Nonequilibrium thermodynamical internal variable description of rheology of solids in the GENERIC framework

Tamás Fülöp, Mátyás Szücs (e-mail: fulop@energia.bme.hu)
Department of Energy Engineering, Budapest University of Technology and Economics, Hungary

The internal variable approach of nonequilibrium thermodynamics, with a symmetric tensorial internal variable, leads to a distinguished model family – the Kluitenberg–Verhás model family [1] (covering the Hooke, Kelvin–Voigt, Maxwell and Jeffrey models as special cases) – for the rheology of solids. This family is significant not only from theoretical perspective but also for experimental applications [2]. GENERIC (General Equation for Nonequilibrium Reversible–Irreversible Coupling) is an attractive general framework for nonequilibrium thermodynamical models (see, e.g., [3], [4]). Whenever a new nonequilibrium thermodynamical model emerges, it is advantageous and recommended to check how it suits the frame of GENERIC. In this poster, we investigate how the internal variable formulation of the Kluitenberg–Verhás model family can be represented in GENERIC.

The internal variable formulation

We work in the small-strain regime ($|\varepsilon| \ll 1$) and, for simplicity, we restrict ourselves to a one-dimensional treatment – the extension to 3D proves straightforward, with each term containing the scalar strain ε replaced by two terms containing the tensors $\boldsymbol{\varepsilon}^{\text{deviatoric}}$ and $\boldsymbol{\varepsilon}^{\text{spherical}}$, respectively. Aspects of objectivity and spacetime compatibility are not addressed here.

In the small-strain regime, density ϱ is constant and the gradient v' of the velocity field v is related to the time derivative of strain: $\dot{\varepsilon} = v'$. Again for simplicity, a constant specific heat c is taken and thermal expansion is neglected, which are simplest to treat and explicitly indicate if, in addition to v and ε, the third variable is temperature T; specific energy is therefore

$$e(v, \varepsilon, T) = \tfrac{1}{2}v^2 + \frac{E^{\|}}{2\varrho}\varepsilon^2 + cT, \tag{1}$$

the middle term being Hookean elastic energy with Young's modulus $E^{\|}$. In parallel, specific entropy is

$$s(v, \varepsilon, T, \xi) = c\ln(T/T_{\text{aux}}) - \tfrac{1}{2}\xi^2 \tag{2}$$

(with appropriate constant T_{aux}), where the fourth variable, the internal variable ξ (a symmetric tensor in 3D), enables modelling rheological aspects.

Rheology also manifests itself in stress σ, hence, in mechanics:

$$\varrho\dot{v} = \sigma' \qquad \text{with} \qquad \sigma = \sigma_{\text{el}} + \sigma_{\text{nel}}, \qquad \sigma_{\text{el}} = E^{\|}\varepsilon, \tag{3}$$

where the internal variable approach ensures positive definiteness of the corresponding entropy production terms

$$(1/T)\sigma_{\text{nel}}v' - \varrho\xi\dot{\xi} \tag{4}$$

via the equations that give the nonelastic stress part σ_{nel}, as well as the time evolution for ξ, as

$$\sigma_{\text{nel}} = l_{11}v' + l_{12}(-\varrho T\xi), \qquad \dot{\xi} = l_{21}v' + l_{22}(-\varrho T\xi). \tag{5}$$

The coefficients l_{ij} – later considered constant for simplicity – must make the matrix l^{S} in the middle of

$$\begin{pmatrix} v' & -\varrho T\xi \end{pmatrix} \begin{pmatrix} l_{11} & l_{12}^{\text{S}} \\ l_{12}^{\text{S}} & l_{22} \end{pmatrix} \begin{pmatrix} v' \\ -\varrho T\xi \end{pmatrix} \tag{6}$$

positive definite, implying $l_{11} \geq 0$, $l_{22} \geq 0$, $\det l^{\text{S}} \geq 0$; note that $l_{12}^{\text{S}} = \tfrac{1}{2}(l_{12} + l_{21})$ is related to irreversibility but the antisymmetric part l^{A} not.

In the GENERIC framework, time evolution of the collection x of fields is given in terms of operators L, M as

$$\dot{x} = L\frac{\delta E}{\delta x} + M\frac{\delta S}{\delta x}, \tag{7}$$

where the term containing functional derivative of the energy functional $E = \int \varrho e \, dV$ represents the reversible part of the dynamics while the irreversible part is provided by the one with the functional derivative of the energy functional $S = \int \varrho s \, dV$. Conditions $L\frac{\delta E}{\delta x} = 0$, $M\frac{\delta S}{\delta x} = 0$ ensure conservation of energy and, for reversible dynamics, of entropy.

For our current rheological model, the time evolution of the variables $x = \begin{pmatrix} v & \varepsilon & T & \xi \end{pmatrix}$ and the functional derivatives are

$$\dot{x} = \begin{pmatrix} \frac{1}{\varrho}(\sigma_{\text{el}} + \sigma_{\text{nel}})' \\ v' \\ \frac{1}{\varrho c}\sigma_{\text{nel}}v' \\ l_{21}v' + l_{22}(-\varrho T\xi) \end{pmatrix}, \quad \frac{\delta E}{\delta x} = \begin{pmatrix} \varrho v \\ E^{\|}\varepsilon \\ \varrho c \\ 0 \end{pmatrix}, \quad \frac{\delta S}{\delta x} = \begin{pmatrix} 0 \\ 0 \\ \frac{\varrho c}{T} \\ -\varrho\xi \end{pmatrix}.$$

We have found two possible choices: if

$$L = \begin{pmatrix} 0 & \frac{1}{\varrho}\partial_r & 0 & 0 \\ \frac{1}{\varrho}\partial_r & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{8}$$

$$M = \begin{pmatrix} -\frac{l_{11}}{\varrho^2}\partial_r(T\partial_r\cdot) & 0 & \frac{l_{11}}{\varrho^2 c}\partial_r(Tv'\cdot) & \frac{l_{12}}{\varrho}\partial_r(T\cdot) \\ 0 & 0 & 0 & 0 \\ -\frac{l_{11}}{\varrho^2 c}Tv'\partial_r & 0 & \frac{l_{11}}{\varrho^2 c^2}Tv'^2 & \frac{l_{12}}{\varrho c}Tv' \\ -\frac{l_{21}}{\varrho}T\partial_r & 0 & \frac{l_{21}}{\varrho c}Tv' & l_{22}T \end{pmatrix} \tag{9}$$

with ∂_r denoting spatial derivative, then $l^{\text{A}} \neq 0$ makes M nonsymmetric (but its symmetric part is positive definite). If

$$L = \begin{pmatrix} 0 & \frac{1}{\varrho}\partial_r & -\frac{l_{12}^{\text{A}}}{\varrho c}\partial_r(Tv'\cdot) & -\frac{l_{12}^{\text{A}}}{\varrho}\partial_r \\ \frac{1}{\varrho}\partial_r & 0 & 0 & 0 \\ -\frac{l_{12}^{\text{A}}}{\varrho c}T\xi\partial_r & 0 & 0 & 0 \\ -\frac{l_{12}^{\text{A}}}{\varrho}\partial_r & 0 & 0 & 0 \end{pmatrix}, \tag{10}$$

$$M = \begin{pmatrix} -\frac{l_{11}}{\varrho^2}\partial_r(T\partial_r\cdot) & 0 & \frac{l_{11}}{\varrho^2 c}\partial_r(Tv'\cdot) & \frac{l_{12}^{\text{S}}}{\varrho}\partial_r(T\cdot) \\ 0 & 0 & 0 & 0 \\ -\frac{l_{11}}{\varrho^2 c}Tv'\partial_r & 0 & \frac{l_{11}}{\varrho^2 c^2}Tv'^2 & \frac{l_{12}^{\text{S}}}{\varrho c}Tv' \\ -\frac{l_{12}^{\text{S}}}{\varrho}T\partial_r & 0 & \frac{l_{12}^{\text{S}}}{\varrho c}Tv' & l_{22}T \end{pmatrix} \tag{11}$$

then, using [5], the Jacobi identity is violated for $l^{\text{A}} \neq 0$. Should we sacrifice Jacobi of L or symmetricity of M?

Also to be done: Instead of T, to use s or e as variable; to generalize by removing all special assumptions concerning thermal expansion, finite deformation, elastic energy, etc.

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