Implementation of a Material Model with Shear Rate and Temperature Dependent Viscosity

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Implementation of a material model with shear rate and temperature dependent viscosity:
Keyword file and FORTRAN code

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Abstract
A user defined material with shear rate and, optionally, temperature dependent viscosity was implemented and validated in reference [1] from 6th European LS-DYNA Users’ Conference, copyright © by Engineering Research AB (ERAB AB). Shear rate dependence was expressed with a Yasuda function and temperature dependence with an Arrhenius function. This document describes the keyword data blocks and the FORTRAN code for the user material model.

1 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.

2 Viscosity, shear rate and temperature
In the user defined material, the equations 1 to 8 are applied in the order of numbering. The normal strain rates are calculated as:

$$\dot{\varepsilon}_{ii} = \frac{\Delta \varepsilon_{ii}}{\Delta t}$$  (1)
The stored shear strains, $\gamma$, are halved to deviatoric strains, $\varepsilon$, in calculation of deviatoric strain rate [2]:

$$\dot{\varepsilon}_{ij} = \frac{1}{2} \dot{\gamma}_{ij} = \frac{\Delta \gamma_{ij}}{2\Delta t}$$  \hspace{1cm} (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 [3, 4]:

$$\mu_{ij}(\dot{\gamma}_{ij}) = \mu_\infty + (\mu_0 - \mu_\infty)(1 + (k \dot{\gamma}_{ij})^a)^{(n-1)/a}$$  \hspace{1cm} (3)

where

- $\mu_\infty$ = lower limit for viscosity at infinite shear rate,
- $\mu_0$ = upper limit for viscosity at zero shear rate,
- $k$ = characteristic time,
- $a, n$ = material constants.

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 [5]:

$$\mu_0(T) = A \exp \left( \frac{E_a}{RT} \right)$$  \hspace{1cm} (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 [5, 6]. Bulk viscosity depends on the viscosity, here average normal viscosity, according to Stokes hypothesis:

$$\mu_B = -\frac{2}{3} \frac{\mu_{kk}}{3}$$  \hspace{1cm} (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:

$$\tau_{ij} = 2\mu_{ij} \dot{\varepsilon}_{ij} - \mu_B \dot{\varepsilon}_{kk} \delta_{ij}$$  \hspace{1cm} (6)

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

$$p = -\frac{\sigma_{kk}}{3} - B \varepsilon_{kk}$$  \hspace{1cm} (7)
Total stress tensor:

\[ \sigma_{ij} = \tau_{ij} - p \delta_{ij} \]  \hspace{1cm} (8)

where
\[ \delta_{ij} = \text{Kronecker delta}, \]
\[ \Delta t = \text{time step}, \]
\[ B = \text{bulk modulus}. \]

3 Key input blocks

Bulk modulus, \( B \), is calculated from Young’s modulus, \( E \), and Poisson’s ratio, \( \nu \) from the relation; \( B = E/(3(1-2\nu)) \). Likewise shear modulus, \( G \), is determined; \( G = E/(2(1+\nu)) \). In the material data shown here, density has been scaled to reduce computation times.

- \( \rho \) = density,
- Young = Young’s modulus,
- Poisson = Poisson’s ratio,
- BULKMOD = bulk modulus,
- SHEARMOD = shear modulus,
- BULKVISC = bulk viscosity,
- CHTIME = \( k \) in equation 3,
- N-EXP = \( n \) in equation 3,
- A-EXP = \( a \) in equation 3,
- MUNINF = \( \mu_{\infty} \) in equation 3,
- MU0 = \( \mu_0 \) in equation 3,
- \( A \) = \( A \) in equation 4,
- ACT-E = \( E_a \) in equation 4,
- MUMAX = upper numerical limit for viscosity,
- BULKVMIN = lower numerical limit for bulk viscosity.

3.1 Isothermal

In an isothermal simulation, the viscosity is calculated with equation 3 with the units \( mm \) and \( MPa \). The data shown in the input block below is for polystyrene at 453 K written according the specifications in reference [3].

```plaintext
*MAT_USER_DEFINED_MATERIAL_MODELS
$ MID 105 43 16 50 0 3 4
$ IVECT 1 0 0 1 1
$ YOUNG 2.4E+03 0.3 2.0E+03 9.23E+02
$ BULKMOD 1E-05 43 43 16 50 0 3 4
$ SHEARMOD 2.4e3 0.3 2.0e3 9.23e2
$ CHTIME 5.18E+000 4.71E-001 2.70E-005 7.82e-002 7.82E-002 0

3
```
3.2 Thermal

In a thermal simulation the viscosity is calculated with equation 4 inserted in equation 3 with the units \( m \) and \( Pa \). The data shown in the input block below is for polystyrene with a temperature from 453 K to 531 K.

```
*MAT_USER_DEFINED_MATERIAL_MODELS
$ MID R0 MT LMC NRV IORTH0 IMLK IG
  1 1e+05 43 16 50 0 3 4
$ IVECT IFAIL ITERM IHYPER IES5
  1 0 1 1
$ YOUNG POISSON BULKMOD SHEARMOD
$ [Pa] [-] [Pa] [Pa]
  2.4e9 0.3 2.0e9 9.23e8
$ CHTIME N-EXP A-EXP MUINF A ACT-E MUMAX BULKVMIN
$ [s] [-] [-] [Pa] [s] [J/mol] [Pa s] [Pa s] [Pa s]
  5.968778 .4815149 2 70 7.573e-11 1.305e+05 7.82e+04 -5.21e+04
```

4 FORTRAN code

The user material model can only handle simulations with solid elements. Here the subroutine added to the FORTRAN file supplied by LSTC, dyn21.f, is printed:

```fortran
C*******************************************************************************
  subroutine umat43 (cm, eps, sig, epsp, hsv, dt1, capa, etype, tt,
    temper, fail, lcrv)
C*******************************************************************************
c  cm(3)=BULKMOD
  cm(09)= CHARTIME
  cm(10)= N-EXP
  cm(11)= A-EXP
  cm(12)= MUINF
  cm(13)= MU0 (isothermal) or A (thermal)
  cm(14)= ACT-E
  cm(15)= MUMAX
  cm(16)= BULKVMIN
  
c  eps(1)=local x strain increment
  eps(2)=local y strain increment
  eps(3)=local z strain increment
  eps(4)=local xy strain increment
  eps(5)=local yz strain increment
  eps(6)=local zx strain increment
  
c  sig(1)=total x stress
  sig(2)=total y stress
  sig(3)=total z stress
```
c sig(4)=total xy stress
c sig(5)=total yz stress
c sig(6)=total zx stress
c
dt1=current time step size
c tt=current problem time
c temper=current temperature
c
c hsv(16..21) = srg(mvi): Shear strain rate gradient
 c hsv(22..27) = mu(mvi): Viscosity
c hsv(28..33) = dst(mvi): Deviatoric stress tensor
c hsv(34) = phyd: Pressure
c hsv(35..40) = sig(mvi): Total stress tensor
c
include 'iounits.inc'
character*5 etype
dimension cm(*),eps(*),sig(*),hsv(*),crv(101,2,*)
real dt1,temper,temp
logical failel
c Local declacrations
dimension sg(6), srg(6), dst(6)
real Rgas, mu(6), mub, phyd
integer kron, mvi
c Gas constant [J/(K*mol)]
Rgas = 8.314510

c Normal strain rate vector
do 20 mvi=1,3
   if(dt1.le.0.or.eps(mvi).eq.0) then
      srg(mvi) = 0
   else
      srg(mvi) = eps(mvi)/dt1
   endif
   hsv(15+mvi)=srg(mvi)
20 continue
c
c Deviatoric strain rate vector
do 25 mvi=4,6
   if(dt1.le.0.or.eps(mvi).eq.0) then
      srg(mvi) = 0
   else
      srg(mvi) = 0.5 * eps(mvi)/dt1
   endif
   hsv(15+mvi)=srg(mvi)
25 continue
Viscosity vector

do 30 mvi=1,6

c  thermal
  if (temper.ge.273) then
    mu(mvi) = cm(12) +
    1 ( cm(13) * exp(cm(14)/(Rgas * temper)) - cm(12) ) /
    2 ( 1.0 + (cm(09) * abs(2*srg(mvi))) **cm(11) )
    3 **((1-cm(10))/cm(11))
  else
    mu(mvi) = cm(12) +
    1 ( cm(13) - cm(12) ) /
    2 ( 1.0 + (cm(09) * abs(2*srg(mvi))) **cm(11) )
    3 **((1-cm(10))/cm(11))
  endif
  if (mu(mvi).gt.cm(15)) then
    mu(mvi) = cm(15)
  endif
  hsv(21+mvi)=mu(mvi)
30 continue

c  isothermal
else
  mu(mvi) = cm(12) +
  1 ( cm(13) - cm(12) ) /
  2 ( 1.0 + (cm(09) * abs(2*srg(mvi))) **cm(11) )
  3 **((1-cm(10))/cm(11))
endif
  if (mu(mvi).gt.cm(15)) then
    mu(mvi) = cm(15)
  endif
  hsv(21+mvi)=mu(mvi)

c  Bulk viscosity
mub = - 2.0/3.0 * (mu(1) + mu(2) + mu(3))/3.0
if (mub.lt.cm(16)) then
  mub = cm(16)
endif

c  Deviatoric stress vector

do 40 mvi=1,6
  if (mvi.le.3) then
    kron=1
  else
    kron=0
  endif
  dst(mvi) = 2 * mu(mvi) * srg(mvi) -
  1 mub * (srg(1) + srg(2) + srg(3)) * kron
  hsv(27+mvi)=dst(mvi)
40 continue

c  Pressure scalar
phyd = -(sig(1) + sig(2) + sig(3))/3 -
  1 cm(3) * (eps(1) + eps(2) + eps(3))
  hsv(34)=phyd

c  Total stress vector

do 70 mvi=1,6

if (mvi.le.3) then
kron=1
else
kron=0
endif

sig(mvi) = - phyd * kron + dst(mvi)

hsv(34+mvi)=sig(mvi)

70 continue

c
return
end

dyn21.f with the subroutine printed above, umat 43, was compiled with Intel FORTRAN compiler.

5 Summary

With the purpose of modelling molten polymers, a user defined material was programmed with a viscosity depending on shear rate by and on temperature. The FORTRAN code was added to the file from LSTC and compiled to a version of LS-DYNA, where the material data was set in input blocks in a keyword file.

References


