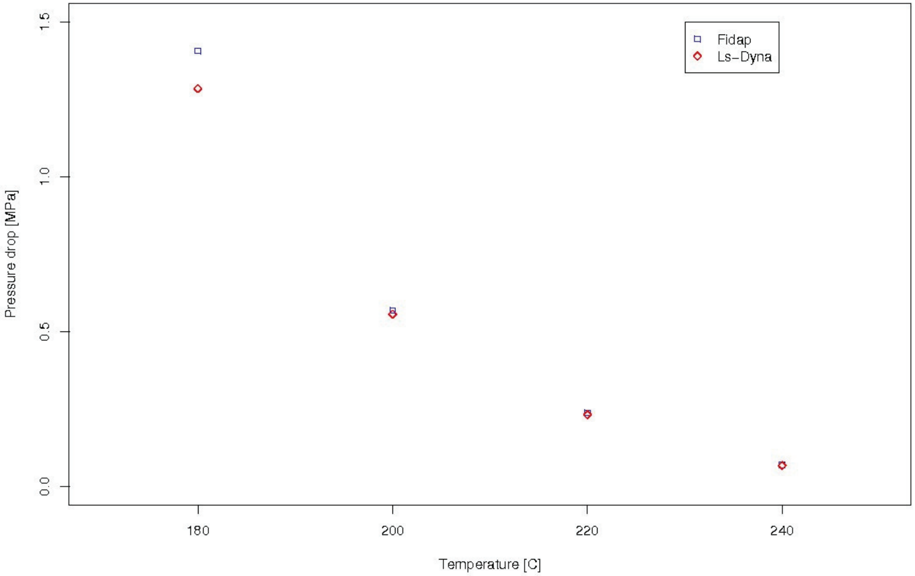

Figure 5: The pressure drops at different temperatures.

Figure 6 shows the outlet x-velocity at the symmetry line, which corresponds to the maximum velocity at the outflow. The increase with temperature of the outlet x-velocity on the symmetry line can be explained by reduced shear thinning which gives a velocity profile closer to a parabola. This is illustrated in figure 3. The deviations between x-velocities from LS-DYNA and FIDAP are for 180°C, 200°C, 220°C and 240°C equal to 24%, 5%, 5% and 4%, respectively. Apart from the simulation at 180°C, where deviation somehow mounts to five times that of other the temperatures, is the agreement acceptable.

The computation times for the implicit steady state simulations were less than a minute with a 32 bit Pentium 4 2.5 GHz processor. For the explicit simulations, the computation times to steady state were longer than two hours on two 64 bit AMD Opteron 2.6 GHz processors with time steps around 7E-6 s.

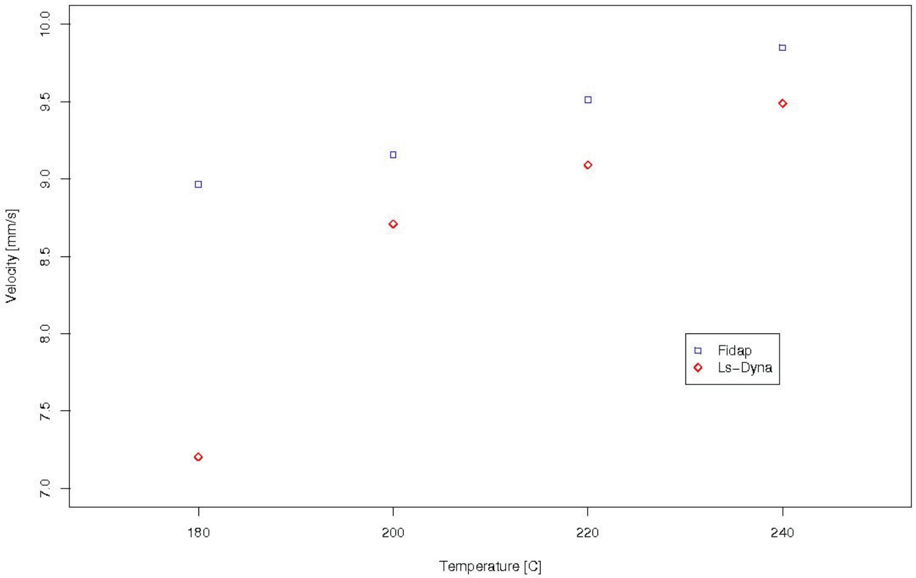

Figure 6: The outlet x-velocities at the symmetry line.

SUMMARY AND CONCLUSIONS

A material model for compressible fluids with a shear rate and temperature dependent viscosity tensor has been implemented.

Data for the viscosity of commercial polystyrene at different shear rates and temperatures were gathered from oscillatory rheometry. A Carreau expression described viscosity as a function of shear rate, when the temperature was constant, and a Carreau expression combined with an Arrhenius function described viscosity from both shear rate and temperature.

Validation of the model has been done on a single element with a prescribed shear rate and temperature course. Simulation of plane Poiseuille flow gave identical results compared to the LS-DYNA material model MAT_NULL.

Flow through a 4:1 contraction was simulated explicit-compressible and implicit-incompressible. Good agreement was found for pressure loss, and the total force at the inlet. For three of the four temperatures, there was good agreement between the maximum outlet velocities as well. However, some deviations must be expected between results from these two widely different simulations. But for practical use, the long computation times, even for models of moderate size, may be a problem.

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