

Numerical modeling of a non-linear viscous flow in order to determine how parameters in constitutive relations influence the entropy production

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Some rheological materials, such as melting polymers, cosmetic creams, ketchup, toothpaste, can be modeled as non-NEWTONian fluids by using a non-linear constitutive relation. An incompressible flow of this kind of amorphous matter can be considered as a thermodynamic process, and a solution for the pressure, velocity and temperature fields describe it fully. Since such flow processes are generally irreversible, entropy is produced leading to dissipation in the system. This energy loss can be measured indirectly in a cone/plate viscometer which is used to determine viscosity of a BINGHAM fluid. While dissipation is an observable quantity we also want to be able to calculate it. Thus the goal of this work is to explain briefly how to compute a transient flow of a viscous fluid in two-dimensional channel under a sinusoidal traction and calculate the dissipated energy for non-NEWTONian fluids.

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1 Introduction and Formulation

Consider a channel treated as an open system defined in two-dimensional space, described by CARTESIAN coordinates $x_i = (x_1, x_2)$. The space is filled up with a viscous fluid. The objective is to determine the mass density ρ , velocity v_i , and the temperature T fields of this matter in space and time. The rational assumption that any process must obey the conservation laws for mass density ρ , linear momentum density ρv_i and internal energy density ρu :

$$\dot{\rho} + \rho \frac{\partial v_i}{\partial x_i} = 0, \quad \rho \dot{v}_i - \frac{\partial \sigma_{ji}}{\partial x_j} = \rho f_i, \quad \rho \dot{u} + \frac{\partial q_i}{\partial x_i} = \sigma_{ij} \frac{\partial v_i}{\partial x_j} + \rho r, \quad (1)$$

leads to a variational formulation with arbitrary test functions δp , δv_i and δT by neglecting volumetric forces f_i and the supply term r :

$$\int_{\Omega} \left(\dot{\rho} + \rho \frac{\partial v_i}{\partial x_i} \right) \delta p \, dv = 0, \quad \int_{\Omega} \left(\rho \dot{v}_i - \frac{\partial \sigma_{ji}}{\partial x_j} \right) \delta v_i \, dv = 0, \quad \int_{\Omega} \left(\rho \dot{u} + \frac{\partial q_i}{\partial x_i} - \sigma_{ij} \frac{\partial v_i}{\partial x_j} \right) \delta T \, dv = 0, \quad (2)$$

where the stress tensor (linear momentum flux) σ_{ij} and heat flux q_i must be given in terms of the unknown fields. Suppose that initially the fluid stands still and maintains a homogeneous temperature and pressure state, and thus has the lowest energy state, i.e., ground state. For a channel geometry, where the bottom is fixed and the top is sheared with a velocity $\hat{v}_i = (A \sin(\omega t), 0)$, the zero velocity field will change. Velocity in the shear direction will vary in the normal to the shear direction. This causes also a change in the temperature field, due to internal friction. If the fluid is incompressible so that the mass density does not alter under these changes, the balance of mass (1)₁ is fulfilled. The pressure field p is the same as the environmental pressure and drops out of the list of unknowns. Assuming linear relations for fluxes and using GIBBS equation for specific internal energy u for a purely viscous fluid:

$$q_i = -\kappa \frac{\partial T}{\partial x_i}, \quad \sigma_{ij} = \mu d_{ij}, \quad T \frac{d\eta}{dt} = \frac{du}{dt} + p \frac{d}{dt} \left(\frac{1}{\rho} \right), \quad \rho|_{x_i,t} = \text{const.} \Rightarrow \dot{u} = T\dot{\eta}, \quad (3)$$

where a constant heat conduction coefficient $\kappa = \text{const.}$, a variable viscosity $\mu = \bar{\mu}(d_{(2)})$, and the specific entropy η (being zero at zero temperature $T = 0$) is assumed. It is of importance that the fluid has a constant volume and a constant pressure in the chosen process and does not store any energy which is recoverable. To get a concrete example, we assume a constant heat conductivity κ and that the viscosity dependency on the second invariant $d_{(2)}$ is expressible by a power law:

$$\mu = a + b(d_{(2)})^c, \quad d_{(2)} = d_{ij}d_{ij}, \quad d_{ij} = \frac{\partial v_{(i}}{\partial x_{j)}} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right). \quad (4)$$

We follow Eckart [1] and use the definition (3)₅ within the equation (1)₃ (and again neglecting r) so that:

$$\rho T \dot{\eta} + \frac{\partial q_i}{\partial x_i} = \sigma_{ij} d_{ij}, \quad \rho \dot{\eta} + \frac{\partial}{\partial x_i} \left(\frac{q_i}{T} \right) = q_i \frac{\partial}{\partial x_i} \left(\frac{1}{T} \right) + \frac{1}{T} \sigma_{ij} d_{ij} = \Sigma. \quad (5)$$

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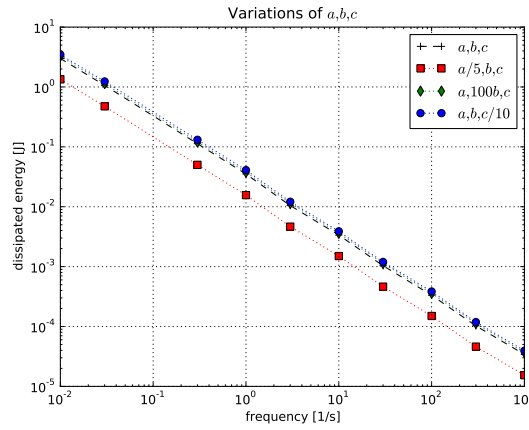


Fig. 1: Logarithmic plot of energy loss vs. frequency under variations of material parameters a, b, c .

This is the balance equation of the entropy density $\rho\eta$ with a positive right hand side, i.e., $\Sigma \geq 0$, which is consistent with the *Second Law* of thermodynamics. Now we use a backwards finite difference for the time discretization:

$$\frac{d}{dt}(\cdot) = \frac{\partial}{\partial t}(\cdot) + \frac{dx_i}{dt} \frac{\partial}{\partial x_i}(\cdot) = \frac{(\cdot) - (\cdot)^0}{t - t^0} + v_i \frac{\partial}{\partial x_i}(\cdot), \quad dt = t - t^0, \quad v_i = \frac{dx_i}{dt} \quad (6)$$

and after employing integration by parts to the derivatives of the fluxes, GALERKIN type finite element for space discretization we obtain:

$$\begin{aligned} & \sum_{\text{elements}} \int_{\Omega^{\text{ele}}} \left(\rho \frac{v_i - v_i^0}{t - t^0} \delta v_i + \rho v_j \frac{\partial v_i}{\partial x_j} \delta v_i + \sigma_{ji} \frac{\partial \delta v_i}{\partial x_j} + \rho T \dot{\eta} \delta T - q_i \frac{\partial \delta T}{\partial x_i} - \sigma_{ij} d_{ij} \delta T \right) dv - \\ & - \oint_{\partial\Omega} \left(\sigma_{ji} \delta v_i n_j - q_i \delta T n_i \right) da. \end{aligned} \quad (7)$$

This can only be solved if for the evolution of specific entropy an approximation from the last time step is used such that it becomes more accurate for smaller time steps:

$$\rho T \dot{\eta} = \sigma_{ij}^0 d_{ij}^0 - \frac{\partial q_i^0}{\partial x_i}. \quad (8)$$

The solution is discrete in time and this is the reason that we can approximate the entropy and thus the solution. The variational form above can be solved within the FEniCS project [2] using the traction free and heat fluxing to the environment boundaries:

$$\sigma_{ji} n_j = 0 \text{ on } \partial\Omega, \quad q_i n_i = h(T - T_{\text{env}}) \text{ on } \partial\Omega. \quad (9)$$

The dissipation function $\Phi = \Sigma T$ is the rate of dissipated energy density [3], hence the loss of energy from the whole system E_{loss} in one period $per = 2\pi/\omega$ reads:

$$E_{\text{loss}} = \sum_{t \in per} (t - t^0) \int_{\Omega} \Phi dv, \quad \Phi = \Sigma T, \quad \Sigma = \frac{\kappa}{T^2} \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_i} + \frac{1}{T} \sigma_{ij} d_{ij}. \quad (10)$$

For some variations of the fictitious material parameters in the Eqs. (3)₂, (4)₁, the energy loss in one cycle of an oscillatory motion is shown in Figure 1. It is possible to measure the dissipated energy from the system such that an appropriate measurement may lead to a fit for the coefficients a, b, c for highly-non-linear materials.

References

- [1] C. Eckart, Phys. Rev. **73**(4), 373–382 (1948).
- [2] A. Logg, K. A. Mardal, and G. Wells (eds.), Automated Solution of Differential Equations by the Finite Element Method, The FEniCS Book (Springer, 2012).
- [3] H. Ziegler and C. Wehrli, Advances in Applied Mechanics, vol. 25, p.183 - 238 (1987).