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GENERALIZED LAGRANGIAN THERMODYNAMICS OF THERMORHEOLOGY

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The thermodynamic principle of virtual dissipation is given a formulation with variations of the field components freed from any constraints. Application of the principle and the introduction of a new state variable called heat content leads to the integro-differential field equations of thermorheology. Rigorous Lagrangian equations are also obtained which avoid the use of the entropy produced as an auxiliary variable while taking into account the heat generated. Quasi-isothermal and quasi-adiabatic evolutions are considered. Attention is called to the completeness of the generalized coordinate description and to implications in finite-element and bifurcation analysis based on the Lagrangian equations.

INTRODUCTION

In a previous work [6] a thermodynamic principle of virtual dissipation was derived and was used to obtain the field differential equations, constitutive equations, and Lagrangian equations of finite thermorheology. Our purpose here is twofold. First, to express the variational principle in a form valid for completely free variations in a domain which includes the boundary. Second, to introduce a new state variable, called the heat content, which eliminates the cumbersome need of introducing the entropy produced as an auxiliary variable for a rigorous description of the state of the system.

After introductory sections recalling a nontensorial description of finite strain, and an evaluation of the basic thermodynamic functions of solids, the principle of virtual dissipation is formulated in two forms, called unmodified and modified. It is pointed that they do not imply the validity of the Onsager relations. The principle is interpreted physically in terms of availability. Its application using the new state variable leads to field equations that are now integro-differential. Rigorous Lagrangian equations are also derived with complete generality. The new formulation leads to drastic simplifications in two important practical cases of evolution which are quasi-isothermal or quasi-adiabatic. The new concepts also clarify the classical theory of linear thermoelasticity. The theory which is first presented in the context of finite thermoelasticity is also applied to a solid with rate-dependent stresses. This includes non-Newtonian fluids. Two kinds of entropy productions are brought out, with or without heat generation. This yields Lagrangian

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equations that take into account the heat generation. They are nonlinear in the rate variables even in the case where the local irreversible thermodynamics is linear.

It is pointed out that the physical descriptions by generalized coordinates is physically complete and rigorous. *They should not be confused with "trial functions." Also, the Lagrangian formulation provides implicitly finite-element methods as well as a new type of bifurcation analysis where the generalized coordinates represent finite departures from a given evolution.*

THE NONTENSORIAL DEFINITION OF FINITE STRAIN AND STRESS

We shall first recall a treatment of finite strain used extensively by the author since 1934 (see, for example, [1] and [2]) and based on virtual work as distinguished from prevailing trends. The treatment includes the tensor definition as a particular case. The procedure is not only simpler but also more general and easily applicable to media with anisotropy. It is ideally suited for thermodynamics. The power and importance of virtual-work methods in continuum mechanics has also been emphasized by Washizu [3].

Consider first a homogeneous deformation. The initial coordinates x_i of the material points become

$$\bar{x}_i = (\delta_{ij} + a_{ij})x_j \tag{1}$$

where δ_{ij} is the unit matrix and a_{ij} are nine coefficients corresponding to nine independent degrees of freedom. One group is represented by three functions of a_{ij} corresponding to a solid rotation. The other group of six functions of a_{ij} represents the strain, and these are denoted by ϵ_{ij}. The notation ij does not imply that these quantities represent a tensor; they constitute only six independent quantities chosen as strain components. A large variety of choice is possible, subject to the condition that these six components are invariant under a rotation. For example, consider rotated axes x_i' for which the transformation (1) becomes

$$\bar{x}_i = (\delta_{ij} + a_{ij}')x_j' \tag{2}$$

in such a way that

$$a_{ij}' = a_{ji}'$$

In this case we define the strain components as [1]

$$\epsilon_{ij} = \epsilon_{ji} = a_{ij}' = a_{ji}' \tag{3}$$

Relative to the axes x_i' the principal directions of strain remain invariant in the transformation (2). We may consider this case to be obtained by considering a unit cube initially oriented along the axes x_i. The cube is rotated rigidly together with the axes x_i', after which the symmetric transformation (2) is applied. The combined rotation and deformation is chosen to be equivalent to the general affine transformation (1).

In another choice the rotated axes x'_i are such that three of the displacements gradients a'_{ij} are put equal to zero, while the six remaining ones represent the strain ϵ_{ij}. This will be the case, for example, if the direction x'_1 is attached to the material while the material initially in the $x'_1x'_2$ plane remains in it. This method is particularly useful for anisotropic materials because the formulation of stress-strain properties may be tailored to the physics of the material and considerably simplified. *It is ideally suited for fiber or laminated composites.*

In this method we must, of course, be able to evaluate the six strain components $\epsilon_{ij}(a_{\ell k})$ as functions of the nine parameters a_{ij}. It was shown that this can easily be done to any order to approximation by a systematic procedure [1, 2]. In practice, for a vast category of problems the second-order approximation is satisfactory. We may also, of course, use Green's tensor

$$\epsilon_{ij} = \tfrac{1}{2}(a_{ij} + a_{ji} + a_{ki}a_{kj}) \tag{4}$$

as a definition of strain. Although it is expressed directly as a function of a_{ij}, in practice it leads to difficulties because it is nonlinearly related to the extension ratios, thereby introducing spurious and unnecessary nonlinear terms in the physical description. Also, the nonlinearities due to the geometry of rotation cannot be clearly separated from those due to the physical properties, which is particularly cumbersome for initially stressed media.

There are six force components τ_{ij} associated with ϵ_{ij}, and these represent the finite stress. They are defined as follows. We consider an initial cubic element of the material of unit size. After deformation defined by the strain components ϵ_{ij} we impose an arbitrary virtual deformation $\delta\epsilon_{ij}$. The virtual work of the forces acting on the faces of the deformed element is written as

$$\delta \mathscr{W} = \tau_{ij}\, \delta\epsilon_{ij} \tag{5}$$

The notation here must be understood to mean a summation extended to the *six independent components* ϵ_{ij}. Relation (5) is used to define the six stress components τ_{ij}. When $\epsilon_{ij} = \epsilon_{ji}$ is a symmetric tensor, in order to conform to usual definitions of τ_{ij} we simply count twice the terms in $\tau_{ij}\, \delta\epsilon_{ij}$ for which $\epsilon_{ij} = \epsilon_{ji}$. The stress $\tau_{ij} = \tau_{ji}$ is then also a symmetric tensor. This definition is completely general and is valid whatever the choice of definition of ϵ_{ij}. The quantity $\delta \mathscr{W}$ is a *physical invariant.* However, the factors τ_{ij} and $\delta\epsilon_{ij}$ are not necessarily tensors. For a nonhomogeneous deformation the initial coordinates x_i become $\bar{x}_i = x_i + u_i$, where the displacements u_i of material points are functions of x_i and the time t. This defines a local homogeneous transformation

$$d\bar{x}_i = (\delta_{ij} + a_{ij})\, dx_j \tag{6}$$

where

$$a_{ij} = \frac{\partial u_i}{\partial x_j} \tag{7}$$

are the displacement gradients. With this value of a_{ij} the local strain, stress, and rotation are defined as for the homogeneous deformation (1).

The virtual work (5) may be written as

$$\delta \mathscr{W} = \tau_{\mu\nu} \frac{\partial \epsilon_{\mu\nu}}{\partial a_{ij}} \delta a_{ij} = T_{ij}\, \delta a_{ij} \tag{8}$$

where

$$T_{ij} = \tau_{\mu\nu} \frac{\partial \epsilon_{\mu\nu}}{\partial a_{ij}} \tag{9}$$

is the Piola tensor. Because of the geometric significance of δa_{ij}, the nine components T_{ij} are the forces along x_i acting on the faces of a rotated and deformed element which is initially a unit cube oriented along the same fixed axes x_i. Only six of the components T_{ij} are independent since they must satisfy three equations of equilibrium of moments obtained by canceling the virtual work of T_{ij} for a rigid rotation of the deformed material. We proceed as follows. Write the variations $\delta \bar{x}_i$ of the transformed coordinates as

$$\delta \bar{x}_i = x_j\, \delta a_{ij} \tag{10}$$

In terms of the final coordinates $\bar{x}_i$, we may write this in the form

$$\delta \bar{x}_i = \bar{x}_j\, \delta \bar{a}_{ij} \tag{11}$$

where $\delta \bar{a}_{ij}$ are suitable coefficients. It is convenient to write the transformation (1) as

$$\bar{x}_j = c_{jk} x_k \tag{12}$$

where $c_{ij} = \delta_{ij} + a_{ij}$. Substitution of this value into (11) yields

$$\delta \bar{x}_i = c_{jk} x_k\, \delta \bar{a}_{ij} \tag{13}$$

Comparing this results with (10), we derive

$$\delta a_{ik} = c_{jk}\, \delta \bar{a}_{ij} \tag{14}$$

With this value of δa_{ij} the virtual work (8) becomes

$$\delta \mathscr{W} = T_{ik} c_{jk}\, \delta \bar{a}_{ij} \tag{15}$$

A virtual rigid rotation after deformation is represented by

$$\begin{aligned} \delta \bar{a}_{ij} &= 0 \qquad \text{for } i = j \\ \delta \bar{a}_{ij} &= -\delta \bar{a}_{ji} \qquad \text{for } i \neq j \end{aligned} \tag{16}$$

Equilibrium requires the virtual work (15) to vanish for this case. This implies that

$$T_{ik}c_{jk} = T_{jk}c_{ik} \tag{17}$$

These three relations between the nine components T_{ij} are required due to equilibrium of moments.

An interesting formula is also obtained for the stress referred to unit areas after deformation along the fixed directions x_i. The virtual work with these stresses is expressed by

$$\delta \mathscr{W} = \sigma_{ij} J\, \delta \bar{a}_{ij} \tag{18}$$

where J is the Jacobian of the transformation (1) and represents the volume of the deformed initial unit cube. Equating the two values (15) and (18) we derive

$$\sigma_{ij} = \sigma_{ji} = \frac{1}{J} T_{ik}c_{jk} \tag{19}$$

The symmetry of σ_{ij} is due to the condition (17) of equilibrium of moments. Finally, with the value (9) of T_{ik} we obtain

$$\sigma_{ij} = \frac{1}{J} \tau_{\mu\nu} c_{jk} \frac{\partial \epsilon_{\mu\nu}}{\partial a_{ik}} \tag{20}$$

a formula which is valid for any choice of definition of $\epsilon_{\mu\nu}$ and $\tau_{\mu\nu}$ *including nontensorial ones*. As pointed out, we note that the repeated indices $\mu\nu$ in the formula (20) indicate a summation with respect to all *six independent* strain components $\epsilon_{\mu\nu}$.

THERMODYNAMIC FUNCTIONS OF FINITE THERMOELASTICITY

The equations of state are the relations between the stress τ_{ij}, the strain ϵ_{ij}, and the temperature T, expressed as

$$\tau_{ij} = \tau_{ij}(\epsilon_{\ell k}, T) \tag{21}$$

where $\epsilon_{\ell k}$ denotes all six components of the strain and is assumed to be known from experiment.

The energy $\mathscr{U}$ and the entropy $\mathscr{S}$ per unit initial volume are state variable functions of ϵ_{ij} and T. They obey the differential relation

$$d\mathscr{U} = \tau_{ij}\, d\epsilon_{ij} + T\, d\mathscr{S} \tag{22}$$

The arbitrary constants in the values of $\mathscr{U}$ and $\mathscr{S}$ are chosen such that $\mathscr{U} = \mathscr{S} = 0$ in the initial undeformed state $\epsilon_{ij} = 0$ at the temperature T_0. The entropy $\mathscr{S}$ may be evaluated when we know the equations of state (21) and one of the heat-capacity coefficients without any additional calorimetric measurement. This important result is obtained by extending to solids the classical Maxwell procedure.

We write the exact differentials

$$d(\mathscr{U} - T\mathscr{S}) = \tau_{ij}\, d\epsilon_{ij} - \mathscr{S}\, dT \tag{23}$$

$$d(\mathscr{U} - T\mathscr{S} - \tau_{ij}\epsilon_{ij}) = -\epsilon_{ij}\, d\tau_{ij} - \mathscr{S}\, dT \tag{24}$$

which imply

$$\left(\frac{\partial \mathscr{S}}{\partial \epsilon_{ij}}\right)_T = -\left(\frac{\partial \tau_{ij}}{\partial T}\right)_\epsilon \qquad \left(\frac{\partial \mathscr{S}}{\partial \tau_{ij}}\right)_T = \left(\frac{\partial \epsilon_{ij}}{\partial T}\right)_\tau \tag{25}$$

The subscripts ϵ and τ indicate that ϵ_{ij} and τ_{ij} are kept constant, respectively, in the differentiation. We now write the entropy differentials

$$d\mathscr{S} = \left(\frac{\partial \mathscr{S}}{\partial \epsilon_{ij}}\right)_T d\epsilon_{ij} + \frac{c_\epsilon}{T}\, dT \tag{26}$$

$$d\mathscr{S} = \left(\frac{\partial \mathscr{S}}{\partial \tau_{ij}}\right) d\tau_{ij} + \frac{c_\tau}{T}\, dT \tag{27}$$

By definition of $\mathscr{S}$ the quantities

$$c_\epsilon = T\left(\frac{\partial \mathscr{S}}{\partial T}\right)_\epsilon \qquad c_\tau = T\left(\frac{\partial \mathscr{S}}{\partial T}\right)_\tau \tag{28}$$

are the heat capacities per unit initial volume at constant strain and constant stress, respectively. They may be measured as functions of ϵ_{ij} and T or of τ_{ij} and T.

Substitution of the values (25) into (26) and (27) yields

$$d\mathscr{S} = -\left(\frac{\partial \tau_{ij}}{\partial T}\right)_\epsilon d\epsilon_{ij} + \frac{c_\epsilon}{T}\, dT \tag{29}$$

$$d\mathscr{S} = \left(\frac{\partial \epsilon_{ij}}{\partial T}\right)_\tau d\tau_{ij} + \frac{c_\tau}{T}\, dT \tag{30}$$

Since these are exact differentials, we derive

$$-\left(\frac{\partial^2 \tau_{ij}}{\partial T^2}\right)_\epsilon = \frac{1}{T}\left(\frac{\partial c_\epsilon}{\partial \epsilon_{ij}}\right)_T \qquad \left(\frac{\partial^2 \epsilon_{ij}}{\partial T^2}\right)_\tau = \frac{1}{T}\left(\frac{\partial c_\tau}{\partial \tau_{ij}}\right)_T \tag{31}$$

Hence, thermodynamics along with the equations of state limit the choice of possible values for c_ϵ and c_τ as functions of ϵ_{ij} and T or of τ_{ij} and T. There is also a relation between these two heat capacities. It is derived by substituting into (30) the differential

$$d\tau_{ij} = \left(\frac{\partial\tau_{ij}}{\partial\epsilon_{\mu\nu}}\right)_T d\epsilon_{\mu\nu} + \left(\frac{\partial\tau_{ij}}{\partial T}\right)_\epsilon dT \tag{32}$$

This yields

$$d\mathscr{S} = \left(\frac{\partial\epsilon_{ij}}{\partial T}\right)_\tau \left(\frac{\partial\tau_{ij}}{\partial\epsilon_{\mu\nu}}\right)_T d\epsilon_{\mu\nu} + \left[\frac{c_\tau}{T} + \left(\frac{\partial\epsilon_{ij}}{\partial T}\right)_\tau \left(\frac{\partial\tau_{ij}}{\partial T}\right)_\epsilon\right] dT \tag{33}$$

By comparing this expression with (29) we find

$$c_\epsilon = c_\tau + T\left(\frac{\partial\epsilon_{ij}}{\partial T}\right)_\tau \left(\frac{\partial\tau_{ij}}{\partial T}\right)_\epsilon \tag{34}$$

Thus when we know the equations of state (21) we may obtain c_ϵ from c_τ, which is much easier to measure.

The differential of the energy is now derived from (22) by substituting into this value one of the differentials (29) or (30) of $\mathscr{S}$. For example, in terms of ϵ_{ij} and T we write

$$d\mathscr{U} = \left[\tau_{ij} - T\left(\frac{\partial\tau_{ij}}{\partial T}\right)_\epsilon\right] d\epsilon_{ij} + c_\epsilon\, dT \tag{35}$$

By integrating (29) and (35) along any suitable path, we obtain the values

$$\mathscr{U} = \mathscr{U}(\epsilon_{ij}, T) \qquad \mathscr{S} = \mathscr{S}(\epsilon_{ij}, T) \tag{36}$$

as functions of ϵ_{ij} and T.

The total energy and entropy of the medium occupying the *initial* domain Ω in the x_i space are

$$U = \int_\Omega \mathscr{U} d\Omega \qquad S = \int_\Omega \mathscr{S} d\Omega \tag{37}$$

The foregoing results concern thermostatic properties for reversible slow deformations. For irreversible transformations with thermal diffusion we consider the heat flux $\dot{H}_i$ *across a deforming material area which in the initial state is equal to unity and normal to x_i* [2]. This heat flux as shown below is a contravariant vector. The total heat flux across a deformed area represented by the surface A in the space of the initial state is

$$\int_A \dot{H}_i n_i \, dA \tag{38}$$

where n_i is the unit normal to A. The dot denotes a time derivative. The time integral H_i of $\dot{H}_i$ with zero initial value will be called the heat fluence vector (previously designated as heat displacement). The time derivative of the entropy is

$$\dot{\mathscr{S}}=\frac{\dot{h}}{T} \qquad \dot{h}=-\frac{\partial \dot{H}_i}{\partial x_i} \tag{39}$$

We may write

$$\dot{\mathscr{S}}=-\frac{\partial}{\partial x_i}\left(\frac{\dot{H}_i}{T}\right)-\frac{\dot{H}_i}{T^2}\frac{\partial T}{\partial x_i} \tag{40}$$

By integrating this expression in a domain Ω of the initial space, assuming no heat flux across the boundary A, we obtain

$$\dot{S}^*=\int_\Omega \dot{\mathscr{S}} d\Omega=-\int_\Omega \frac{\dot{H}_i}{T^2}\frac{\partial T}{\partial x_i}d\Omega \tag{41}$$

Obviously this is the rate of entropy produced in the solid. Use of the symbol $\dot{S}^*$ instead of $\dot{S}$ is to indicate that it represents an entropy *produced.* Since this is true for an arbitrary domain, the rate of entropy produced per unit initial volume is [2]

$$\dot{s}^*=-\frac{\dot{H}_i}{T^2}\frac{\partial T}{\partial x_i} \tag{42}$$

This generalizes for a deformable solid the formally similar expression derived by Meixner for a rigid medium [4].

The law of thermal diffusion is expressed as

$$\dot{H}_i=-K_{ij}\frac{\partial T}{\partial x_i} \qquad \frac{\partial T}{\partial x_i}=-\Lambda_{ij}\dot{H}_j \tag{43}$$

where $K_{ij}(\epsilon_{\ell k}, T)$ and $\Lambda_{ij}(\epsilon_{\ell k}T)$ are functions of the strain and temperature. They are, respectively, the thermal conduction and the resistivity tensor generalized to the contravariant heat flux. With relations (43), the rate of entropy production (42) becomes

$$\dot{s}^*=\frac{1}{T^2}K_{ij}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_j}=\frac{1}{T^2}\Lambda_{ij}\dot{H}_i\dot{H}_j \tag{44}$$

These relations are completely general and show that K_{ij} is a contravariant tensor while its inverse Λ_{ij} is covariant.

In the absence of a magnetic field or Coriolis forces of very high intensity, Onsager's reciprocity relations [5] are expressed by the symmetry properties

$$K_{ij} = K_{ji} \qquad \Lambda_{ij} = \Lambda_{ji} \tag{45}$$

Note that the validity of the present theory *does not require that these reciprocity relations be verified,* since expression (44) involves only the symmetric part of Λ_{ij}.

For an isotropic material with reciprocity relations (45), we must choose a symmetric definition of ϵ_{ij} given by (3) or (4). The energy $\mathscr{U}$ and entropy $\mathscr{S}$ then become functions of the three invariants of ϵ_{ij} and the temperature. The symmetric resistivity (45) for this case is

$$\Lambda_{ij} = \left(\frac{1}{k} + F_1 \epsilon_{kk}\right) \delta_{ij} + F_2 \epsilon_{ij} + F_3 \epsilon_{ik} \epsilon_{jk} \tag{46}$$

where F_1, F_2, F_3 are functions of the invariants and the temperature, and k is the thermal conductivity at zero strain. This equation is invariant under rotation of axes x_i or x_i'. Principal directions coincide, and for axes oriented along these directions it is immediately evident that the relation satisfies isotropy and is the most general. In practice, only linear terms with F_1 and F_2 functions of the temperature only will generally be adequate.

GENERALIZED FORM OF THE PRINCIPLE OF VIRTUAL DISSIPATION

Consider an irreversible evolution of a thermoelastic medium occupying the initial domain Ω. The evolution of the system is described by the field u_i of material point displacements and by the temperature field T as functions of time. We *freeze the system* at any particular instant and apply variations δu_i and δH_i. The variation δu_i is arbitrary. However, we impose upon the variation δH_i the condition that its normal component vanishes at the boundary A of Ω. In other words there is no *virtual* heat transfer across the boundary. Note that this condition is only virtual in the frozen state and *does not imply that in the actual evolution there is no heat flow across the boundary.*

Let us first assume that there are no inertia forces. Under these conditions we may write

$$\delta U = \delta W \tag{47}$$

where δU is the variation of the total energy (37) of the medium and δW is the virtual work of the external forces acting on the medium. Also, from (40), replacing $\dot{H}_i$ by δH_i and $\dot{\mathscr{S}}$ by $\delta \mathscr{S}$ we obtain

$$\delta S = \delta S^* \tag{48}$$

where δS is the variation of the total entropy (37) while δS^* is the variation of the entropy produced. Equation (41) shows that

$$\delta S^* = \int_\Omega \delta s^* \, d\Omega \tag{49}$$

where

$$\delta s^* = -\frac{1}{T^2}\frac{\partial T}{\partial x_i}\delta H_i = \frac{\Lambda_{ij}}{T^2}\dot{H}_j \delta H_i \tag{50}$$

is the virtual entropy produced per unit initial volume.

It follows from (47) and (48) that we may write the variational principle

$$\delta V + T_o \delta S^* = \delta W \tag{51}$$

where T_o is an arbitrary constant having the dimension of a temperature and

$$V = U - T_o S \tag{52}$$

is the thermoelastic potential of the whole medium. We may also write

$$V = \int_\Omega \mathscr{V} d\Omega \tag{53}$$

where

$$\mathscr{V} = \mathscr{U} - T_o \mathscr{S} \tag{54}$$

is the thermoelastic potential per unit initial volume. From the value (22) of $d\mathscr{U}$ we also derive the important differential relation

$$d\mathscr{V} = \tau_{ij} d\epsilon_{ij} + \theta \, d\mathscr{S} \tag{55}$$

where

$$\theta = T - T_o \tag{56}$$

Until now we have assumed δH_i to be subject to the constraint of no virtual heat transfer at the boundary. For the sake of generality it is important to remove this constraint. This is accomplished as follows. We write relations (39) and (55) in variational form as

$$\delta \mathscr{V} = \tau_{ij} \delta \epsilon_{ij} + \theta \delta \mathscr{S} \tag{57}$$

$$\delta \mathscr{S} = -\frac{1}{T}\frac{\partial}{\partial x_i}\delta H_i \tag{58}$$

Hence

$$\delta \mathscr{V} = \tau_{ij}\delta\epsilon_{ij} - \frac{\theta}{T}\frac{\partial}{\partial x_i}\delta H_i \tag{59}$$

Consider now variations δH_i which are arbitrary in the domain Ω except in a thin layer Ω' near the boundary A where the normal component drops rapidly to zero as we approach this boundary. We denote by $\delta\mathscr{V}_c$ the variation which obeys this constraint and by $\delta\mathscr{V}$ the variation which is free. The integral of $\delta\mathscr{V}_c$ over the volume Ω may be split into two terms by writing

$$\int_\Omega \delta\mathscr{V}_c\, d\Omega = \int_{\Omega-\Omega'} \delta\mathscr{V} d\Omega + \int_{\Omega'} \delta\mathscr{V}_c\, d\Omega \tag{60}$$

In the second integral the term containing $(\theta/T)(\partial/\partial x_i)\delta H_i$ becomes infinite as the thickness of the layer Ω' tends to zero. However, the infinity may be removed by integration by parts. In the limit where the layer Ω' vanishes we obtain

$$\int_\Omega \delta\mathscr{V}_c\, d\Omega = \int_\Omega \delta\mathscr{V} d\Omega + \int_A \frac{\theta}{T}\delta H_i n_i\, dA \tag{61}$$

where $\delta H_i n_i$ is the normal component of δH_i at the boundary. On the right-hand side of this equation the variations δH_i are now completely free in Ω as well as at the boundary A. We put

$$\delta W^{TH} = -\int \frac{\theta}{T}\,\delta H_i n_i\, dA \tag{62}$$

which may be considered as the *virtual work of the thermal forces* at the boundary. As a consequence we may write the variational principle (51) as

$$\delta V + T_0\delta S^* = \delta W + \delta W^{TH} \tag{63}$$

where the variations δu_i and δH_i are now completely free and arbitrary in a domain including the boundary.

The variational principle may be extended to dynamical systems. Following d'Alembert's principle, the virtual work of the external forces may include the work of the reversed inertia forces which play the same role as body forces. These inertial body forces per unit initial volume are $\rho\ddot{u}_i$, where $\ddot{u}_i$ is the acceleration and ρ is the initial density of the material elements. If we denote by

$$\delta W^{IN} = \int_\Omega \rho\ddot{u}_i\delta u_i\, d\Omega \tag{64}$$

the virtual work of the inertia forces, we can replace δW by $\delta W - \delta W^{IN}$ in Eq. (63). We obtain

$$\delta W^{IN} + \delta V + T_o \delta S^* = \delta W + \delta W^{TH} \tag{65}$$

This constitutes a generalized form of the *unmodified* principle of virtual dissipation announced earlier for irreversible thermodynamics [6].

If the external forces are partly derived from a mechanical potential G such as gravity, we write

$$G = \int_\Omega \rho\, \mathscr{G}(\bar{x}_i)\, d\Omega \tag{66}$$

where $\mathscr{G}(\bar{x}_i)$ is the body force potential per unit mass at the displaced point $\bar{x}_i = x_i + u_i$ and ρ is the initial density at x_i. We introduce a mixed collective potential [6]

$$\mathscr{P} = V + G \tag{67}$$

and write the variational principle (65) as

$$\delta W^{IN} + \delta \mathscr{P} + T_o \delta S^* = \delta W^M + \delta W^{TH} \tag{68}$$

where δW^M is now the virtual work of the remaining external mechanical forces, namely the forces applied at the boundary. In which case, we may write

$$\delta W^M = \int_A f_i \delta u_i \, dA \tag{69}$$

where f_i is the force per unit initial area at the boundary A.

The term $T_o \delta S^*$ represents a virtual dissipation. While this is not essential, we shall assume the reciprocity relations (45) to be satisfied and introduce a dissipation function

$$\mathscr{D} = \frac{1}{2} T_o \dot{s}^* = \frac{1}{2} \frac{T_o}{T^2} \Lambda_{ij} \dot{H}_i \dot{H}_j \tag{70}$$

With this definition, the values (49) and (50) yield

$$T_o \delta S^* = \int_\Omega T_o \delta s^* \, d\Omega \tag{71}$$

with

$$T_o \delta s^* = \frac{\partial \mathscr{D}}{\partial \dot{H}_i} \delta H_i \tag{72}$$

The principle of virtual dissipation (68) may now be written

$$\delta W^{IN} + \delta \mathscr{P} + T_o \int_\Omega \delta s^* \, d\Omega = \delta W^M + \delta W^{TH} \tag{73}$$

where $T_o \delta s^*$ is expressed by (72) in terms of the dissipation function (70).

Another form of the variational principle is also obtained by introducing a different dissipation function, defined as

$$\mathscr{D}_{in} = \tfrac{1}{2} T \dot{s}^* = \tfrac{1}{2} T \Lambda_{ij} \dot{S}_i \dot{S}_j \tag{74}$$

where $\dot{S}_i = \dot{H}/T$ is the entropy flux. In this case we may write

$$T \delta s^* = \frac{\partial \mathscr{D}_{in}}{\partial \dot{S}_i} \delta S_i \qquad \delta S_i = \frac{\delta H_i}{T} \tag{75}$$

Also

$$\mathscr{S} = \frac{\partial S_i}{\partial x_i} + s^* \tag{76}$$

where S_i is the entropy fluence vector defined as the time integral of $\dot{S}_i$ and s^* is the total entropy produced. We then vary arbitrarily δu_i and δS_i. It can easily be shown [6] that the variational principle (73) becomes

$$\delta W^{IN} + \delta_r \mathscr{P} + \int_\Omega T \delta s^* = \delta W^M + \delta W^{TH} \tag{77}$$

where $T \delta s^*$ is given by (75) while

$$\delta W^{TH} = - \int_A \theta \, \delta S_i \, n_i \, dA \tag{78}$$

The term $\delta_r \mathscr{P}$ is a variation obtained by putting $\delta \mathscr{S} = -(\partial/\partial x_i) \delta S_i$. We shall call (77) the *modified form* of the principle of virtual dissipation. We also refer to $\mathscr{D}$ and $\mathscr{D}_{in}$, respectively, as the *relative* and *intrinsic* dissipation functions. They obey the relation

$$\mathscr{D} = \frac{T_o}{T} \mathscr{D}_{in} \tag{79}$$

The reason for this appellation will be discussed in the next section along with the physical interpretation of the virtual dissipation $T_o \delta S^*$.

If the Onsager reciprocity relations are not satisfied, the virtual dissipations $T_o \delta s^*$ and $T \delta s^*$ contain an antisymmetric term analogous to a gyrostatic force in mechanics where the virtual work principle retains its validity *although the force performs no physical work. This validity extends to the virtual dissipation.*

PHYSICAL SIGNIFICANCE OF THE THERMOELASTIC POTENTIAL

The foregoing derivation is based on the introduction of an arbitrary chosen constant T_0, which has the dimension of a temperature. A fundamental physical interpretation of the thermoelastic potential is obtained by adjoining to the system Ω a large isothermal thermal well TW at the temperature T_0. The system Ω + TW constitutes a hypersystem [6].

We start from a ground state of this hypersystem where Ω is stress free and at the temperature T_0. The hypersystem is then subjected to an arbitrary reversible transformation where work is performed on it by external forces without any exchange of heat from outside this system. However, heat is provided to Ω by transfer from the thermal well by the use of reversible heat pumps. Since the transformation is reversible, the total increase of entropy of the hypersystem is zero. Therefore, if S is the entropy of Ω the entropy of the thermal well is $-S$ and its energy is $-T_0 S$. With U denoting the energy of Ω, the total energy of the hypersystem is

$$V = U - T_0 S \tag{80}$$

This provides the physical interpretation of the thermoelastic potential. The same interpretation is also obtained by considering the differential (55) of $\mathscr{V}$, where the term $\tau_{ij} d\epsilon_{ij}$ is the work of the stresses on an element, while $\theta d\mathscr{S}$ represents the work required by a reversible heat pump extracting heat from the thermal well and injecting into the element a quantity of heat $T d\mathscr{S}$ at the temperature T. As indicated earlier [7], the heat pump may operate through a Carnot cycle, or without any cycling, by pumping pure heat, using a blackbody radiation pump.

Further physical interpretation of the variational principle (68) is obtained by replacing the variations by time derivatives. We may write this in the form

$$\dot{\mathscr{T}} + \dot{\mathscr{P}} = -T_0 \dot{S}^* + \dot{W}^M + \dot{W}^{TH} \tag{81}$$

where

$$\mathscr{T} = \frac{1}{2} \int_\Omega \rho \dot{u}_i \dot{u}_i \, d\Omega \tag{82}$$

is the kinetic energy and

$$\dot{W}^M = \int_A f_i \dot{u}_i \, dA \qquad \dot{W}^{TH} = -\int_A \frac{\theta}{T} \dot{H}_i n_i \, dA \tag{83}$$

The quantity $\mathscr{P} + \mathscr{T}$ may be considered as a generalized "availability" representing the useful energy available in the presence of a thermal well at the temperature T_0 which may be identified with an environment. On the right-hand side, $\dot{W}^{IN}$ and $\dot{W}^{TH}$ represent the influx of availability through the work of external forces and heat influx from the environment. For an irreversible transformation the term $-T_0\dot{S}^*$ is always negative since $\dot{S}^*$ is the rate of entropy production. It represents a loss of availability and is a minimum for a reversible transformation.

This also provides an interpretation of the two dissipation functions (70) and (74) considered above. The intrinsic dissipation rate $2\mathscr{D}_{in}$ represents the loss of availability in the presence of a thermal well whose temperature is equal to the local temperature T. It is a total loss of useful energy. However, in the presence of a thermal well at a lower temperature T_0 the relative rate of dissipation $2\mathscr{D} = 2(T_0/T)\mathscr{D}_{in}$ represents only a partial loss of useful energy. This distinction between intrinsic and relative dissipation was discussed earlier in a more general context [6].

Use of the potential V as the *key potential for irreversible thermodynamics* was introduced and developed by the author in a series of publication originating in 1954. It was referred to at the time as a generalized free energy because for an isothermal transformation it coincides with the Hel~~oh~~holtz free energy. The term "exergy" was later used by others to designate this potential. /m

DERIVATION OF FIELD EQUATIONS FROM THE VARIATIONAL PRINCIPLES

Differential field equations are obtained directly from the unmodified principle of virtual dissipation (68) by varying arbitrarily the fields u_i and H_i *inside* the domain Ω. We obtain the field equations

$$\rho\ddot{u}_i - \frac{\partial}{\partial x_j}\left(\tau_{\mu\nu}\frac{\partial\epsilon_{\mu\nu}}{\partial a_{ij}}\right) + \rho\frac{\partial\mathscr{G}}{\partial\bar{x}_i} = 0 \tag{84}$$

$$\frac{\partial T}{\partial x_i} + \Lambda_{ij}\dot{H}_j = 0 \tag{85}$$

Equations (84) express momentum balance, while Eqs. (85) govern heat conduction. Since $\dot{H}_i$ is not a state variable, a complete description requires the auxiliary equations (38), namely

$$T\dot{\mathscr{S}} + \frac{\partial\dot{H}_i}{\partial x_i} = 0 \tag{86}$$

A scalar formulation is obtained by solving Eqs. (85) for $\dot{H}_i$ and substituting these values into (86). We obtain

$$T\dot{\mathscr{S}} = \frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial T}{\partial x_j}\right) \tag{87}$$

This involves second derivatives and may not be as convenient for numerical work as the vectorial form (85) which satisfies flow continuity and involves only first spatial derivatives.

We may also use the modified form (77) of the variational principle using arbitrary variations of u_i and S_i. This leads to field equations for these variables. Since S_i is not a state variable, an accurate description requires the evaluation of s^* which satisfies the auxiliary equation (74), namely

$$\dot{s}^* = \Lambda_{ij}\dot{S}_i\dot{S}_j \tag{88}$$

These equations also lead to the form (85) with $\dot{H}_i$ by substituting $\dot{S}_i = \dot{H}_i/T$. However, use of the variables S_i has the advantage that we may often neglect the auxiliary equation (88) while preserving flow continuity and the first spatial derivatives. In the next section we shall introduce new state variables that provide a rigorous vectorial formulation preserving flow continuity without the need for auxiliary equations.

THE HEAT CONTENT AS A NEW STATE VARIABLE

As we have seen, use of the vectors H_i or S_i as field variables, while preserving flow continuity, does not provide a complete description of the state of the system without the use of an additional unknown obeying either (86) or (87) as auxiliary equations. In order to avoid this inconvenience we will introduce a new state variable, which we shall call the *heat content.* It is a generalization of a similar concept already used earlier in the more restricted context of pure heat transfer [8].

This may be accomplished in two ways. Starting from a given uniform initial temperature T_o the energy of an element is

$$\mathscr{U} = \mathscr{U}(\epsilon_{ij}, \theta) \tag{89}$$

where $\theta = T - T_o$. We first consider an adiabatic transformation. The temperature increase θ^A for such a transformation is a function only of the strain ϵ_{ij}. The corresponding energy

$$\mathscr{U}(\epsilon_{ij}, \theta^A) = \mathscr{U}^A(\epsilon_{ij}) \tag{90}$$

is also a function only of ϵ_{ij}. The energy (89) may then be written

$$\mathscr{U}(\epsilon_{ij}, \theta) = \mathscr{U}^A(\epsilon_{ij}) + h^A \tag{91}$$

where h^A is the heat to be added *under constant strain* in order to reach a temperature $T = T_o + \theta$. Hence

$$h^A(\epsilon_{ij}, \theta) = \mathscr{U}(\epsilon_{ij}, \theta) - \mathscr{U}^A(\epsilon_{ij}) \tag{92}$$

is a state variable function of ϵ_{ij} and θ. We shall call h^A the *heat content of the first kind.*

The same reasoning applies when we start with an isothermal transformation at a uniform constant temperature T_o for which the energy $\mathscr{U}^B$, the entropy $\mathscr{S}^B$, and the thermoelastic potential $\mathscr{V}^B$ are functions only of ϵ_{ij}. We write

$$\begin{aligned} h^\epsilon &= \mathscr{U}(\epsilon_{ij}, \theta) - \mathscr{U}^B(\epsilon_{ij}) \\ h^B &= h^\epsilon + \mathscr{S}^B T_o = \mathscr{U}(\epsilon_{ij}, \theta) - \mathscr{V}^B \end{aligned} \tag{93}$$

where h^ϵ is the heat to be added under constant strain in order to reach the temperature $T_o + \theta$. We call h^B the *heat content of the second* kind. It is a state variable.

The same formalism may be used for both cases denoting by h^C the heat content, where C is either A or B. With this notation we may write (92) and (93) in the same form as

$$h^C = \mathscr{U}(\epsilon_{ij}, \theta) - \mathscr{V}^C(\epsilon_{ij}) \tag{94}$$

We denote by $\tau_{ij}{}^A(\epsilon_{\varrho k})$ and $\tau_{ij}{}^B(\epsilon_{\varrho k})$ the stress for the adiabatic and isothermal transformations, respectively. Again, they are functions only of the strain. Using the notation $\tau_{ij}{}^C$ where C is either A or B, we may write the differential

$$d\mathscr{V}^C = \tau_{ij}{}^C d\epsilon_{ij} \tag{95}$$

Hence (94) yields

$$d\mathscr{U} = \tau_{ij}{}^C d\epsilon_{ij} + dh^C \tag{96}$$

where ϵ_{ij} and h^C are now *state variables.* The temperature is obtained by solving Eqs. (94) for θ. Note that the differential (96) corresponds to an incremental change in the vicinity of a state of deformation ϵ_{ij} at the temperature $T = T_o + \theta$. We denote by τ_{ij} the actual stress in this state. The energy differential may also be written as

$$d\mathscr{U} = \tau_{ij} d\epsilon_{ij} + dh \tag{97}$$

where dh is the heat to be added to obtain the increments $d\epsilon_{ij}$ and dT. By equating the two values (96) and (97), we obtain

$$dh = (\tau_{ij}{}^C - \tau_{ij}) d\epsilon_{ij} + dh^C \tag{98}$$

With time derivatives, this is written as

$$\dot{h} = (\tau_{ij}{}^C - \tau_{ij}) \dot{\epsilon}_{ij} + \dot{h}^C \tag{99}$$

We may also introduce three contravariant vector fields $\dot{H}_i^+$, $\dot{H}_i$, and $\dot{H}_i^C$ defined per unit initial area in the deformed solid by

$$(\tau_{ij}{}^C - \tau_{ij}) \dot{\epsilon}_{ij} = -\frac{\partial \dot{H}_i^+}{\partial x_i} \tag{100}$$

$$\dot{h} = -\frac{\partial \dot{H}_i}{\partial x_i} \qquad \dot{h}^C = -\frac{\partial \dot{H}_i^C}{\partial x_i} \tag{101}$$

Equation (99) is then satisfied if we put

$$\dot{H}_i = \dot{H}_i^+ + \dot{H}_i^C \tag{102}$$

Integrating $\dot{h}^C$ with respect to time with zero initial values, we obtain

$$h^C = \frac{\partial H_i^C}{\partial x_i} \tag{103}$$

Since h^C is a state variable, the vector H_i^C along with u_i determines the state of the system. Hence H_i^C *is also a state variable.* We shall call H_i^C the *heat content fluence,* $\dot{H}_i^C$ the *heat content flux,* $\dot{H}_i$ the *total heat flux,* and $\dot{H}_i^+$ the *auxiliary heat flux.*

We may write Eq. (100) as

$$\frac{\partial \dot{H}_i^+}{\partial x_i} = \dot{h}^+ \qquad \dot{h}^+ = (\tau_{ij} - \tau_{ij}^C)\dot{e}_{ij} \tag{104}$$

where $\dot{h}^+$ behaves as a fictitious heat source per unit initial volume.

Equation (104) does not define a unique field $\dot{H}_i^+$ in terms of $\dot{h}^+$. A possible choice is obtained by introducing a singular vector field $g_i(x_\ell, x_\ell^+)$ which represents the flux due to a unit source at the point x_ℓ^+. In other words, it satisfies the equation

$$\frac{\partial g_i}{\partial x_i} = \delta(x_\ell, x_\ell^+) \tag{105}$$

where $\delta(x_\ell, x_\ell^+)$ is Dirac's function. A field $\dot{H}_i^+$ is then

$$\dot{H}_i^+ = \int_{\Omega^+} g_i(x_\ell, x_\ell^+)\dot{h}^+ \, d\Omega^+ \tag{106}$$

where integration is over the space Ω^+ of initial coordinates x_ℓ^+.

Note that $\dot{H}_i^+$ as well as g_i still possess a large amount of arbitrariness. They may be chosen, for example, to satisfy conditions of vanishing flow across certain portions of the deformed boundary in the space of initial coordinates.

We now derive the field equations for u_i and H_i^C by applying the unmodified principle of virtual dissipation (68) and varying arbitrarily these two vector fields. From (102) we may write the variation

$$\delta H_i^C = \delta H_i - \delta H_i^+ \tag{107}$$

where

$$\delta H_i^+ = \int_{\Omega^+} g_i(x_\ell, x_\ell^+)\,(\tau_{\mu\nu} - \tau_{\mu\nu}^C)\delta\epsilon_{\mu\nu}\,d\Omega^+ \tag{108}$$

as implied by (104) and (106). Since δH_i^+ is determined by δu_i, we may choose δH_i to vary arbitrarily instead of δH_i^C. With arbitrary variations δH_i and δu_i inside the domain Ω, the variational principle (68) leads to the same field equations (84) and (85) as before, except that the total heat flux $\dot{H}_i$ is now replaced by

$$\dot{H}_i = \int_{\Omega^+} g_i(x_\ell, x_\ell^+)\,(\tau_{\mu\nu} - \tau_{\mu\nu}^C)\dot{\epsilon}_{\mu\nu}\,d\Omega^+ + \dot{H}_i^C \tag{109}$$

Hence the field equations for u_i and H_i^C become integro-differential equations, where the local state variables are ϵ_{ij} and $h^C = -\partial H_i^C/\partial x_i$. These variables completely determine the history of evolution of the system and the auxiliary equation (86) is not needed. The same result is also obtained by using the modified form of the variational principle.

GENERALIZED LAGRANGIAN EQUATIONS

In the past we have derived Lagrangian equations from the modified form (77) of the virtual dissipation principle using the entropy fluence vector S_i as a field variable. A rigorous description of the system in this formulation required the introduction of the entropy produced, s^*, as an additional variable, with an auxiliary equation. While this auxiliary variable could be neglected in first approximation, its elimination should provide a fundamental improvement. This can now be accomplished by using the heat content fluence H_i^C as a state variable which preserves the flux continuity. By this procedure the principle of virtual dissipation in its unmodified form (65) leads to rigorous Lagrangian equations of evolution which involve no approximation.

We express the vector fields

$$u_j = u_j(q_i, x_\ell) \qquad H_i^C = H_i^C(q_i, x_\ell) \tag{110}$$

as functions of the initial coordinates x_i and a finite number of generalized coordinates q_i, which are unknown functions of time to be determined. The functions u_j and H_i^C may also contain the time as an explicit variable if need be, but this variable is omitted here for simplicity. The local state variables ϵ_{ij} and h^C may be expressed here as functions of q_i and x_i, and the mixed collective potential $\mathscr{P}(q_i)$ becomes a function of q_i. We may write

$$\delta\mathscr{P} = \frac{\partial\mathscr{P}}{\partial q_i}\,\delta q_i \tag{111}$$

with arbitrary variations δq_i. The variations of the fields (110) are

$$\delta u_j = \frac{\partial u_j}{\partial q_i}\,\delta q_i \qquad \delta H_j^C = \frac{\partial H_j^C}{\partial q_i}\,\delta q_i \tag{112}$$

From (102), (104), (106), (108), and (112) we also derive

$$\delta H_j = \mathscr{L}_{ji}\delta q_i \qquad \dot{H}_j = \mathscr{L}_{ji}\dot{q}_i \tag{113}$$

where

$$\mathscr{L}_{ji}(q_k, x_\varrho) = \int_{\Omega^+} g_j(x_\varrho, x_\varrho^+)(\tau_{\mu\nu} - \tau_{\mu\nu}^C)\frac{\partial \epsilon_{\mu\nu}}{\partial q_i} d\Omega^+ + \frac{\partial H_j^C}{\partial q_i} \tag{114}$$

This quantity is a function of the set of q_i's and the initial coordinates x_ϱ. The virtual work of the mechanical and thermal boundary force is

$$\delta W^M = Q_i^M \delta q_i \qquad \delta W^{TH} = Q_i^{TH}\delta q_i \tag{115}$$

with corresponding generalized forces

$$Q_i^M = \int_A f_j \frac{\partial u_j}{\partial q_i} dA \qquad Q_i^{TH} = -\int_A \frac{\theta}{T}\mathscr{L}_{ji} n_j \, dA \tag{116}$$

Consider next the virtual relative dissipation of the whole system. According to (113) we may write

$$\frac{\partial \dot{H}_j}{\partial \dot{q}_i} = \mathscr{L}_{ji} \qquad \delta H_j = \frac{\partial \dot{H}_j}{\partial \dot{q}_i}\delta q_i \tag{117}$$

For simplicity we shall assume the validity of the reciprocity relations. However, as pointed out this is not required, since antisymmetric terms may be introduced in the virtual dissipation.

In this case the virtual dissipation (71) becomes

$$T_0 \delta S^* = \int_\Omega \frac{\partial \mathscr{D}}{\partial \dot{H}_j}\frac{\partial \dot{H}_j}{\partial \dot{q}_i}\delta q_i \, d\Omega = \frac{\partial D}{\partial \dot{q}_i}\delta q_i \tag{118}$$

with a total relative dissipation function

$$D = \int_\Omega \mathscr{D} \, d\Omega \tag{119}$$

This dissipation function is a positive-definite quadratic form in q_i:

$$D = \tfrac{1}{2} b_{ij}\dot{q}_i\dot{q}_j \tag{120}$$

where the coefficients b_{ij} are functions of the set of q_i's.

Finally, using a classical procedure [8] we express the virtual work of the inertia forces as

$$\delta W^{IN} = \int_\Omega \rho \ddot{u}_i \delta u_i \, d\Omega = \left[\frac{d}{dt}\left(\frac{\partial \mathscr{T}}{\partial \dot{q}_i}\right) - \frac{\partial \mathscr{T}}{\partial q_i}\right] \delta q_i \tag{121}$$

where

$$\mathscr{T} = \frac{1}{2}\int_\Omega \rho \dot{u}_i \dot{u}_i \, d\Omega = \frac{1}{2} m_{ij} \dot{q}_i \dot{q}_j \tag{122}$$

is the kinetic energy of the medium as a positive-definite quadratic form in $\dot{q}_i$ with the coefficients m_{ij} functions of the q_i's.

We now substitute the values (111), (115), (118), and (121) into the unmodified form (65) of the principle of virtual dissipation. Since δq_i is arbitrary, this yields the Lagrangian equations

$$\frac{d}{dt}\left(\frac{\partial \mathscr{T}}{\partial \cancel{q}_i}\right) - \frac{\partial \mathscr{T}}{\partial q_i} + \frac{\partial D}{\partial \dot{q}_i} + \frac{\partial \mathscr{P}}{\partial q_i} = Q_i \tag{123}$$

$/\dot{q}_i$

where $Q_i = Q_i^M + Q_i^{TH}$ is the generalized thermomechanical force exerted by the environment. Through (110), the q_i's are now state variables and the Lagrangian equations describe completely the evolution of the dynamical and thermodynamic system in a potential field G such as a gravity field.

Note that, by integration with respect to time, equations (123) lead to a variational principle in *Hamiltonian form*

$$\int_t \left[\delta(\mathscr{T} + \mathscr{P}) + \left(\frac{\partial D}{\partial \dot{q}_i} - Q_i\right)\delta q_i\right] dt = 0 \tag{124}$$

THE CASE OF PURE HEAT TRANSFER

If the work of deformation is negligible in comparison with the heat flow, we may put $\epsilon_{ij} = 0$. Hence the only state variable is

$$H_i = H_i^C \qquad h = h^C = -\frac{\partial H_i}{\partial x_i} \tag{125}$$

In this case the concept of heat content h^C becomes identical with the same concept introduced earlier for pure heat transfer [8]. Since there is no deformation, the heat fluence vector H_i is now an ordinary cartesian vector. Putting $\mathscr{T} = G = 0$, the Lagrangian equations (123) become

$$\frac{\partial V}{\partial q_i} + \frac{\partial D}{\partial \dot{q}_i} = Q_i \tag{126}$$

where Q_i now reduces to the thermal force Q_i^{TH} and V is given by

$$V = \int_\Omega \mathscr{V} d\Omega \qquad \mathscr{V} = \int_0^h \frac{\theta}{T} dh \tag{127}$$

In this particular case an alternative formulation is obtained where the factor 1/T is eliminated from the integrands for $\mathscr{V}$ and Q_i^{TH}. This is shown by expressing the principle of virtual dissipation (65) in terms of arbitrary variations δH_i. After integration by parts using the relation $\partial(\theta/T)/\partial x_i = -(T_o/T^2)\partial\theta/\partial x_i$ and canceling the factor T_o/T^2 in the integrand, we obtain

$$\int_\Omega \left(\frac{\partial\theta}{\partial x_i} + \Lambda_{ij}\dot{H}_j\right) \delta H_i \, d\Omega = 0 \tag{128}$$

which implies that the integrand vanishes. Another integration by parts then yields

$$\int_\Omega (\theta\,\delta h + \Lambda_{ij}\dot{H}_j\delta H_i)\, d\Omega = -\int_A \theta n_i \delta H_i \, dA \tag{129}$$

which is the variational principle of heat transfer derived earlier [8]. It leads to the Lagrangian equations (126) with a thermal potential V, a dissipation function D, and a generalized thermal force Q, expressed as

$$V = \int_\Omega d\Omega \int_0^h \theta \, dh \qquad D = \frac{1}{2}\int_\Omega \Lambda_{ij}\dot{H}_i\dot{H}_j \, d\Omega \qquad Q_i = -\int_A \theta \frac{\partial H_i}{\partial q_i} n_i \, dA \tag{130}$$

Applications of the variational principle (129) and the corresponding Lagrangian equations were discussed extensively in a monograph [8]. In this context, attention should be called to special formulations such as that of associated fields which lead to the direct use of the scalar temperature field as the unknown instead of H_i and the treatment of boundary heat transfer to a moving fluid using the concept of *trailing function.* The latter eliminates the inconsistencies of standard methods and is well suited to the Lagrangian treatment.

It should also be noted that in the present treatment the variational principle is used to derive the field equations of heat conduction and not the reverse, as is done by standard variational procedures. Also, the Lagrangian equations are obtained directly from a general thermodynamic variational principle without using the field differential equations.

QUASI-ADIABATIC AND QUASI-ISOTHERMAL CASE

There are two important practical cases leading to drastic simplification. One is where the temperature is nearly equal to its uniform initial value T_0. In this case we choose the heat content h^B as the state variable. Since $\tau_{ij} - \tau_{ij}^B$ is negligible we may put

$h^+ = H_i^+ = 0$. In this case the field $H_i = H_i^B$ becomes a state variable and may be expressed in terms of generalized coordinates q_i. The Lagrangian equations are correspondingly simplified. This case was the object of an extensive discussion earlier [2].

The other case of practical importance is where the deformation is almost adiabatic. Again, we neglect $\tau_{ij} - \tau_{ij}^A$ and $H_i = H_i^A$ becomes a state variable with a similar simplification of the Lagrangian equations.

NEW INSIGHT IN LINEAR THERMOELASTICITY

The linear theory with small strain $\epsilon_{ij} = e_{ij}$ and small temperature increment θ has become classical. Some new light is provided in this case by the present analysis. The linear equations of state are

$$\tau_{ij} = C_{ij}^{\mu\nu} e_{\mu\nu} - \beta_{ij}\theta \tag{131}$$

The energy and entropy differentials $d\mathscr{U}$ and $d\mathscr{S}$ obtained from exact values (29) and (35) are integrated retaining only first- and second-order terms. We obtain

$$\mathscr{U} = \tfrac{1}{2} C_{ij}^{\mu\nu} e_{ij} e_{\mu\nu} + T_o s \tag{132}$$

$$\mathscr{S} = s \cancel{+} \frac{1}{2} c \frac{\theta^2}{T_o{}^{2}} \tag{133}$$

$/ -$

$\checkmark 2$

where

$$s = \beta_{ij} e_{ij} + \frac{c\theta}{T_o} \tag{134}$$

$/ \frac{}{T_o}$

and c is a constant heat capacity per unit volume. We also derive the thermoelastic potential,

$$\mathscr{V} = \mathscr{U} - T_o \mathscr{S} = \frac{1}{2} C_{ij}^{\mu\nu} e_{ij} e_{\mu\nu} + \frac{1}{2} \frac{c\theta^2}{T_o} \tag{135}$$

It is interesting to note the disappearance of the linear terms in the value of $\mathscr{V}$. This remains true even if we assume a linear dependence of c on the temperature. In addition, $\mathscr{V}$ remains unaffected. We also note the *dual role* of the entropy, first as a linear state variable s and second as a nonlinear quantity $\mathscr{S}$ analogous to a potential with quadratic terms.

We now introduce the heat content of the second kind, $h^B = -\partial H^B/\partial x_i$, as a state variable. A comparison of Eqs. (93), (132), and (135) yields

$$h^B = -\frac{\partial H^B}{\partial x_i} = T_o s \tag{136}$$

According to (99) we may also write

$$\dot{h} = ({\tau_{ij}}^B - \tau_{ij})\dot{e}_{ij} + \dot{h}^B \tag{137}$$

Hence, to the first order we have

$$h = h^B \qquad H_i = H_i^B \tag{138}$$

and in the linear approximation we may use h and H_i as state variables with

$$h = -\frac{\partial H_i}{\partial x_i} = T_o s \tag{139}$$

This justifies the procedure used in the linear theory.

The foregoing analysis brings out and explains a particular feature of the linear theory regarding energy conservation, namely that the use of the linearized state variable h instead of h^B does not yield a correct value of the energy valid to the second order. This may be verified by writing the time derivative $\dot{\mathscr{U}}$ of the energy (132) and substituting the approximate linearized value (139) of $T_o s$. We obtain

$$\dot{\mathscr{U}} = {\tau_{ij}}^B \dot{e}_{ij} + \dot{h} \tag{140}$$

which is *incorrect* to the second order. However, repeating this evaluation using the exact value (136) of $T_o s$ yields

$$\dot{\mathscr{U}} = {\tau_{ij}}^B \dot{e}_{ij} + \dot{h}^B \tag{141}$$

By introducing the value of $\dot{h}^B$ derived from Eq. (137) this becomes

$$\dot{\mathscr{U}} = \tau_{ij}\dot{e}_{ij} + \dot{h} \tag{142}$$

which is the correct value of the power input.

EXTENSION TO VISCOELASTICITY

Consider the stress to be partially dependent on the rate of deformation $\dot{\epsilon}_{ij}$. We separate the stress into two terms,

$$\tau_{ij} = \tau_{ij}^V + \tau_{ij}^E \tag{143}$$

where $\tau_{ij}^E(\epsilon_{\mu\nu}, T)$ is the elastic part for slow reversible deformations while $\tau_{ij}^V(\epsilon_{\mu\nu}, \dot{\epsilon}_{\mu\nu}, T)$ is the rate dependent part. We may write the time derivative of the energy as

$$\dot{\mathscr{U}} = \tau_{ij}\dot{\epsilon}_{ij} - \frac{\partial \dot{H}_i}{\partial x_i} = \tau_{ij}^E \dot{\epsilon}_{ij} + T\dot{\mathscr{S}} \tag{144}$$

We derive

$$\mathscr{S} = \frac{1}{T} \tau_{ij}{}^{V} \dot{\epsilon}_{ij} - \frac{1}{T} \frac{\partial \dot{H}_i}{\partial x_i} = \dot{s}^* - \frac{\partial \dot{S}_i}{\partial x_i} \tag{145}$$

with

$$\dot{s}^* = \frac{1}{T} \tau_{ij}{}^{V} \dot{\epsilon}_{ij} - \frac{\dot{H}_i}{T^2} \frac{\partial T}{\partial x_i} \qquad \dot{S}_i = \frac{\dot{H}_i}{T} \tag{146}$$

where $\dot{s}^*$ is the rate of entropy production per unit initial volume and $\dot{S}_i$ is the entropy flux. The rate of intrinsic dissipation is

$$T\dot{s}^* = \tau_{ij}{}^{V} \dot{\epsilon}_{ij} + T\Lambda_{ij} \dot{S}_i \dot{S}_j \tag{147}$$

The corresponding virtual dissipation is

$$T\delta s^* = \tau_{ij}{}^{V} \delta \epsilon_{ij} + T\Lambda_{ij} \dot{S}_j \delta S_i \tag{148}$$

Further physical clarification of the entropy produced is obtained by considering an adiabatic deformation producing a certain temperature rise. The differential of the energy in this case is

$$d\mathscr{U} = (\tau_{ij}{}^{V} + \tau_{ij}{}^{E}) d\epsilon_{ij} \tag{149}$$

If the same deformation and temperature rise are produced reversibly with an injection of heat dh, the differential of the energy is

$$d\mathscr{U} = \tau_{ij}{}^{E} d\epsilon_{ij} + dh \tag{150}$$

Hence

$$dh = \tau_{ij}{}^{V} d\epsilon_{ij} \qquad \text{or} \qquad \dot{h} = \tau_{ij}{}^{V} \dot{\epsilon}_{ij} \tag{151}$$

This intrinsic dissipation yields an entropy production $\dot{s}^* = \dot{h}/T$ and is obtained by a calorimetric measurement. It corresponds to the concept of uncompensated heat of Clausius. We note here that there are *two types of entropy productions*, represented by the two terms of Eq. (147). The first is due to the generation of heat, while the second represents a dissipation *without heat production.*

In order to obtain field and Lagrangians equations, we proceed exactly as in the section on the derivation of field equations from the variational principles using the heat content fluence H_i^C as a state variable and an auxiliary field H_i^+ satisfying equation (100). The only difference is that we must substitute the total stress $\tau_{ij} = \tau_{ij}{}^{V} + \tau_{ij}{}^{E}$. Hence the variation (107) and the heat flux (109) become

$$\delta H_i = T\delta S_i = \int_{\Omega^+} g_i(x_\varrho, x_\varrho^+)(\tau_{\mu\nu}{}^{V} + \tau_{\mu\nu}{}^{E} - \tau_{\mu\nu}{}^{C}) \delta \epsilon_{\mu\nu} \, d\Omega^+ + \delta H_i^C \tag{152}$$

$$\dot{H}_i = T\dot{S}_i = \int_{\Omega^+} g_i(x_\ell, x_\ell^+)\,(\tau_{\mu\nu}{}^V + \tau_{\mu\nu}{}^E - \tau_{\mu\nu}{}^C)\dot{\epsilon}_{\mu\nu}\, d\Omega^+ + \dot{H}_i^C \tag{153}$$

Field equations are readily obtained by using the principle of virtual dissipation in its modified form (77), with arbitrary variations δu_i and δS_i inside the domain. In this procedure we must also put

$$\delta\mathscr{S} = -\frac{\partial}{\partial x_i}\delta S_i \tag{154}$$

in the variation $\delta_R\mathscr{P}$. We obtain the field equations

$$\rho\ddot{u}_i - \frac{\partial}{\partial x_j}\left[(\tau_{\mu\nu}{}^V + \tau_{\mu\nu}{}^E)\,\frac{\partial\epsilon_{\mu\nu}}{\partial a_{ij}}\right] + \rho\frac{\partial\mathscr{G}}{\partial\bar{x}_i} = 0 \tag{155}$$

$$\frac{\partial T}{\partial x_i} + T\Lambda_{ij}\dot{S}_j = 0 \tag{156}$$

In the second set of equations we replace $T\dot{S}_i$ by its value (153). Hence these field equations are integro-differential equations where the only unknown variables are the state variables u_i and H_i^C. Auxiliary equations such as (86) or (88) are not needed for $\mathscr{S}$ or s^*.

Lagrangian equations using expressions (110) of the fields u_i and H_i^C in terms of generalized coordinates may be obtained directly from the unmodified principle of virtual dissipation (65). In this case we must evaluate the virtual relative dissipation

$$T_o\delta S^* = T_o\int_\Omega \delta s^* d\Omega = \int_\Omega\left(\frac{T_o}{T}\tau_{\mu\nu}{}^V\delta\epsilon_{\mu\nu} + \frac{T_o}{T^2}\,\Lambda_{ij}\dot{H}_i\delta H_j\right)d\Omega \tag{157}$$

This may be expressed in terms of generalized coordinates by using expressions (110). We may write

$$\delta\epsilon_{\mu\nu} = \frac{\partial\epsilon_{\mu\nu}}{\partial q_i}\delta q_i \qquad \delta H_j = (\mathscr{L}_{ji}^V + \mathscr{L}_{ji})\delta q_i \qquad \dot{H}_j = (\mathscr{L}_{ji}^V + \mathscr{L}_{ji})\dot{q}_i \tag{158}$$

where

$$\mathscr{L}_{ji}{}^V(\dot{q}_k, q_k, x_\ell) = \int_{\Omega^+} g_i(x_\ell, x_\ell^+)\tau_{\mu\nu}{}^V\,\frac{\partial\epsilon_{\mu\nu}}{\partial q_i}\,d\Omega^+ \tag{159}$$

Because $\tau_{\mu\nu}{}^V$ is rate-dependent, this expression is a function of $\dot{q}_i$. The virtual dissipation (157) may now be written as

$$T_o\delta S^* = (R_i^V + R_i^{TH})\delta q_i + \frac{\partial D}{\partial\dot{q}_i}\delta q_i \tag{160}$$

where

$$R_i^V(\dot{q}_k, q_k) = \int_\Omega \frac{T_o}{T} \tau_{\mu\nu}{}^V \frac{\partial \epsilon_{\mu\nu}}{\partial q_i} \delta q_i \, d\Omega \tag{161}$$

$$R_i^{TH}(\dot{q}_k, \dot{q}_k) = \int_\Omega \frac{T_o}{T^2} \Lambda_{kj} (\mathscr{L}_{k\ell}{}^V \mathscr{L}_{ji}{}^V + \mathscr{L}_{k\ell} \mathscr{L}_{ji}^V + \mathscr{L}_{k\ell}{}^V \mathscr{L}_{ji}) \dot{q}_\ell \, d\Omega \tag{162}$$

are rate-dependent dissipative forces. The generalized thermal force (115) at the boundary now becomes

$$Q_i^{TH} = - \int_A \frac{\theta}{T} (\mathscr{L}_{ji}^V + \mathscr{L}_{ji}) n_j \, dA \tag{163}$$

With these values the Lagrangian equations are written as

$$\frac{d}{dt}\left(\frac{\partial \mathscr{T}}{\partial \cancel{q}_i}\right) + \frac{\partial \mathscr{T}}{\partial q_i} + R_i^V + R_i^{TH} + \frac{\partial D}{\partial \dot{q}_i} + \frac{\partial \mathscr{P}}{\partial Q_i} = Q_i \tag{164}$$

$\dot{q}_i$

For simplicity, we have assumed the reciprocity relations (44) to be valid, which implies a dissipation function. But the more general case is not excluded. It is interesting to note the physical significance of the new dissipative forces in the present case. The force $R_i{}^V$ corresponds to the loss of availability due to viscous heat production, while $R_i{}^{TH}$ corresponds to an additional loss of availability due to the fact that the heat produced is transferred by conduction. Finally, the term $\mathscr{L}_{ji}{}^V$ in (163) represents the loss of availability of the frictional heat to the environment.

The results are applicable to a large variety of constitutive properties including nonlinear creep and non-Newtonian fluids *and take into account the frictional heat production.* For a Newtonian fluid if we neglect the heat produced, the equations are of the same type as (123) with a single dissipation function D which embodies both the viscosity and the heat conduction [6].

As pointed out, we may write Lagrangian equations where q_i represent *deviations from a given evolution* with $Q_i = 0$. This corresponds to a nonlinearized bifurcation analysis with a time-dependent dissipation function. For the creeping motion of viscous incompressible fluids, the Lagrangian equations are reduced to

$$\frac{\partial D}{\partial \dot{q}_i} = 0 \tag{165}$$

Unstable solutions may be obtained as, for example, in the case of a nonhomogeneous layered viscous solid [6]. Note that Helmholtz's theorem stating that the evolution tends to a stable steady state (see [9], p. 619) is not applicable to nonhomogeneous fluids. The thermal conduction tensor K_{ij} for a viscous fluid as a function of the deformation has been evaluated [6] using the invariance property of the dissipation.

COMPLETENESS OF THE GENERALIZED COORDINATE DESCRIPTION, IMPLICIT FINITE ELEMENTS, AND BIFURCATION ANALYSIS

Fundamentally, the generalized coordinates are not simply "trial functions," as mistakenly believed, but from the standpoint of physics provide an accurate and complete description of the physical system. This can be seen by dividing the system into a network of cells, where the generalized coordinates are field components at the nodes. Values in the cells are obtained by polynomial interpolation. The cells are always finite in number, and their size may be assumed small enough to reach a *"resolution threshold"* [8] below which the macroscopic laws break down. Hence, from this standpoint the Lagrangian equations provide a *rigorous formulation of the physical evolution.* By the same token this viewpoint provides implicitly a large variety of finite-element methods with suitably chosen cells. We may use linear, or higher degree, interpolation. Quadratic interpolation similar to Simpson's method should provide high accuracy without requiring small-size cells.

A bifurcation analysis with generalized coordinates, representing a *finite departure* from a given time-dependent evolution, is also implicit using Lagrangian equations for the bifurcation coordinates q_i as exemplified by Eq. (165). This procedure is completely general and constitutes a powerful tool for a stability analysis. It may also be used to test the accuracy of a given solution by evaluating the magnitude of possible departures.

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