

4.4 Continuum Thermomechanics

The classical thermodynamics is now extended to the thermomechanics of a continuum. The state variables are allowed to vary throughout a material and processes are allowed to be irreversible and move far from thermal and mechanical equilibrium. Some schools of thought would question whether entropy is a state function at all under these conditions. Here, we simply accept the fact that it is. This is part of the **rational thermodynamics** approach and is generally accepted in the solid mechanics community.

4.4.1 The First Law

The first law of thermodynamics is, in rate form,

$$P_{ext} + Q^* = \dot{U} + \dot{K} \quad (4.4.1)$$

where P_{ext} is the power of the external forces, Q^* is the rate at which heat is supplied (called the **thermal power**, the **non-mechanical power**, or the **rate of thermal work**), \dot{U} is the rate of change of the internal energy and \dot{K} is the rate of change of kinetic energy. The superscript “*” is used here and in what follows to indicate rates of change of quantities which are not state functions.

Recall from Part III, Eqn 3.8.2, the mechanical energy balance,

$$P_{ext} + P_{int} = \dot{K} \quad (4.4.2)$$

Eliminating P_{ext} and \dot{K} from these equations leads to

$$-P_{int} + Q^* = \dot{U} \quad (4.4.3)$$

Heat supply

It is convenient to write the total heat supply to a finite volume of material as an integral over the volume. This is done by defining the **heat flux** \mathbf{q} to be the rate at which heat is conducted from interior to exterior per unit area, Fig. 4.4.1. The rate of heat *entering* is thus $-\int_s \mathbf{q} \cdot \mathbf{n} ds$. Let there also be a source of heat supply inside the material, for example a radiator of heat. Let $\int_v r dv$ be the rate of such heat supply, where the scalar r is the **heat source**, the rate of heat generated per unit volume. Thus, with the divergence theorem,

$$Q^* = -\int_v \text{div} \mathbf{q} dv + \int_v r dv \quad (4.4.4)$$

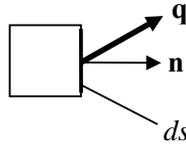


Figure 4.4.1: heat flux vector and normal vector to a surface element

Recall also from Part III, Eqns. 3.8.15, the stress power

$$P_{\text{int}} = -\int_v \boldsymbol{\sigma} : \mathbf{d}dv \quad (4.4.5)$$

Combining Eqns. 4.4.3-5, and expressing the strain energy rate in the form of an integral (see Part III, Eqn. 3.8.15) leads to

$$\int_v \boldsymbol{\sigma} : \mathbf{d}dv - \int_v \text{div} \mathbf{q} dv + \int_v r dv = \int_v \rho \dot{u} dv \quad (4.4.6)$$

Since this holds for all volumes v , one has the local form

$$\boxed{\boldsymbol{\sigma} : \mathbf{d} - \text{div} \mathbf{q} + r = \rho \dot{u}} \quad \text{The First Law} \quad (4.4.7)$$

4.4.2 The Second Law

Entropy

The entropy $S(\mathbf{x}, t)$ is defined as the scalar property

$$S = \int_v \rho s dv \quad (4.4.8)$$

where s is the specific entropy or **entropy density**. The change in entropy is due to two quantities. First, very like the heat transferred into a body, Eqn. 4.4.4, define the entropy supply $S^{(r)*}$ to be the rate of entropy input,

$$S^{(r)*} = -\int_s \mathbf{s}_q \cdot \mathbf{n} ds + \int_v s_r dv \quad (4.4.9)$$

where \mathbf{s}_q is the **entropy flux** through the element surface and s_r is entropy supply due to sources within the element. Further, the entropy flux is taken to be proportional to the heat flux, and the proportionality factor is the reciprocal of the non-negative scalar **absolute temperature** θ (and similarly for the density s_r and the heat supply density r) so that, using the divergence theorem,

$$\begin{aligned}
 S^{(r)*} &= -\int_s \frac{\mathbf{q}}{\theta} \cdot \mathbf{n} ds + \int_v \frac{r}{\theta} dv \\
 &= -\int_v \operatorname{div} \left(\frac{\mathbf{q}}{\theta} \right) dv + \int_v \frac{r}{\theta} dv
 \end{aligned}
 \tag{4.4.10}$$

Define the entropy production $S^{(i)*}$ to be the difference between the rate of change of entropy and the entropy supply:

$$S^{(i)*} = \dot{S} - S^{(r)*} \tag{4.4.11}$$

The second law of thermodynamics states that the entropy production is a non-negative quantity,

$$S^{(i)*} \geq 0 \tag{4.4.12}$$

The Clausius-Duhem Inequality

Thus one has the **Clausius-Duhem inequality**:

$$S^{(i)*} = \frac{d}{dt} \int_v \rho s dv + \int_v \operatorname{div} \left(\frac{\mathbf{q}}{\theta} \right) dv - \int_v \frac{r}{\theta} dv \geq 0 \tag{4.4.13}$$

In local form, the Clausius-Duhem inequality reads as (introducing a specific entropy production, $s^{(i)*}$)

$$s^{(i)*} = \dot{s} + \frac{1}{\rho} \operatorname{div} \left(\frac{\mathbf{q}}{\theta} \right) - \frac{r}{\rho \theta} \geq 0 \tag{4.4.14}$$

or, equivalently {▲ Problem 1},

$$\boxed{s^{(i)*} = \dot{s} - \frac{r}{\rho \theta} + \frac{1}{\rho \theta} \operatorname{div} \mathbf{q} - \frac{1}{\rho \theta^2} (\mathbf{q} \cdot \nabla \theta) \geq 0} \quad \text{The Second Law} \tag{4.4.15}$$

This is the continuum statement of the Second Law.

4.4.3 The Dissipation Inequality

Eliminating $\operatorname{div} \mathbf{q}$ (and r) from both the first and second laws leads to the **dissipation inequality**

$$\boxed{\theta s^{(i)*} = \theta \dot{s} - \dot{u} + \frac{1}{\rho} (\boldsymbol{\sigma} : \mathbf{d}) - \frac{1}{\rho \theta} (\mathbf{q} \cdot \nabla \theta) \geq 0} \quad \text{Dissipation Inequality} \tag{4.4.16}$$

The term $\theta s^{(i)*}$ is the specific dissipation (or **internal dissipation**) and is denoted by the symbol ϕ . The Clausius-Duhem inequality can simply be written as

$$\phi \equiv \theta s^{(i)*} \geq 0 \quad (4.4.17)$$

Multiplying Eqn. 4.4.16 across by the density leads to

$$\rho \theta s^{(i)*} = [\rho \dot{\theta} s - \rho \dot{u} + \boldsymbol{\sigma} : \mathbf{d}] + \left[-\frac{1}{\theta} (\mathbf{q} \cdot \nabla \theta) \right] \geq 0 \quad (4.4.18)$$

Each term here has units of power per unit (current) volume. The term inside the first bracket is called the **mechanical dissipation** (per unit volume). The term inside the second bracket is the dissipation due to temperature gradients, i.e. heat flow, and is called the **thermal dissipation** (per unit volume). Note that the thermal dissipation will always be positive if \mathbf{q} and $\nabla \theta$ are of opposite sign. Integrating over a volume v leads to

$$\int_v \rho \theta s^{(i)*} dv = \int_v \{ \boldsymbol{\sigma} : \mathbf{d} - \rho \dot{u} + \rho \dot{\theta} s \} dv + \int_v \left\{ -\frac{1}{\theta} (\nabla \theta \cdot \mathbf{q}) \right\} dv \quad (4.4.19)$$



dissipation



mechanical
dissipation



thermal
dissipation

The term $\rho \theta s^{(i)*}$ in Eqn. 4.4.18 is often denoted by the symbol γ and also termed the dissipation. This is a dissipation per unit volume. When the deformations are small, the volume changes are negligible. When the deformations are appreciable, however, the volume and density change, and it is better to work with specific quantities such as ϕ .

The dissipation inequality 4.4.16 is in terms of the internal energy. In terms of the specific free energy $\psi = u - s\theta$, one has

$$\phi = \theta s^{(i)*} = -s\dot{\theta} - \dot{\psi} + \frac{1}{\rho} (\boldsymbol{\sigma} : \mathbf{d}) - \frac{1}{\rho\theta} (\mathbf{q} \cdot \nabla \theta) \geq 0 \quad (4.4.20)$$

4.4.4 The Clausius-Plank Inequality

In many applications the thermal dissipation is very much smaller than the mechanical dissipation (in fact it is zero in many important applications – see section 4.4.7 below). If this is the case then the thermal dissipation rate can be ignored, and one has the stronger form of the second law, in terms of internal energy and free energy,

$$\boxed{\begin{aligned}\phi &= \theta \dot{s} - \dot{u} + \frac{1}{\rho} (\boldsymbol{\sigma} : \mathbf{d}) \geq 0 \\ \phi &= -s \dot{\theta} - \dot{\psi} + \frac{1}{\rho} (\boldsymbol{\sigma} : \mathbf{d}) \geq 0\end{aligned}}$$

Clausius-Plank inequality (4.4.21)

which is known as the **Clausius-Plank inequality**.

Equivalently, one can argue that the processes of mechanical dissipation and heat flow are independent, so that each are separately required to be non-negative, again leading to Eqn. 4.4.21. This issue will be explored more fully in Part IV, where it will indeed be shown that the thermal dissipation is very often decoupled from the mechanical dissipation, with both being required to be separately positive.

Using the first law, Eqn. 4.4.21 can be rewritten in the alternative form

$$\theta \dot{s} = \phi + \frac{1}{\rho} r - \frac{1}{\rho} \operatorname{div} \mathbf{q} \quad (4.4.22)$$

which is an **evolution equation** for s (showing how it evolves over time).

4.4.5 Special Thermodynamic Processes

Some important limiting processes are considered next.

Reversible Processes

In a reversible process, $\phi = s^{(i)*} = 0$. The Clausius-Plank inequality now becomes

$$\dot{u} = \theta \dot{s} + \frac{1}{\rho} (\boldsymbol{\sigma} : \mathbf{d}) \quad \text{or} \quad \dot{\psi} = -s \dot{\theta} + \frac{1}{\rho} (\boldsymbol{\sigma} : \mathbf{d}) \quad (4.4.23)$$

From the First Law,

$$\rho \dot{s} = -\frac{\operatorname{div} \mathbf{q}}{\theta} \quad (4.4.24)$$

This is the entropy supply (with zero temperature gradients) and corresponds to the classical thermodynamic (for which, also, $\nabla \theta = 0$) expression $dS^{(r)} = \delta Q / \theta$.

Isentropic Conditions

For an isentropic process, the entropy is constant and remains constant, so $\dot{s} = 0$. In this case, the dissipation is

$$\phi = -\dot{u} + \frac{1}{\rho}(\boldsymbol{\sigma} : \mathbf{d}) - \frac{1}{\rho\theta}(\mathbf{q} \cdot \nabla\theta) \geq 0 \quad (4.4.25)$$

Isothermal Conditions

In an isothermal process, the absolute temperature remains constant, $\dot{\theta} = 0$. This can be achieved, for example, by keeping the material's surroundings at constant temperature, and loading the material very slowly, so that any temperature differences which arise between the material and surroundings are allowed to disappear.

The Clausius-Plank inequality becomes

$$\phi = \theta\dot{s} - \dot{u} + \frac{1}{\rho}(\boldsymbol{\sigma} : \mathbf{d}) \geq 0 \quad \text{or} \quad \phi = -\dot{\psi} + \frac{1}{\rho}(\boldsymbol{\sigma} : \mathbf{d}) \geq 0 \quad (4.4.26)$$

Equilibrium Conditions

As mentioned in §4.2.3, a material which is unaffected by external conditions has no work done to it or heat supplied and the first law then states that the internal energy is constant. In that case, when the entropy has reached a maximum and the dissipation is zero, there is no more change in any of the state variables, and equilibrium has been reached.

Adiabatic Conditions

In an adiabatic process, $\mathbf{q} = \mathbf{0}$. This can be achieved, for example, by very rapid loading, so that there is no time for heat exchange with the surroundings.

Under these conditions (and taking also $r = 0$), the first law reads $\boldsymbol{\sigma} : \mathbf{d} = \rho\dot{u}$ (recall that the internal energy change is equal to the work done in an adiabatic process). The dissipation inequality reduces to

$$s^{(i)*} = \dot{s} \geq 0 \quad (4.4.27)$$

or

$$\phi = \theta\dot{s} \geq 0 \quad (4.4.28)$$

If the process is both adiabatic and isentropic, then $\phi = \dot{s} = 0$. An adiabatic reversible process is equivalent to an isentropic reversible process.

4.4.6 Summary

A summary of the thermomechanical theory, showing the various laws and relations which are involved, and how they are interconnected, is given in Fig. 4.4.2 below.

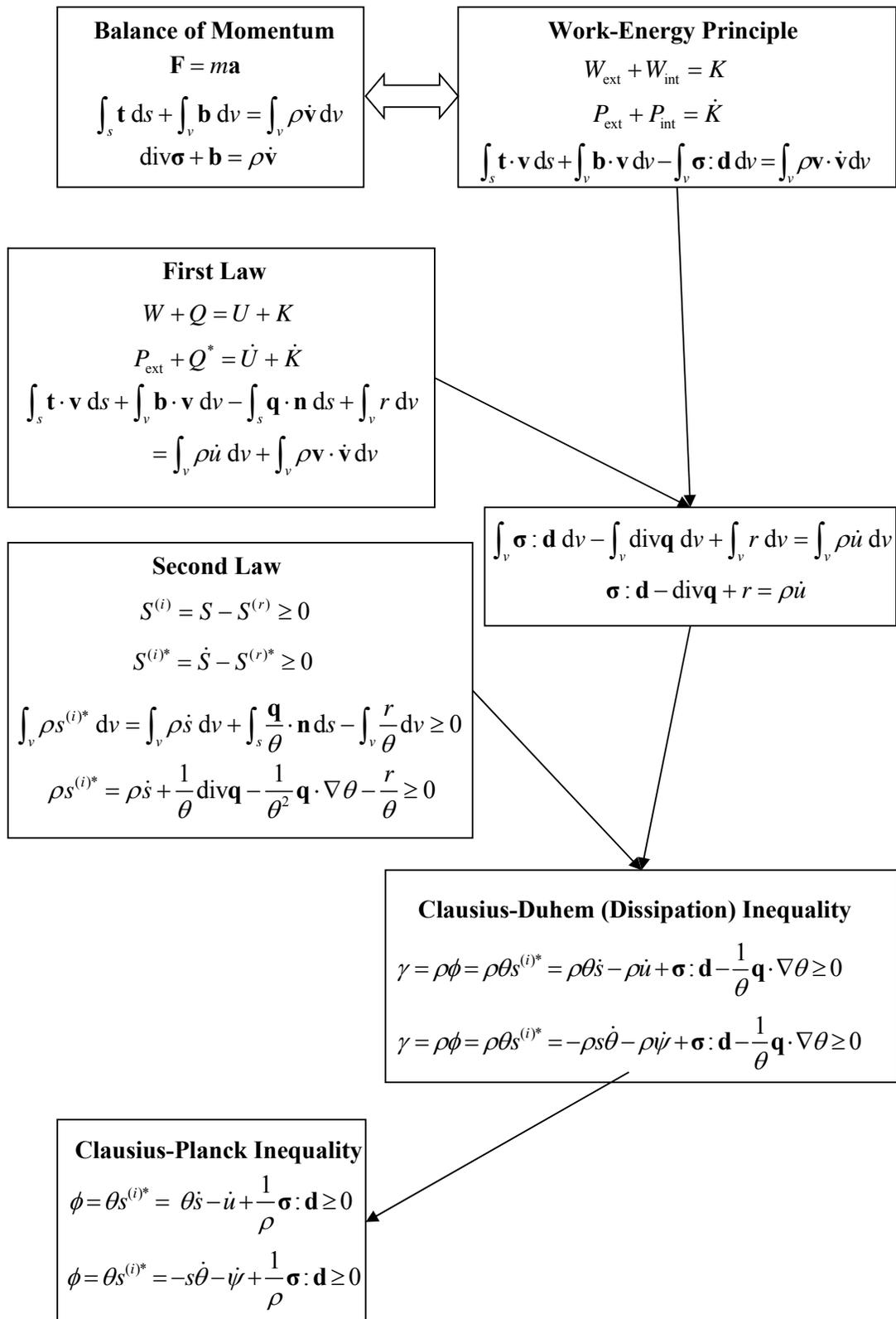


Figure 4.4.2: Thermomechanics

4.4.7 The use of Thermomechanics in Developing Material Models

Material models and the consequences of the laws of thermomechanics will be discussed in depth in Part IV. Here, as an introduction, the case of small-strain elastic/thermoelastic materials will be touched upon briefly.

The classical thermodynamic expression for the work done to a system is $\delta W = -pdV$. This was generalised to the continuum statement for the power exerted on an infinitesimal element, $\boldsymbol{\sigma} : \mathbf{d}$. In the same way, the kinematic variable of the classical thermodynamic system, V , is generalised to the case of a continuum by considering the state to be a function of the *strains*.

When the strains are small, the rate of deformation is equivalent to the time rate of change of the small strain tensor:

$$\mathbf{d} = \dot{\boldsymbol{\varepsilon}}, \quad d_{ij} = \dot{\varepsilon}_{ij} \quad (4.4.29)$$

The dissipation inequalities are then

$$\begin{aligned} \phi = \theta \dot{s} - \dot{u} + \frac{1}{\rho} \sigma_{ij} \dot{\varepsilon}_{ij} - \frac{1}{\rho \theta} q_i \theta_{,i} \geq 0, \quad \phi = \theta \dot{s} - \dot{u} + \frac{1}{\rho} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{1}{\rho \theta} \mathbf{q} \cdot \nabla \theta \geq 0 \\ \text{or} \\ \phi = -s \dot{\theta} - \dot{\psi} + \frac{1}{\rho} \sigma_{ij} \dot{\varepsilon}_{ij} - \frac{1}{\rho \theta} q_i \theta_{,i} \geq 0, \quad \phi = -s \dot{\theta} - \dot{\psi} + \frac{1}{\rho} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{1}{\rho \theta} \mathbf{q} \cdot \nabla \theta \geq 0 \end{aligned} \quad (4.4.30)$$

Reversible Process

In the case of reversible processes:

$$\begin{aligned} \theta \dot{s} - \dot{u} + \frac{1}{\rho} \sigma_{ij} \dot{\varepsilon}_{ij} - \frac{1}{\rho \theta} q_i \theta_{,i} = 0, \quad \theta \dot{s} - \dot{u} + \frac{1}{\rho} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{1}{\rho \theta} \mathbf{q} \cdot \nabla \theta = 0 \\ \text{or} \\ -s \dot{\theta} - \dot{\psi} + \frac{1}{\rho} \sigma_{ij} \dot{\varepsilon}_{ij} - \frac{1}{\rho \theta} q_i \theta_{,i} = 0, \quad -s \dot{\theta} - \dot{\psi} + \frac{1}{\rho} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{1}{\rho \theta} \mathbf{q} \cdot \nabla \theta = 0 \end{aligned} \quad (4.4.31)$$

Consider now a material whose state is completely defined by the set of state variables $(\theta, \varepsilon_{ij})$, so the free energy state function is $\psi = \psi(\theta, \varepsilon_{ij})$. This defines the **thermoelastic material**. The internal energy is expressed in canonical form as $u = u(s, \varepsilon_{ij})$ (see section 4.3). One then has

$$\dot{u} = \frac{\partial u}{\partial s} \dot{s} + \frac{\partial u}{\partial \varepsilon_{ij}} \dot{\varepsilon}_{ij} \quad \text{and} \quad \dot{\psi} = \frac{\partial \psi}{\partial \theta} \dot{\theta} + \frac{\partial \psi}{\partial \varepsilon_{ij}} \dot{\varepsilon}_{ij} \quad (4.4.32)$$

Thus

$$\begin{aligned}
 \left(\theta - \frac{\partial u}{\partial s}\right) \dot{s} + \left(\frac{1}{\rho} \sigma_{ij} - \frac{\partial u}{\partial \varepsilon_{ij}}\right) \dot{\varepsilon}_{ij} + \frac{1}{\rho \theta} q_i \theta_{,i} &= 0 \\
 \left(\theta - \frac{\partial u}{\partial s}\right) \dot{s} + \left(\frac{1}{\rho} \boldsymbol{\sigma} - \frac{\partial u}{\partial \boldsymbol{\varepsilon}}\right) : \dot{\boldsymbol{\varepsilon}} + \frac{1}{\rho \theta} \mathbf{q} \cdot \nabla \theta &= 0 \\
 \text{or} \\
 -\left(s + \frac{\partial \psi}{\partial \theta}\right) \dot{\theta} + \left(\frac{1}{\rho} \sigma_{ij} - \frac{\partial \psi}{\partial \varepsilon_{ij}}\right) \dot{\varepsilon}_{ij} - \frac{1}{\rho \theta} q_i \theta_{,i} &= 0 \\
 -\left(s + \frac{\partial \psi}{\partial \theta}\right) \dot{\theta} + \left(\frac{1}{\rho} \boldsymbol{\sigma} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}\right) : \dot{\boldsymbol{\varepsilon}} - \frac{1}{\rho \theta} \mathbf{q} \cdot \nabla \theta &= 0
 \end{aligned} \tag{4.4.33}$$

Consider now the free energy equation here (the argument which follows applies also to the internal energy equation). The state variables are $(\theta, \varepsilon_{ij})$ and the other properties are state functions of these variables; these include all the terms inside the brackets, that is, s, ψ, σ_{ij} and also the partial derivatives. For any particular state, these properties will have certain values. On the other hand, no matter the state, the variables $\dot{\theta}, \dot{\varepsilon}_{ij}, \theta_{,i}$ can (in theory) be assigned arbitrary values: negative, zero or positive. The terms which pre-multiply $\dot{\theta}, \dot{\varepsilon}_{ij}$ are *completely independent* of these variables – indeed, this fact is built into the model under consideration: the state is a function of $(\theta, \varepsilon_{ij})$ only and is not, for example, dependent on the values of $\dot{\theta}, \dot{\varepsilon}_{ij}, \theta_{,i}$. On the other hand, \mathbf{q} is not a state function and in fact may be a function of the temperature gradients. The only way that Eqn. 4.4.33 can be satisfied in general, then, is for

$$\nabla \theta = 0 \tag{4.4.34}$$

and the following relations must hold (compare these with 4.3.3 and 4.3.8):

$$\boxed{\theta = \frac{\partial u}{\partial s}, \quad \sigma_{ij} = \rho \frac{\partial u}{\partial \varepsilon_{ij}}} \quad \text{and} \quad \boxed{s = -\frac{\partial \psi}{\partial \theta}, \quad \sigma_{ij} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij}}} \tag{4.4.35}$$

Constitutive Relations for Small-Strain Reversible Processes

Note that the density (and volume) changes for small strains may be neglected, so that the density in 4.4.35 can be taken to be the current density or the density in the undeformed configuration, ρ_0 .

4.4.8 Thermomechanics in the Material Form

The dissipation inequality is derived here for the case of the material description.

The First Law

In order to rewrite the energy balance equations in material form, first introduce the scalars (what follows is analogous to the definitions of traction and stress with respect to the current and reference configurations)

$$\begin{aligned} q^{(n)} &= -\mathbf{q} \cdot \mathbf{n} \\ Q^{(N)} &= -\mathbf{Q} \cdot \mathbf{N} \end{aligned} \quad (4.4.36)$$

Here \mathbf{q} is the **Cauchy heat flux** of Eqn. 4.4.4, defined per unit current surface area ds with outward normal \mathbf{n} , and \mathbf{Q} the **Piola-Kirchhoff heat flux**, defined per unit reference surface area dS and outward normal \mathbf{N} .

The rate of heat transfer into the material can now be written as either of

$$-\int_s \mathbf{q} \cdot \mathbf{n} ds = -\int_S \mathbf{Q} \cdot \mathbf{N} dS \quad (4.4.37)$$

Using Nanson's formula, Part III, Eqn. 2.2.59, $\mathbf{n} ds = \mathbf{J}\mathbf{F}^{-T}\mathbf{N} dS$, the Cauchy and Piola-Kirchhoff heat flux vectors are related through $\mathbf{Q} = \mathbf{J}\mathbf{F}^{-1}\mathbf{q}$.

The combination of the mechanical energy balance with the first law, i.e. Eqn. 4.4.3, then reads (see also Part III, Eqn. 3.8.26)

$$\int_V \mathbf{P} : \dot{\mathbf{F}} dV - \int_V \text{Div} \mathbf{Q} dV + \int_V R dV = \int_V \rho_0 \dot{u} dV \quad (4.4.38)$$

where $\int_V R dV = \int_v r dv$, or, in local form,

$$\mathbf{P} : \dot{\mathbf{F}} - \text{Div} \mathbf{Q} + R = \rho_0 \dot{u} \quad (4.4.39)$$

or

$$\mathbf{S} : \dot{\mathbf{E}} - \text{Div} \mathbf{Q} + R = \rho_0 \dot{u} \quad (4.4.40)$$

Note that, comparing the spatial and material forms,

$$\int_V \text{Div} \mathbf{Q} dV = \int_v \text{div} \mathbf{q} dv, \quad \text{Div} \mathbf{Q} = J \text{div} \mathbf{q}, \quad \frac{1}{\rho_0} \text{Div} \mathbf{Q} = \frac{1}{\rho} \text{div} \mathbf{q} \quad (4.4.41)$$

The Second Law

Analogous to Eqn. 4.4.13, the second law can be expressed in material form as

$$\frac{d}{dt} \int_V \rho_0 s dV + \int_V \text{Div} \left(\frac{\mathbf{Q}}{\theta} \right) dV - \int_V \frac{R}{\theta} dV \geq 0 \quad (4.4.42)$$

or, analogous to 4.4.16, one has the dissipation inequality

$$\theta s^{(i)*} = \theta \dot{s} - \dot{u} + \frac{1}{\rho_0} (\mathbf{P} : \dot{\mathbf{F}}) - \frac{1}{\rho_0 \theta} (\mathbf{Q} \cdot \text{Grad} \theta) \geq 0 \quad (4.4.43)$$

Isothermal Conditions

In an isothermal process,

$$\phi = \theta \dot{s} - \dot{u} + \frac{1}{\rho_0} (\mathbf{P} : \dot{\mathbf{F}}) \geq 0 \quad \text{or} \quad \phi = -\dot{\psi} + \frac{1}{\rho_0} (\mathbf{P} : \dot{\mathbf{F}}) \geq 0 \quad (4.4.44)$$

The second of these can be written as

$$\mathbf{P} : \dot{\mathbf{F}} = \rho_0 \dot{\psi} + \rho_0 \phi \quad \text{with} \quad \phi \geq 0 \quad (4.4.45)$$

where the rate of free energy ($\rho_0 \dot{\psi}$) and the dissipation ($\rho_0 \phi$) are per unit reference volume.

4.4.9 Objectivity

By definition, the scalars heat Q , internal energy U , entropy S and temperature θ are objective, that is they remain unchanged under an observer transformation 2.8.7. It follows that the heat flux vector \mathbf{q} is also objective, transforming according to 2.8.10. By definition, the vector entropy flux \mathbf{s}_q is objective, that is it transforms according to 2.8.10.

4.4.10 Problems

1. Show that $\text{div} \left(\frac{\mathbf{q}}{\theta} \right) = \frac{1}{\theta} \text{div} \mathbf{q} - \frac{1}{\theta^2} (\mathbf{q} \cdot \nabla \theta)$
2. Show that the relation $\mathbf{Q} = J \mathbf{F}^{-1} \mathbf{q}$ is consistent with the relation 4.4.41, $\text{Div} \mathbf{Q} = J \text{div} \mathbf{q}$.