RATE EQUATIONS COMPATIBLE WITH THERMODYNAMICS

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1 Introduction

Rate equations are commonly applied to describe microstructural effects on the macromotion or memory features associated with motion and thermal behaviour of the body. Scalar, vector, and tensor quantities governed by rate equations are generally named internal variables. They trace back to Duhem [1], §I.8, and Bridgman [2]. The first analysis within continuum thermodynamics seems to be that given in [3] while a review on the subject is given in [4]. Rate equations with higher-order spatial derivatives are investigated in [5].

To fix ideas look at a solid and suppose that the set of independent variables consists of the deformation gradient $\mathbf{F}$, the temperature θ, the temperature gradient $\mathbf{g}$ and an internal (scalar, vector, or tensor) variable α so that the evolution is given by

$$\dot{\alpha} = f(\mathbf{F}, \theta, \mathbf{g}, \alpha), \tag{1}$$

the stress $\mathbf{T}$, the Helmholtz free energy ψ, the entropy η, and the heat flux $\mathbf{q}$ too being functions of the same variables.

Two questions arise in connection with (1) and, generally, with the rate equations. Owing to the constitutive character, f is required to be compatible with thermodynamics. Now we express the entropy inequality by assuming that

$$\rho\dot{\eta} \geq -\nabla \cdot \frac{\mathbf{q}}{\theta} + \frac{\rho r}{\theta}, \tag{2}$$

where r is the energy supply (per unit mass) and a superposed dot denotes the material (or total) time derivative. The statement of the second law is expressed by saying that, for all set of physically-admissible constitutive functions satisfying the balance equations, the inequality (2) must hold for all times t and point $\mathbf{x}$. We then have to determine the restrictions placed by the second law on f as well as on the other constitutive functions.

The second question is related to the time derivative occurring in (1). It may happen that the material properties indicate a more involved derivative. Furthermore, if the internal variable is a vector or a tensor then the material time derivative is not objective (or frame-indifferent). The literature exhibits several objective time derivatives. It is then conceptually of interest to check the compatibility of objective rate equations (1) with the second law in the form (2) since the time derivative in (2) is necessarily the material one.

It is the purpose of this paper to examine the compatibility, with the second law of thermodynamics, of some rate equations involving objective time derivatives.

2 Rate equations and Clausius-Duhem inequality

The local balance of mass, linear momentum, and energy read

$$\dot{\rho} + \rho\nabla \cdot \mathbf{v} = 0,$$

$$\rho\dot{\mathbf{v}} = \nabla \cdot \mathbf{T} + \rho\mathbf{b},$$

$$\rho\dot{\varepsilon} = \mathbf{T} \cdot \mathbf{D} - \nabla \cdot \mathbf{q} + \rho r,$$

where ρ is the mass density, $\mathbf{v}$ is the velocity, $\mathbf{b}$ is the body force, ε is the internal energy, and $\mathbf{D}$ is the stretching tensor. For the present purposes there is no loss in generality by letting $\phi = \mathbf{q}/\theta$. Hence substitution of $\rho r - \nabla \cdot \mathbf{q}$ from the balance of energy allows eq. (2) to be written in the form

$$-\dot{\psi} - \eta\,\dot{\theta} + \frac{1}{\rho}\mathbf{T} \cdot \mathbf{D} - \frac{1}{\rho\theta}\mathbf{q} \cdot \mathbf{g} \geq 0,$$

where $\psi = \varepsilon - \theta\eta$. Upon evaluation of $\dot{\psi}$ and using the arbitrariness of $\dot{\mathbf{g}}, \dot{\theta}, \dot{\mathbf{F}}$ we find

$$\partial_{\mathbf{g}}\psi = 0, \qquad \eta = -\partial_\theta\psi, \qquad \mathbf{T} = \rho\,\partial_{\mathbf{F}}\psi\mathbf{F}^T,$$

$$-\partial_\alpha\psi f - \frac{1}{\rho\theta}\mathbf{q} \cdot \mathbf{g} \geq 0.$$

If, in particular, f is independent of $\mathbf{g}$ then we have

$$\partial_\alpha\psi f \leq 0,$$

that is a condition on $\partial_\alpha\psi$ and on the evolution function f.

This is so if α is a scalar. Now let α be the pair of a vector $\mathbf{u}$ and a tensor $\mathbf{K}$, possibly $\mathbf{u} = \mathbf{q}, \mathbf{K} = \mathbf{T}$, and take the rate equations

$$\dot{\mathbf{u}} = \hat{\mathbf{u}}(\mathbf{F}, \theta, \mathbf{g}, \mathbf{D}, \mathbf{u}, \mathbf{K}), \qquad \dot{\mathbf{K}} = \hat{\mathbf{K}}(\mathbf{F}, \theta, \mathbf{g}, \mathbf{D}, \mathbf{u}, \mathbf{K}).$$

Hence the Clausius-Duhem inequality yields

$$\partial_{\mathbf{D}}\psi = 0, \qquad \partial_{\mathbf{g}}\psi = 0, \qquad \eta = -\partial_\theta\psi$$

and

$$\frac{1}{\rho}\mathbf{T}\cdot\mathbf{D}-\frac{1}{\rho\theta}\mathbf{q}\cdot\mathbf{g}-\partial_{\mathbf{u}}\psi\cdot\hat{\mathbf{u}}-\partial_{\mathbf{K}}\psi\cdot\hat{\mathbf{K}}\geq 0.$$

For definiteness, by generalizing rate equations for heat conduction and viscosity we let

$$\hat{\mathbf{u}}=-\nu\,\mathbf{u}-\gamma\mathbf{g},\qquad \hat{\mathbf{K}}=-\Lambda\mathbf{K}+\Gamma\mathbf{D},$$

where ν,γ,Λ, and Γ are functions of $\mathbf{F}$ and θ. Upon substitution, the arbitrariness of $\mathbf{D}$ and $\mathbf{g}$ implies that the inequality holds if and only if

$$\mathbf{T}=\rho\,\partial_{\mathbf{F}}\psi\mathbf{F}^T+\rho\,\Gamma\partial_{\mathbf{K}}\psi,\qquad \mathbf{q}=\rho\,\theta\gamma\partial_{\mathbf{u}}\psi,$$

and

$$\nu\,\partial_{\mathbf{u}}\psi\cdot\mathbf{u}+\Lambda\partial_{\mathbf{K}}\psi\cdot\mathbf{K}\geq 0.$$

A simple model arises by taking ψ in the additive form

$$\psi=\Psi(\mathbf{F},\theta)+\psi_w(\mathbf{w}^2)+\psi_K(\mathbf{K}^2).$$

As a consequence, ψ satisfies the inequality if and only if

$$\psi_w'\geq 0,\qquad \psi_K'\geq 0$$

while

$$\mathbf{T}=\rho\,\partial_{\mathbf{F}}\psi\mathbf{F}^T+2\rho\,\Gamma\psi_K'\mathbf{K},\qquad \mathbf{q}=2\rho\,\theta\gamma\psi_u'\mathbf{u}.$$

We now examine the corresponding model by replacing the material time derivative with frame-indifferent derivatives. Indeed we restrict attention to the following widely-used derivatives in continuum mechanics.

Corotational (or Green-Naghdi) time derivative. Look at the corotational time derivatives

$$\overset{\square}{\mathbf{u}}=\dot{\mathbf{u}}-\Omega\mathbf{u},\qquad \overset{\square}{\mathbf{K}}=\dot{\mathbf{K}}-\Omega\mathbf{K}+\mathbf{K}\Omega,$$

and state the evolution equations as

$$\overset{\square}{\mathbf{u}}=\hat{\mathbf{u}},\qquad \overset{\square}{\mathbf{K}}=\hat{\mathbf{K}}.$$

Hence, from

$$\frac{1}{\rho}\mathbf{T}\cdot\mathbf{D}-\frac{1}{\rho\theta}\mathbf{q}\cdot\mathbf{g}-\partial_{\mathbf{u}}\psi\cdot\dot{\mathbf{u}}-\partial_{\mathbf{K}}\psi\cdot\dot{\mathbf{K}}\geq 0$$

we have

$$\frac{1}{\rho}\mathbf{T}\cdot\mathbf{D}-\frac{1}{\rho\theta}\mathbf{q}\cdot\mathbf{g}-\partial_{\mathbf{u}}\psi\cdot(\hat{\mathbf{u}}+\Omega\mathbf{u})-\partial_{\mathbf{K}}\psi\cdot(\hat{\mathbf{K}}+\Omega\mathbf{K}-\mathbf{K}\Omega)\geq 0.$$

Quite naturally one expects that the contribution of the spin tensor Ω to the dissipation is zero in that the choice of the frame of reference should not affect the entropy growth. Of course we are not interested in the trivial case $\partial_{\mathbf{u}}\psi=0$, $\partial_{\mathbf{K}}\psi=0$. Hence we let ψ be a function of the invariants $\mathbf{u}^2,\mathbf{u}\cdot\mathbf{K}\mathbf{u}$, and $\mathbf{K}^2$, where $\mathbf{K}^2=\mathbf{K}\cdot\mathbf{K}$. Since

$$\partial_{\mathbf{u}}\psi=2\partial_{\mathbf{u}^2}\psi\mathbf{u}+\partial_{\mathbf{u}\cdot\mathbf{K}\mathbf{u}}\psi(\mathbf{K}+\mathbf{K}^T)\mathbf{u},\qquad \partial_{\mathbf{K}}\psi=\partial_{\mathbf{u}\cdot\mathbf{K}\mathbf{u}}\psi\mathbf{u}\otimes\mathbf{u}+\partial_{\mathbf{K}^2}\psi\mathbf{K},$$

we find

$$\begin{aligned}\partial_{\mathbf{u}}\psi\cdot\Omega\mathbf{u}+\partial_{\mathbf{K}}\psi\cdot(\Omega\mathbf{K}-\mathbf{K}\Omega)&=2\partial_{\mathbf{u}^2}\psi\mathbf{u}\cdot\Omega\mathbf{u}+\partial_{\mathbf{K}^2}\psi\mathbf{K}\cdot(\Omega\mathbf{K}-\mathbf{K}\Omega)\\&+\partial_{\mathbf{u}\cdot\mathbf{K}\mathbf{u}}\psi[(\omega\mathbf{u})\cdot(\mathbf{K}+\mathbf{K}^T)\mathbf{u}+(\mathbf{u}\otimes\mathbf{u})\cdot(\Omega\mathbf{K}-\mathbf{K}\Omega)].\end{aligned}$$

By the skew-symmetry of Ω it follows that $\mathbf{u}\cdot\Omega\mathbf{u}=0$. Moreover,

$$\mathbf{K}\cdot(\Omega\mathbf{K}-\mathbf{K}\Omega)=(\mathbf{K}\mathbf{K}^T)\cdot\Omega-(\mathbf{K}^T\mathbf{K})\cdot\Omega.$$

Since $\mathbf{K}\mathbf{K}^T$ and $\mathbf{K}^T\mathbf{K}$ are symmetric tensors, again in view of the skew-symmetry of Ω we obtain

$$\mathbf{K}\cdot(\Omega\mathbf{K}-\mathbf{K}\Omega)=0.$$

Now, some rearrangements show that

$$\begin{aligned}(\Omega\mathbf{u})\cdot(\mathbf{K}+\mathbf{K}^T)\mathbf{u}+(\mathbf{u}\otimes\mathbf{u})\cdot(\Omega\mathbf{K}-\mathbf{K}\Omega)&=(\Omega\mathbf{u})\cdot(\mathbf{K}\mathbf{u})\\&+(\Omega\mathbf{u})\cdot(\mathbf{K}^T\mathbf{u})-(\Omega\mathbf{u})\cdot(\mathbf{K}\mathbf{u})-(\Omega\mathbf{u})\cdot(\mathbf{K}^T\mathbf{u})=0.\end{aligned}$$

Accordingly, if the free energy depends on the internal variables $\mathbf{u},\mathbf{K}$ via the invariants $\mathbf{u}^2,\mathbf{u}\cdot\mathbf{K}\mathbf{u}$, and $\mathbf{K}^2$,

$$\psi=\psi(\mathbf{F},\theta,\mathbf{u}^2,\mathbf{u}\cdot\mathbf{K}\mathbf{u},\mathbf{K}^2),$$

then the contribution of the corotational derivative to the entropy inequality equals that of the material time derivative via the evolution functions $\hat{\mathbf{u}},\hat{\mathbf{K}}$.

By merely replacing the generic spin tensor Ω with the spin tensor of the velocity field $\mathbf{W}$ we are dealing with the Jaumann derivative. We then say that also with the Jaumann derivative, $\overset{\circ}{\mathbf{u}},\overset{\circ}{\mathbf{K}}$, the contribution to the entropy inequality equals that of the material time derivative via the evolution functions $\hat{\mathbf{u}},\hat{\mathbf{K}}$.

Compatibility with the second law of thermodynamics holds depending on the functions $\hat{\mathbf{u}}$ and $\hat{\mathbf{K}}$.

The *Truesdell rate* and the *upper convected Oldroyd derivative* are better investigated within the material description.

3 Rate equations in the material description

We now address attention to a thermoelastic material with memory for the heat conduction. The heat flux is subject to a rate equation of the form

$$\overset{\diamond}{\mathbf{q}} + \lambda\mathbf{q} = -\alpha\nabla\theta \tag{3}$$

where

$$\overset{\diamond}{\mathbf{q}} = \dot{\mathbf{q}} - \mathbf{L}\mathbf{q} + (\nabla\cdot\mathbf{v})\mathbf{q}$$

is the Truesdell rate of the vector $\mathbf{q}$ and $\lambda > 0$.

The corresponding material field $\mathbf{q}_R$ of $\mathbf{q}$ is given by

$$\mathbf{q}_R = J\mathbf{q}\mathbf{F}^{-T}, \qquad J = \det\mathbf{F}.$$

Moreover we have

$$J\,\overset{\diamond}{\mathbf{q}}\,\mathbf{F}^{-T} = \overline{J\mathbf{q}\mathbf{F}^{-T}}^{\cdot} = \dot{\mathbf{q}}_R. \tag{4}$$

Right multiplication of (3) by $J\mathbf{F}^{-T}$ and use of (4 give

$$\dot{\mathbf{q}}_R + \lambda\mathbf{q}_R = -\alpha J\nabla\theta\mathbf{F}^{-T}.$$

Let $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ denote the right Cauchy-Green tensor. Since

$$\nabla\theta = \nabla_{\mathbf{X}}\theta\mathbf{F}^{-1}, \qquad \nabla\theta\mathbf{F}^{-T} = \nabla_{\mathbf{X}}\theta\mathbf{C}^{-1}$$

then the rate equation becomes

$$\dot{\mathbf{q}}_R + \lambda\mathbf{q}_R = -\alpha J\mathbf{C}^{-1}\nabla_{\mathbf{X}}\theta. \tag{5}$$

The material stress field $\mathbf{T}_{RR}$ (second Piola stress) is given by

$$\mathbf{T}_{RR} = J\mathbf{F}^{-1}\mathbf{T}\mathbf{F}^{-T}.$$

Hence the Clausius-Duhem inequality in the material description can be given the form [6; 7]

$$-\rho_R(\dot{\psi} + \eta\dot{\theta}) + \tfrac{1}{2}\mathbf{T}_{RR}\cdot\dot{\mathbf{C}} - \frac{1}{\theta}\mathbf{q}_R\cdot\nabla_{\mathbf{X}}\theta \geq 0. \tag{6}$$

To describe the thermoelastic solid we let

$$\theta, \mathbf{C}, \nabla_{\mathbf{X}}\theta, \mathbf{q}_R$$

be the independent variables and $\psi, \eta, \mathbf{T}_{RR}$ the constitutive functions while $\dot{\mathbf{q}}_R$ is given by (5). Upon evaluation of $\dot{\psi}$ and substitution in (6) we obtain

$$-\rho_R(\partial_\theta\psi + \eta)\dot{\theta} + (\tfrac{1}{2}\mathbf{T}_{RR} - \rho_R\partial_{\mathbf{C}}\psi)\cdot\dot{\mathbf{C}} - \rho_R\partial_{\nabla_{\mathbf{X}}\theta}\psi\cdot\nabla_{\mathbf{X}}\dot{\theta}$$
$$+\rho_R\partial_{\mathbf{q}_R}\psi\cdot(\lambda\mathbf{q}_R + \alpha J\mathbf{C}^{-1}\nabla_{\mathbf{X}}\theta) - \frac{1}{\theta}\mathbf{q}_R\cdot\nabla_{\mathbf{X}}\theta \geq 0.$$

Hence it follows that

$$\partial_{\nabla_{\mathbf{X}}\theta}\psi = 0, \qquad \mathbf{T}_{RR} = 2\rho_R\partial_{\mathbf{C}}\psi, \qquad \eta = -\partial_\theta\psi \tag{7}$$

and

$$\partial_{\mathbf{q}_R}\psi\cdot\mathbf{q}_R \geq 0, \qquad \frac{1}{\theta}\mathbf{q}_R = \alpha J\rho_R\mathbf{C}^{-1}\partial_{\mathbf{q}_R}\psi.$$

Accordingly,

$$\psi = \Psi(\theta, \mathbf{C}) + \frac{1}{2\theta J\rho_R\alpha}\mathbf{q}_R\cdot\mathbf{C}\mathbf{q}_R \tag{8}$$

and

$$\partial_{\mathbf{q}_R}\psi\cdot\mathbf{q}_R = \frac{1}{\theta J\rho_R\alpha}\mathbf{q}_R\cdot\mathbf{C}\mathbf{q}_R \geq 0$$

in view of the positive definiteness of $\mathbf{C}$. Hence the whole scheme is compatible with thermodynamics provided ψ has the form (8) and $\mathbf{T}_{RR}, \eta$ are given by (7).

The advantage of the material rate equation (5) versus the spatial rate equation (3) is that we can solve easily eq. (5) to find

$$\mathbf{q}_R(t) = -\int_{-\infty}^{t} \exp(-\int_s^t \lambda(\xi)d\xi)\,\alpha(s)J(s)\nabla\theta(s)\mathbf{F}^{-T}(s)ds$$

whence

$$\mathbf{q}(t) = -\frac{1}{J(t)}\int_{-\infty}^{t} \exp(-\int_s^t \lambda(\xi)d\xi)\,\alpha(s)J(s)\nabla\theta(s)\mathbf{F}^{-T}(s)ds\,\mathbf{F}^T(t). \tag{9}$$

It is a natural consistency requirement that the solution (9) is independent of the choice of the reference configuration. In this connection let $\mathcal{R}_0$ be the reference configuration considered so far. Let $\mathcal{R}_1$ be an intermediate configuration such that

$$\mathcal{R}_0 \to \mathcal{R}_1 \to \mathcal{E}$$

and $\mathbf{F}_0$ and $\mathbf{F}_1$ be the deformation gradients from $\mathcal{R}_0$ to $\mathcal{R}_1$ and from $\mathcal{R}_1$ to $\mathcal{E}$. Hence

$$\mathbf{F}(t) = \mathbf{F}_1(t)\mathbf{F}_0, \qquad J(t) = J_1(t)J_0.$$

Upon substitution we obtain

$$\mathbf{q}(t) = -\frac{1}{J_1(t)}\int_{-\infty}^{t} \exp(-\int_s^t \lambda(\xi)d\xi)\,\alpha(s)J_1(s)\nabla\theta(s)\mathbf{F}_1^{-T}(s)ds\,\mathbf{F}_1^T(t)$$

thus proving the invariance.

4 Conclusions and remarks

The corotational derivative proves to be consistent with thermodynamics, subject to requirements on the evolution functions $\hat{\mathbf{u}}, \hat{\mathbf{K}}$. The Truesdell rate is shown to be compatible with thermodynamics, the compatibility being ascertained within the material description of the balance equations and the second law.

It is worth pointing out that here the occurrence of rates in the constitutive equations is taken in the normal form (1) and the compatibility involves both the derivative and the constitutive function f. There are approaches where appropriate rates of the unknown fields enter the state space (or the set of independent variables). This is done both with the material time derivative [8], e.g.

$$\eta = \hat{\eta}(\varepsilon, \upsilon, \dot{\varepsilon}, \dot{\upsilon}), \qquad \upsilon = 1/\rho,$$

and with the corotational time derivative [9; 10]. In such cases the thermodynamic analysis is based on a generalized Gibbs equation, with the occurrence of additional “intensive quantities” [8] or Lagrange multipliers [9], thus introducing difficulties on the physical interpretation of the model.

REFERENCES

[1] C. Truesdell, Rational Thermodynamics, Springer, New York (1984), ch. 5

[2] P.W. Bridgman, The Nature of Thermodynamics, Harvard University Press, Cambridge, MA, 1961.

[3] B.D. Coleman, M.E. Gurtin, Thermodynamics with internal state variables, J. Chem. Phys. 47, 597-613 (1967).

[4] G.A. Maugin, W. Muschik, Thermodynamics with internal variables. Part I. General concepts, J. Non-Equilib. Thermodyn. 19, 217-249 (1994).

[5] V.A. Cimmelli, P. Ván, The effects of nonlocality on the evolution of higher order fluxes in nonequilibrium thermodynamics, J. Math. Phys. 46, 112901 (2005).

[6] A. Morro, Evolution equations and thermodynamic restrictions for dissipative solids, Math. and Comp. Modelling 52, 1869-1876 (2010).

[7] A. Morro, Evolution equations for non-simple viscoelastic solids, J. Elasticity 105, 93-105 (2011).

[8] S.I. Serdyukov, Extended irreversible thermodynamics and the Jeffreys type constitutive equations, Phys. Letters A 316, 177-183 (2003).

[9] V.A. Cimmelli, Different thermodynamic theories and different heat conduction laws, J. Non-Equilib. Thermodyn. 34, 299-333 (2009).

[10] D. Jou, J. Casa-Vázquez, M. Criado-Sancho, Thermodynamics of Fluids under Flow, Springer, Berlin, 2001, p. 6.