



Sandia National Laboratories

Operated for the U.S. Department of Energy by

Sandia Corporation

Albuquerque, New Mexico 87185

date: March 4, 2015

to: Distribution

from: Kevin N. Long (1554), Kurtis R. Ford (1526), and William Scherzinger (1554)

subject: Modeling a Newtonian Fluid with a Rate-Dependent, Von Mises Plasticity Model for Solid Mechanics Applications

Executive Summary

This memo derives a particular use of a rate-dependent, perfectly plastic Von Mises Plasticity constitutive model that represents a Newtonian (or Bingham) fluid. Only two parameters are needed: the viscosity and bulk modulus to complete the model parameterization. Under certain deformations, the model exactly represents a Newtonian fluid. Under others, the model shear thins. A Newtonian fluid representation may be used in confined flow applications in which a fluid-solid interaction is desired but code coupling is not.

Contents

1	Introduction	2
2	Rate Dependent Constitutive Model Theory	3
3	Model Behavior under Pure Shear Conditions	4
4	Model Behavior Under Simple Shear Conditions	4
5	Simple Shear Example	7
6	Sierra Solid Mechanics Input Syntax Example	10
7	Summary	11
	References	11

Figures

1	Simple Shear Normalized Shear Stress vs. Associated Deviatoric Rate of Deformation Component	7
2	Simple Shear Normalized Shear Stress and Viscosity	8
3	Simple Shear Normalized Viscosity vs. Log Shear Deformation Parameter	8

1 Introduction

On occasion, analysts need to represent confined fluid flow behavior in components. The usual approach is to use a nearly incompressible elastic material that essentially has no shear resistance. While this formalism may be satisfactory in some applications, it is poor if the fluid stresses exerted on surrounding materials are desired. In this memo, we present an alternative approach that uses a rate dependent J_2 (Von Mises) plasticity model which produces Newtonian Fluid-like behavior under certain conditions, and we provide an example on how to calibrate it.

First, let us define the shear stress response of a Newtonian fluid,

$$\text{dev}\boldsymbol{\sigma} = 2\eta \text{dev}\boldsymbol{d}, \quad (1)$$

wherein $\boldsymbol{\sigma}$ is the Cauchy stress, \boldsymbol{d} is the spatial rate of deformation (symmetric part of the spatial velocity gradient), η is the viscosity, and “dev” denotes a deviatoric operator (see reference [2]). The viscosity is constant for a Newtonian fluid. Notice that the deviatoric Cauchy stress is proportional to the shear strain *rate*, and not the shear strain, as it would be for an elastic material. Thus, for a constant shear strain rate (deviatoric rate of deformation), the deviatoric part of the Cauchy stress is *constant*. In contrast, consider a linear elastic isotropic constitutive response:

$$\text{dev}\boldsymbol{\sigma} = 2\mu \text{dev}\boldsymbol{\epsilon}, \quad (2)$$

where μ is the shear modulus and $\boldsymbol{\epsilon}$ is the small strain tensor. In the small strain limit, where we can ignore objectivity of the stress rate, an isotropic linear elastic solid responds to a constant deviatoric strain rate with a constant rate of increase of the deviatoric stress response such as:

$$\text{dev}\dot{\boldsymbol{\sigma}} = 2\mu \text{dev}\dot{\boldsymbol{\epsilon}}., \quad (3)$$

Clearly, Equation 3 is not equivalent to Equation 1 even in the small deformation limit. Therefore, an elastic solid can never represent a Newtonian fluid.

However, qualitatively, plastic flow resembles fluid flow. We shall show that we can more accurately approximate a Newtonian fluid with the proper choice of a rate dependent Von Mises plasticity constitutive model. We will consider an isotropic perfectly plastic model using a hyperelastic formulation (due to its theoretical simplicity) for this work compared with hypoelastic formulations built into the LAME constitutive model library (see [4]). In this memo, isotropic J_2 plasticity is considered under perfectly plastic (zero hardening) conditions. The rate dependence is chosen to give a constant viscosity.

2 Rate Dependent Constitutive Model Theory

First, we discuss the hyperelastic-plastic formulation in which the deformation gradient is multiplicatively split into elastic and plastic parts. We develop a rate dependent form that extends a standard form in the literature (see for example [3]). The deformation gradient is split as:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p. \quad (4)$$

The elastic response is determined by the elastic left Cauchy-Green deformation tensor through the following constitutive function written in terms of the Kirchoff stress:

$$\mathbf{b}^e = \mathbf{F}^e \mathbf{F}^{eT}, \quad (5)$$

$$\boldsymbol{\tau} = \frac{\kappa}{2}(J_e - J_e^{-1})\mathbf{1} + \mu \text{dev}(\bar{\mathbf{b}}^e), \quad (6)$$

where $J_e = \det \mathbf{F}^e = \det \mathbf{F}$ under isochoric plastic flow conditions such as occurs in a Newtonian fluid motion. Here, κ is the initial bulk modulus and μ is the initial shear modulus. This response linearizes to an isotropic linear elastic model in the small deformation limit. Finally, $\bar{\mathbf{b}}^e$ is the unimodular part of \mathbf{b}^e given by,

$$\bar{\mathbf{b}}^e = J_e^{-\frac{2}{3}} \mathbf{b}^e. \quad (7)$$

The elastic state is bounded by the yield condition, which for an isotropic perfectly plastic rate dependent form may be given by:

$$\phi = \sqrt{3}J_2 - R\tau_Y \leq 0, \quad (8)$$

wherein τ_Y is the initial yield strength in uniaxial tension/compression for a rate coefficient, R , of 1. In Equation 8, J_2 is the second invariant of the deviatoric part of the Kirchoff stress defined as:

$$J_2 = \sqrt{\frac{1}{2} \text{dev} \boldsymbol{\tau} : \text{dev} \boldsymbol{\tau}}, \quad (9)$$

such that $\sqrt{3}J_2$ is the Von Mises Stress invariant of the Kirchoff stress. The form of the yield condition in Equation 8 is consistent with the `RATE_PLASTICITY` model used in this analysis. The rate coefficient, R , is a user-specified function of the deviatoric rate of deformation,

$$R = R[\dot{\boldsymbol{\varepsilon}}] \quad \text{where} \quad \dot{\boldsymbol{\varepsilon}} = \sqrt{\frac{2}{3} \text{dev} \mathbf{d} : \text{dev} \mathbf{d}} \quad (10)$$

Under perfectly plastic conditions, the yield strength changes only through the rate coefficient R , and so we anticipate that by setting the form of R appropriately, we can represent the desired behavior.

Note that because the shear modulus must be specified, there will always be an elastic strain regime, the size of which depends on the ratio of the yield strength to the shear modulus. It may be desirable, as in the case of thermoplastics near melt [1], to have a relatively large elastic regime to represent a bingham fluid. Other than making the shear modulus and yield strength comparable in magnitude, no adjustments to the model formulation are required to represent such behavior. However, we will focus on Newtonian fluid behavior for the rest of this memo.

3 Model Behavior under Pure Shear Conditions

First, we consider the constitutive response under pure shear conditions in stress space. Under these conditions, the constitutive response exactly replicates a Newtonian fluid for finite strains and any strain rate. Our approach is to prescribe the Cauchy stress under pure shear conditions and then compute the resulting rate of deformation tensor. The prescribed Cauchy stress is deviatoric. Since we are considering isotropic materials, a deviatoric stress state produces no volume change so that the Cauchy and Kirchoff stresses are the same. The prescribed Cauchy stress, which we project onto a Cartesian coordinate system, and its second deviatoric invariant are:

$$\text{for } t \geq 0, \quad \boldsymbol{\sigma} = \begin{bmatrix} \sigma_0 & 0 & 0 \\ 0 & -\sigma_0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad J_2 = \sigma_0. \quad (11)$$

Given our Newtonian fluid constitutive model in Equation 1, the corresponding rate of deformation and equivalent strain rate from Equation 10 are:

$$\text{for } t \geq 0, \quad \mathbf{d} = \frac{\dot{\gamma}}{2} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \text{where } \dot{\gamma} = \frac{\sigma_0}{\eta}. \quad (12)$$

$$\dot{\epsilon} = \frac{\dot{\gamma}}{\sqrt{3}} \quad (13)$$

Next, we must select the yield surface rate function. Suppose we choose:

$$R[\dot{\epsilon}] = 3\dot{\epsilon}c_R = \sqrt{3}\dot{\gamma}c_R, \quad (14)$$

where $c_R = 1 \text{ sec}$ is a material constant that enforces correct units since the rate function is dimensionless. Then, during fluid flow when the yield condition from Equation 8 is exactly satisfied (under perfectly plastic conditions as stated before), we have:

$$\phi = \sqrt{3}J_2 - R\tau_Y = 0 \rightarrow \sigma_0 = \dot{\gamma}c_R\tau_Y, \quad (15)$$

Hence, according to Equation 1 for the 11 and 22 components:

$$\frac{\text{dev}\tau_{11}}{\text{dev}d_{11}} = \frac{\sigma_0}{\dot{\gamma}/2} = 2\eta = 2c_R\tau_Y \rightarrow \eta = c_R\tau_Y. \quad (16)$$

Thus, under pure shear conditions, the rate dependent perfectly plastic constitutive equation exactly replicates a Newtonian fluid response outside the elastic regime provided the rate function in Equation 14 is used.

4 Model Behavior Under Simple Shear Conditions

In many confined flow applications that might be of interest in structural analysis, the pure shear boundary value problem may not be particularly representative. So we turn our attention to simple shear, which is a specific homogenous motion boundary value problem that might be more

appropriate for confined flow scenarios. The motion during simple shear is isochoric and relevant to rheology since it is equivalent to the steady shear response of parallel plates. From a solid mechanics perspective, we consider a unit cube, which is fixed on one face while the opposite face is uniformly moved transversely to the normals of the two faces. Unlike the pure shear problem of the previous section, simple shear is a fully displacement controlled boundary value problem. Thus, we prescribe the motion and, consequently, the deformation gradient tensor left Cauchy-Green deformation tensor and its unimodular part directly. Projecting these tensors into a Cartesian coordinate system aligned with the axes of the unit cube, they are:

$$\text{for } t \geq 0, \quad \mathbf{F} = \begin{bmatrix} 1 & \dot{\gamma}t & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{b} = \bar{\mathbf{b}} = \begin{bmatrix} 1 + (\dot{\gamma}t)^2 & \dot{\gamma}t & 0 \\ \dot{\gamma}t & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (17)$$

where $\dot{\gamma}$ is the constant shear deformation rate parameter and t represents time starting from the undeformed cube state. Second rank tensors are subsequently projected onto this same coordinate system in this section. Note that this motion is isochoric as \mathbf{F} and \mathbf{b} are unimodular (unit determinants). Hence, there is no pressure response for the isotropic constitutive models that we are considering here. The rate of deformation, its deviatoric part, and the deviatoric part of $\bar{\mathbf{b}}$ are:

$$\text{for } t \geq 0, \quad \mathbf{d} = \text{dev}\mathbf{d} = \frac{\dot{\gamma}}{2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (18)$$

$$\text{dev}\bar{\mathbf{b}} = \begin{bmatrix} \frac{2}{3}(\dot{\gamma}t)^2 & \dot{\gamma}t & 0 \\ \dot{\gamma}t & -\frac{1}{3}(\dot{\gamma}t)^2 & 0 \\ 0 & 0 & -\frac{1}{3}(\dot{\gamma}t)^2 \end{bmatrix}. \quad (19)$$

The fact that Equation 19 contains diagonal terms while the rate of deformation does not is problematic. This indicates we should expect normal stress (11) and (22) that have no associated deviatoric rate of deformation quantity. These normal stresses ultimately poison the Newtonian fluid response at large deformations where $\dot{\gamma}t \geq 1$.

From Equation 18 and 10, the equivalent strain rate is given by:

$$\dot{\epsilon} = \frac{\dot{\gamma}}{\sqrt{3}}. \quad (20)$$

Our analysis proceeds by considering the response right at the transition between elastic and plastic behavior. Consider the *elastic* response first. Since $J = J_e = 1$, the Kirchoff and Cauchy stresses are identical. According to the Neo-Hookean constitutive response, both stress tensors are given (in the original Cartesian basis) by Equation 6 and their common J_2 invariant as:

$$J_2 = \mu \dot{\gamma}t \sqrt{1 + \frac{(\dot{\gamma}t)^2}{3}}. \quad (21)$$

To relate the response to Newtonian flow, we will need the shear stress response in the elastic regime:

$$\tau_{12} = \sigma_{12} = \mu \dot{\gamma}t. \quad (22)$$

Using the same rate dependence of the yield function as in the pure shear case (Equation 14) let us consider when the stress state first meets the yield surface ($\phi = 0$). From Equation 8, we require:

$$J_2 = c_R \dot{\gamma} \tau_Y. \quad (23)$$

Since the yield condition changes with strain rate, we require that the perfectly plastic yield condition must hold. Thus, we require that:

$$\frac{\partial \phi}{\partial \dot{\gamma}} \Big|_{\phi=0} = 0 \rightarrow \frac{\partial J_2}{\partial \dot{\gamma}} - c_R \tau_Y = 0, \quad (24)$$

However, from Equation 21 within the elastic regime, just when the material reaches the yield surface, we derive that:

$$\frac{\partial J_2}{\partial \dot{\gamma}} = \mu t \left(\sqrt{1 + \frac{(\dot{\gamma} t)^2}{3}} + \frac{(\dot{\gamma} t)^2}{3\sqrt{1 + \frac{(\dot{\gamma} t)^2}{3}}} \right). \quad (25)$$

Of course, following Equation 1 we are ultimately interested in:

$$\frac{\partial \text{dev} \tau_{12}}{\partial \text{dev} d_{12}} = \frac{\partial \tau_{12}}{\partial \dot{\gamma}/2} = 2 \left(\frac{\partial \tau_{12}}{\partial J_2} \right) \frac{\partial J_2}{\partial \dot{\gamma}} = 2c_R \tau_Y \left(\sqrt{1 + \frac{\tau_{12}^2}{3\mu^2}} + \frac{\tau_{12}^2}{3\mu^2 \sqrt{1 + \frac{\tau_{12}^2}{3\mu^2}}} \right)^{-1}, \quad (26)$$

which we have arrived at by computing $\left(\frac{\partial J_2}{\partial \tau_{12}} \right)$ using Equations 21 and 22 and then using Equation 26. Under small strain conditions, where $\dot{\gamma} t \ll 1$ or $\tau_{12} \ll \mu$, the radial yield surface grows linearly in time according to Equation 21. Its sensitivity to strain rate is constant according to Equation 25. As $\dot{\gamma} t \approx 1$, the radial yield surface is now quadratic in the shear strain while its sensitivity to shear strain rate becomes linear. Thus, at finite shear strains, this constitutive model *softens* under simple shear and hence would represent a shear thinning fluid.

Returning to our goal, a Newtonian fluid behavior requires that the right-hand side of Equation 26 is a constant (the viscosity), which it is clearly not under finite strain considerations. In the small strain, Equation 26 linearizes to:

$$\frac{\partial \text{dev} \tau_{12}}{\partial \text{dev} d_{12}} = \frac{\partial \tau_{12}}{\partial \dot{\gamma}/2} = 2\eta = 2c_R \tau_Y. \quad (27)$$

Hence, under *small shearing strains*, a Newtonian fluid behavior is recovered. Recall that $c_R = 1$ time unit, which is used simply to maintain units consistency. Therefore, to set the viscosity under the small deformation condition, one need only choose the yield strength parameter multiplied by the appropriate time unit to be the viscosity.

5 Simple Shear Example

Consider the following example. Suppose we wish to model a very viscous Newtonian fluid with a viscosity of 5100 Pascal seconds. For reference, honey and water at room temperature have approximate viscosities of 40 and 1E-3 Pascal seconds respectively [1][2]. This high viscosity could be associated with thermoplastics near melt or thermosetting polymers near gelation. Ideally, we would model a rigid elastic-plastic response in which there would be negligible plastic deformation. In practice, we must avoid numerical issues associated with large changes in material stiffness. Therefore we consider a shear modulus that is 100 times that of the initial yield strength (in uniaxial stress conditions), and we choose a poisson ratio of 0.45 to be near the incompressible regime. During loading, the shear stress response normalized to the yield strength parameter (σ_{12}/τ_{Y0}) versus the simple shear deformation parameter ($\gamma = \dot{\gamma}t$) is plotted for a few different strain rates in Figure 1. The magenta circles denote the normalized shear stress at first

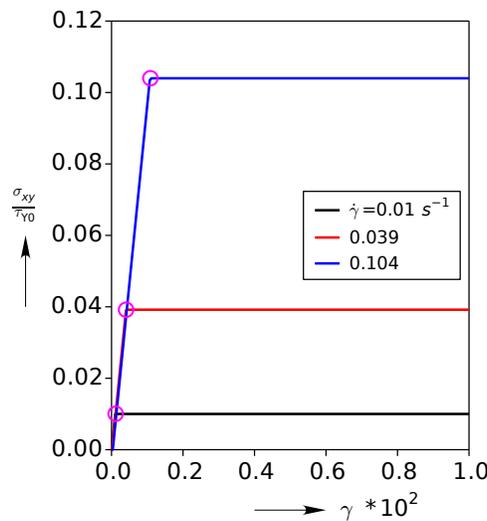


Figure 1. Shear stress normalized to the yield strength parameter vs. the associated shear component of the deformation gradient in simple shear. The strain axis has been modified by the factor of 10^2 to show the elastic region, which is otherwise very small.

yield calculated from the viscosity derived from the model theory in Equation 26 multiplied by twice the associated component of the rate of deformation from Equation 18. Agreement is excellent at small shearing strains. Newtonian fluid behavior is observed where the shear stress is constant for a given strain rate in the plastic regime. If we extract the shear stress after yielding and plot this response as a function of shear strain rate as well as the corresponding slope, we may determine the viscosity as a function of strain rate in Figure 2.

It appears that the viscosity drops off quickly at larger strain rates. However, this behavior is just a consequence of leaving the small strain regime. The appropriate way to understand the model response is to look at the predicted viscosity from Equation 26 against the simple shear deformation parameter γ , which is shown in Figure 3 for several decades of shear strain. For simple shear shear deformation parameters smaller than 0.3, the viscosity is constant, and the response is

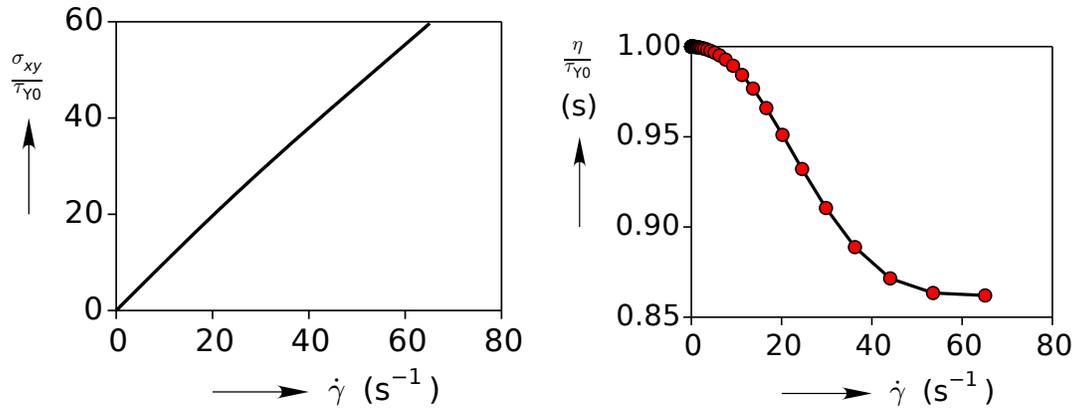


Figure 2. Shear stress post yield normalized by the yield strength parameter vs. shearing strain rate and normalized viscosity under simple shear conditions

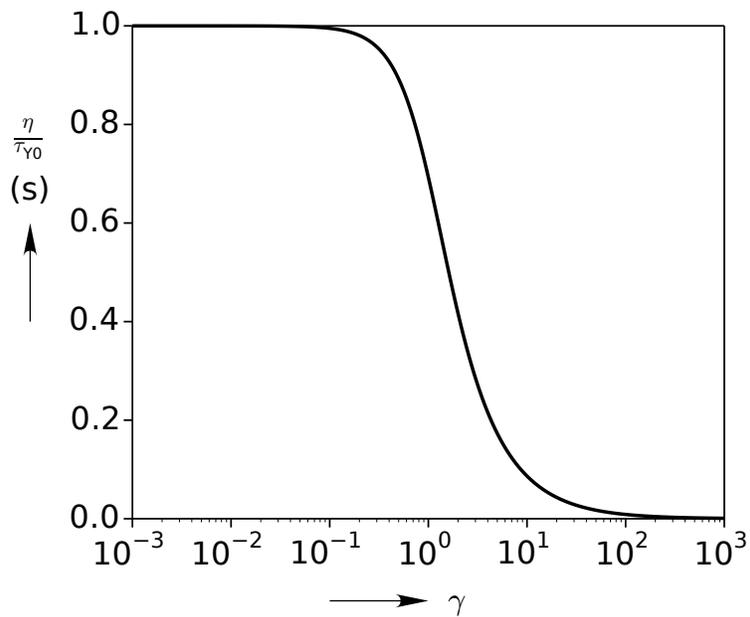


Figure 3. Simple Shear Normalized Viscosity vs. Log Shear Deformation Parameter

Newtonian. When $\gamma \approx 2$, the viscosity is approximately half of the user supplied viscosity. And when $\gamma \approx 10$, the viscosity is approximately just one tenth of the user supplied target. These results are independent of strain rate. We note that when $\gamma = 1$, one axis of the unit cube has been sheared by a 45 degree angle relative to its initial axis corresponding to a very large state of shear, and $\gamma \gg 1$ would correspond to dramatically distorted finite elements that are unusable in practice.

6 Sierra Solid Mechanics Input Syntax Example

We include an example material model input that uses a rate-dependent, Von Mises plasticity model with perfect plasticity (no hardening). The user need only specify the bulk modulus and viscosity up front in the APREPRO definitions. See [4].

```
# Zero, define your material properties. NOTE, The user must input:
# 1)  VISCOSITY (Pa * seconds for example)
# 2)  KBULK (Pa) the bulk modulus.
#
# The shear modulus should be large relative to the yield stress,
# but not too large for time step reasons.
# We suggestion 100*YIELDSTRESS
#{GSHEAR = 100.0*VISCOSITY}
# cR is assumed to be 1 second
#{CR = 1} # second
#{YIELDSTRESS = VISCOSITY/CR}

# First, define the yield condition rate function
begin function newtonianfluidratefun
  type is analytic
  evaluate expression is "3.0*x"
end function newtonianfluidratefun

# Second, define the hardening function (perfect plasticity so no hardening)
begin definition for function nohardfun
  type is piecewise linear
  begin values
    0.0      {YIELDSTRESS}
    1.0E9    {YIELDSTRESS}
  end values
end definition for function nohardfun

# Finally, define the material model
begin material fluidmat
  density = 1000 # kg / m^3. The user should change this parameter!
  begin parameters for model rate_plasticity
    shear modulus      = {GSHEAR}
    bulk modulus       = {KBULK}
    yield stress       = {YIELDSTRESS}
    hardening function = nohardfun
    rate function      = newtonianfluidratefun
  end parameters for model rate_plasticity
end material fluidmat
```

7 Summary

We have presented the use of a rate-dependent, perfectly plastic Von Mises Plasticity model as a representation of a Newtonian fluid, which may be useful represent confined fluid flow in solid mechanics applications. Under certain conditions, this constitutive model exactly represents a Newtonian fluid, such as under pure shear. However, under other conditions, such as simple shear which may be more relevant to confined fluid flow, this constitutive equation quickly becomes non-Newtonian and its viscosity diminishes at finite strains. These results were derived within a Hyper elastic-plastic formulation because the theoretical developments are more straightforward. However, under hypo elastic plastic conditions, which represents the majority of elastic-plastic constitutive models used within the LAME constitutive model library [4], the same results arise for pure shear while qualitatively similar results will be produced under simple shear conditions. That is, under pure shear, the constitutive response is exactly Newtonian for both hypo and hyper elastic plastic models while under simple shear, both model types will produce shear thinning behavior at finite strains but with different dependencies on the finite strain amplitude.

As a last note, this approach of using a rate dependent plasticity model to represent a Newtonian (or Bingham) fluid features compressibility, but it will not represent cavitation phenomena should the pressure become tensile [2]. We caution the users against pushing the model too far. It is best used for qualitative purposes.

References

- [1] <http://en.wikipedia.org/wiki/Viscosity>. Viscosity, March 2015.
- [2] Pijush K. Kundu and Ira M. Cohen. *Fluid Mechanics*. Elsevier, 4 edition, 2008.
- [3] J. C. Simo. A framework for finite strain elastoplasticity based on maximum plastic dissipation and the multiplicative decomposition .1. continuum formulation. *Computer Methods in Applied Mechanics and Engineering*, 66(2), 1988. Times Cited: 247.
- [4] SIERRA Solid Mechanics Team. *Sierra/SolidMechanics 4.34 User's Guide*. Computational Solid Mechanics and Structural Dynamics Department Engineering Sciences Center Sandia National Laboratories, Box 5800 Albuquerque, NM 87185-0380, 4.34 edition, October 2014.

Acknowledgment

The authors appreciate helpful discussions with Rekha Rao (1515) and to Lauri Williams (1555) for her review.

Internal Distribution:

MS-0840	J. Redmond	1550
MS-0840	E. Fang	1554
MS-0840	J. Pott	1555
MS-0346	D. Peebles	1526
MS-9042	J. Ostien	8256
MS-0346	K. Ford	1526
MS-0346	D. Vangoethem	1526
MS-0346	R. Chambers	1526
MS-0346	B. Elisberg	1526
MS-0840	B. Reedlun	1554
MS-0840	W. Scherzinger	1554
MS-0840	N. Breivik	1554
MS-0840	T. Hinnerichs	1554
MS-0840	C. Lo	1554
MS-0840	J. Bean	1554
MS-0840	E. Corona	1554
MS-0840	J. Bishop	1554
MS-0840	S. Grange	1554
MS-0840	K. Gwinn	1554
MS-0840	J. Cox	1554
MS-0845	M. Tupek	1542
MS-0845	K. Pierson	1542
MS-0845	N. Crane	1542
MS-0836	R. Rao	1515