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VARIATIONAL THERMODYNAMICS OF VISCOUS COMPRESSIBLE HEAT-CONDUCTING FLUIDS*

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Abstract. A new variational principle of virtual dissipation generalizing d'Alembert's principle to nonlinear irreversible thermodynamics is applied to compressible heat-conducting fluids with Newtonian and non-Newtonian viscosity. The principle is applied in the context of Eulerian formalism where the flow is described with reference to a fixed coordinate system. New concepts of entropy displacement and mass displacement are used as well as a new definition of the chemical potential which avoids the usual ambiguities of the classical thermodynamic approach. The variational principle is used to derive a novel form of field differential equations for the coupled fluid dynamics and convective heat transfer.

1. Introduction. A new variational principle which we have referred to as the *principle of virtual dissipation* of wide generality has been shown to govern dissipative thermodynamic systems both linear and nonlinear [1]. It was applied to a new fundamental approach to the thermorheology of continua including Newtonian and non-Newtonian viscous, compressible, heat-conducting fluids [2]. However, the treatment was based on a material description where the coordinates of the fluid particle ξ_i are considered as functions of their initial coordinates x_i :

$$\xi_i = \xi_i(x_i, t). \quad (1)$$

In such a material description the density ρ per unit initial volume depends on the initial coordinates x_i , so that the treatment is applicable to a fluid which is nonhomogeneous at rest.

In the present treatment we shall consider a fluid which is homogeneous at rest with a uniform value of the density ρ_0 , the pressure p_0 and the temperature T_0 . For such a case it is possible to express the principle of virtual dissipation in Eulerian form, where the space coordinates ξ_i and the time are the independent variables.

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The unknowns are now new variables $S_i(\xi_k, t)$ and $M_i(\xi_k, t)$ introduced below ((23), (24)) and representing fields of entropy and mass displacements. New definitions are obtained for the chemical potential and the fluid pressure which avoid the usual ambiguities of the classical treatment.

Field differential equations in novel form are derived from the variational principle for the coupled dynamics and convective heat transfer. This is *in contrast to current procedures of deriving variational principles from the differential equations*.

2. Principle of virtual dissipation in Eulerian form. In its Eulerian form the principle of virtual dissipation is expressed by

$$\int_{\Omega} (\delta_R \mathcal{P} - \rho \mathcal{B}_i \delta u_i + \rho a_i \delta u_i + T \delta s^*) d\Omega = 0 \quad (2)$$

where the integration is over a domain Ω of space defined by the fixed coordinates ξ_i with the element of volume $d\Omega = d\xi_1 d\xi_2 d\xi_3$ and no variations at the boundary. At a given time t and at the fixed point ξ_i , \mathcal{B}_i is the body force, ρ the fluid density, T the absolute temperature and δu_i a virtual material displacement. Per unit volume at point ξ_i and time t , \mathcal{P} is the cell potential as defined previously ([1, 2]) and s^* is the entropy produced. The symbol δ_R denotes a restricted variation for which $\delta s^* = 0$. With the velocity v_i the fluid acceleration is

$$a_i = \frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial \xi_i} \quad (3)$$

It should be noted that, in contrast with the previous treatment, the unit element is not a material cell but a fixed cell of unit dimension in space with matter flowing through its boundaries. From the viewpoint of thermodynamics it is an *open cell*.

In order to formulate explicitly the variational principle in its Eulerian form we must introduce the concepts of mass and entropy displacement as well as a new approach to the definition of chemical potential which avoids some of the difficulties and ambiguities involved in classical thermodynamics.

3. Chemical potential and entropy displacement. The cell potential of the unit volume may be written

$$\mathcal{P} = \rho \bar{\mathcal{P}} \quad (4)$$

where

$$\bar{\mathcal{P}} = \bar{u} - T \bar{s} \quad (5)$$

and where $\bar{\mathcal{P}}$, \bar{u} and \bar{s} are respectively the cell potential, the internal energy, and the entropy per unit mass. The variation is

$$\delta \mathcal{P} = \bar{\mathcal{P}} \delta \rho + \rho \delta \bar{\mathcal{P}} \quad (6)$$

According to a previous result ([1, 2]) we write

$$\delta \bar{\mathcal{P}} = -p \delta \left(\frac{1}{\rho} \right) + \theta \delta \bar{s} \quad (7)$$

where p is the fluid pressure as a known function of ρ and \bar{s} under static conditions. Note

that this definition is purely thermodynamic and does not involve the viscous stresses, while $\theta = T - T_r$ is the excess temperature over the initial equilibrium temperature T_r . Combining (5), (6) and (7) yields

$$\delta\Phi = \mu \delta\rho + \theta \delta S \quad (8)$$

where $S = \rho\bar{s}$ is the entropy per unit volume and

$$\mu = \bar{u} - T\bar{s} + \frac{p}{\rho} \quad (9)$$

is the chemical potential which is a known function $\mu(\rho\bar{s})$ of ρ and S . It is completely defined and does not contain any arbitrary constant since it is assumed that $\bar{u} = \bar{s} = 0$ in the initial equilibrium state. From (8) we derive

$$\partial\Phi/\partial\rho = \mu, \quad \partial\Phi/\partial\theta = S, \quad (10)$$

thus providing a new definition of μ .

We shall also need the concept of entropy displacement already introduced earlier in a more restricted form [3]. Consider the material time derivative of \bar{s} multiplied by ρ :

$$\rho \frac{D\bar{s}}{Dt} = \rho \frac{\partial\bar{s}}{\partial t} + \rho v_i \frac{\partial\bar{s}}{\partial\xi_i} \quad (11)$$

Taking into account the conservation of mass condition

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial\xi_i}(\rho v_i) = 0, \quad (12)$$

(11) becomes

$$\rho \frac{D\bar{s}}{Dt} = \frac{\partial}{\partial t}(\rho\bar{s}) + \frac{\partial}{\partial\xi_i}(\rho v_i\bar{s}). \quad (13)$$

On the other hand, the same material derivative times ρ may be written

$$\rho \frac{D\bar{s}}{Dt} = -\frac{1}{T} \frac{\partial J_i}{\partial\xi_i} + \dot{s}_v^* = \frac{\partial}{\partial\xi_i} \left(\frac{J_i}{T} \right) - \frac{1}{T^2} J_i \frac{\partial\theta}{\partial\xi_i} + \dot{s}_v^* \quad (14)$$

where J_i is the rate of heat flow by *conduction* per unit area and \dot{s}_v^* is the rate of entropy production per unit volume due to viscosity. Equating expressions (13) and (14) yields

$$\frac{\partial}{\partial t}(\rho\bar{s}) = -\frac{\partial}{\partial\xi_i} \left(\rho v_i\bar{s} + \frac{J_i}{T} \right) - \frac{1}{T^2} J_i \frac{\partial\theta}{\partial\xi_i} + \dot{s}_v^*. \quad (15)$$

We define the *entropy displacement vector* as

$$S_i = S_i^c + S_i^T \quad (16)$$

where the time derivatives

$$\dot{S}_i^c = \rho v_i\dot{\bar{s}}, \quad \dot{S}_i^T = J_i/T \quad (17)$$

are respectively the rates of entropy displacements by convection and conduction. Furthermore,

$$\dot{s}_v^* = -\frac{1}{T^2} J_i \frac{\partial\theta}{\partial\xi_i} \quad (18)$$

is the rate of entropy production per unit volume due to thermal conduction. Hence, integrating (15) with respect to time with zero initial conditions, we obtain

$$S = -\frac{\partial S_i}{\partial \xi_i} + s^* \quad (19)$$

where

$$s^* = s_T^* + s_s^* \quad (20)$$

is the total entropy produced per unit volume. Eq. (19) may be considered as an entropy conservation equation in terms of the entropy S per unit volume and the total entropy displacement field S_i . The term

$$s = -\partial S_i / \partial \xi_i \quad (21)$$

will be called the *entropy supplied* per unit volume. Relation (21) constitutes a fundamental *holonomic conservation constraint* between s and S_i . We may also write (19) as

$$S = s + s^*, \quad (22)$$

i.e. the total entropy of the unit volume is the sum of the entropy produced and the entropy supplied by convection and conduction.

4. Variational derivation of the field equations. The field will be defined by seven variables. Six of the variables are represented by two vectors, one being the *entropy displacement*

$$S_i = S_i(\xi_k, t); \quad (23)$$

the other is the *mass displacement*

$$M_i = M_i(\xi_k, t) \quad (24)$$

defined by the relation

$$\dot{M}_i = \rho v_i. \quad (25)$$

It satisfies the mass conservation equation (12) which may be written

$$\rho = -\partial M_i / \partial \xi_i \quad (26)$$

The seventh variable is the scalar s^* representing the entropy produced per unit volume.

When applying the variational principle (2) we vary the vectors S_i and M_i . The various terms in the integrand of (2) are obtained as follows. According to (8) and (22) we write

$$\delta \mathcal{P} = \mu \delta \rho + \theta \delta \mathcal{P} = \mu \delta \rho + \theta \delta (s + s^*). \quad (27)$$

In order to obtain the restricted variation δ_R we put $\delta s^* = 0$. Hence

$$\delta_R \mathcal{P} = \mu \delta \rho + \theta \delta s. \quad (28)$$

The virtual displacement δu_i of a fluid particle may be written

$$\delta u_i = \delta M_i / \rho. \quad (29)$$

The thermal conduction of the fluid is expressed by

$$J_i = T \dot{S}_i^T = -k(\partial\theta/\partial\xi_i) \quad (30)$$

where k is the thermal conductivity of the fluid at point ξ , and time t . Hence (18) becomes

$$\dot{s}_T^* = \frac{1}{k} \dot{S}_i^T \dot{S}_i^T. \quad (31)$$

The thermal conductivity k is a function of the local density ρ and local entropy s :

$$k = k(\rho, s). \quad (32)$$

The virtual dissipation due to thermal conduction is

$$T \delta s_T^* = \frac{T}{k} \dot{S}_i^T \delta S_i^T. \quad (33)$$

The virtual dissipation due to viscosity is

$$T \delta s_v^* = \sigma_{ij}' \frac{\partial}{\partial \xi_i} \left(\frac{\delta M_i}{\rho} \right) \quad (34)$$

where σ_{ij}' is the *viscous stress* dependent on the strain rate tensor e_{ij}' . For a Newtonian fluid σ_{ij}' may be expressed as

$$\sigma_{ij}' = \partial \mathfrak{D}_v / \partial e_{ij}' \quad (35)$$

where the dissipation function is

$$\mathfrak{D}_v = \frac{1}{2} (\lambda' e'^2 + 2\eta e_{ij}' e_{ij}') \quad (36)$$

with viscosity coefficients λ' and η and the volumetric strain rate $e' = e_{ii}'$. The viscosity coefficients are functions of the local density ρ and local entropy s :

$$\lambda' = \lambda'(\rho, s), \quad \eta = \eta(\rho, s). \quad (37)$$

The strain rate is

$$e_{ij}' = \frac{1}{2} \left[\frac{\partial}{\partial \xi_i} \left(\frac{\dot{M}_j}{\rho} \right) + \frac{\partial}{\partial \xi_j} \left(\frac{\dot{M}_i}{\rho} \right) \right]. \quad (38)$$

For a non-Newtonian fluid we have shown by a very simple derivation that the viscous stress is expressed by

$$\sigma_{ij}' = F_1 \delta_{ij} + F_2 e_{ij}' + F_3 e_{ik}' e_{kj}'. \quad (39)$$

where

$$F_k = F_k(\rho, s, I_1, I_2, I_3), \quad (40)$$

are functions of ρ , s and the three invariants

$$I_1 = e_{ii}', \quad I_2' = e_{ij}' e_{ij}', \quad I_3' = e_{ij}' e_{jk}' e_{ki}'. \quad (41)$$

The total virtual dissipation is

$$T \delta s^* = T(\delta s_T^* + \delta s_v^*) = \frac{T}{k} \dot{S}_i^T \delta S_i^T + \sigma_{ij}' \frac{\partial}{\partial \xi_i} \left(\frac{\delta M_j}{\rho} \right). \quad (42)$$

With expressions (28) (29) and (42) for the variations, the variational principle (2) becomes

$$\int_{\Omega} \left[\mu \delta \rho + \theta \delta s - (\mathfrak{B}_i - a_i) \delta M_i + \frac{T}{k} \dot{S}_i^T \delta S_i^T + \sigma_{ij}' \frac{\partial}{\partial \xi_j} \left(\frac{\delta M_i}{\rho} \right) \right] d\Omega = 0. \quad (43)$$

An essential step is due to the relations

$$\delta \rho = -\frac{\partial}{\partial \xi_i} \delta M_i, \quad \delta s = -\frac{\partial}{\partial \xi_i} \delta S_i \quad (44)$$

derived from the holonomic conservation constraints (21) and (26). We introduce these values in the integrand of Eq. (43) and assume arbitrary variations δM_i and δS_i different from zero inside Ω . Integration by parts then yields

$$\int_{\Omega} \left[\left(\frac{\partial \mu_i}{\partial \xi_i} - \frac{1}{\rho} \frac{\partial \sigma_{ij}'}{\partial \xi_j} - \mathfrak{B}_i + a_i \right) \delta M_i + \frac{\partial \theta}{\partial \xi_i} \delta S_i + \frac{T}{k} \dot{S}_i^T \delta S_i^T \right] d\Omega = 0. \quad (45)$$

It remains to evaluate δS_i^T in terms of δM_i and δS_i . Eq. (17),

$$\dot{S}_i^c = \rho v_i \bar{s} = \bar{s} \dot{M}_i, \quad (46)$$

implies

$$\delta S_i = \bar{s} \delta M_i. \quad (47)$$

Hence from Eq. (16) we obtain

$$\delta S_i^T = \delta S_i - \bar{s} \delta M_i. \quad (48)$$

Introducing the values (47) and (48) into (45), we obtain

$$\int_{\Omega} \left[\left(\frac{\partial \mu}{\partial \xi_i} - \frac{1}{\rho} \frac{\partial \sigma_{ij}'}{\partial \xi_j} - \mathfrak{B}_i + a_i + \bar{s} \frac{\partial \theta}{\partial \xi_i} \right) \delta M_i + \left(\frac{\partial \theta}{\partial \xi_i} + \frac{T}{k} \dot{S}_i^T \right) \delta S_i \right] d\Omega. \quad (49)$$

The variations δM_i and δS_i being arbitrary and independent, this result implies the field equations

$$\begin{aligned} \frac{\partial \mu}{\partial \xi_i} - \frac{1}{\rho} \frac{\partial \sigma_{ij}'}{\partial \xi_j} - \mathfrak{B}_i + a_i + \bar{s} \frac{\partial \theta}{\partial \xi_i} &= 0, \\ \frac{\partial \theta}{\partial \xi_i} + \frac{T}{k} \dot{S}_i^T &= 0. \end{aligned} \quad (50)$$

These equations may be further transformed as follows. From Eqs. (5) and (9) we derive

$$d\mu = d\bar{\mathcal{P}} + d\left(\frac{p}{\rho}\right) - d(\theta \bar{s}). \quad (51)$$

Introducing the value (7) of $\bar{\mathcal{P}}$, we obtain

$$d\mu = \frac{dp}{\rho} - \bar{s} d\theta. \quad (52)$$

Hence

$$\frac{\partial \mu}{\partial \xi_i} = \frac{1}{\rho} \frac{\partial p}{\partial \xi_i} - \bar{s} \frac{\partial \theta}{\partial \xi_i}. \quad (53)$$

Furthermore, from (48) we write

$$\dot{S}_i^* = \dot{S}_i - \bar{s}\dot{M}_i \quad (54)$$

By substituting the values (53) and (54) the field equations (50) become

$$\begin{aligned} \frac{1}{\rho} \left(\frac{\partial p}{\partial \xi_i} - \frac{\partial \sigma_{i,i'}}{\partial \xi_i} \right) - \mathfrak{B}_i + a_i &= 0, \\ k \frac{\partial \theta}{\partial \xi_i} + T(\dot{S}_i - \bar{s}\dot{M}_i) &= 0. \end{aligned} \quad (55)$$

These six equations contain the seven unknowns S_i, M_i and s^* . The additional equation may be obtained from (42) and expresses the local dissipation

$$T\dot{s}^* = \frac{T}{k} (\dot{S}_i - \bar{s}\dot{M}_i)(\dot{S}_i - \bar{s}\dot{M}_i) + \sigma_{i,i'} \frac{\partial}{\partial \xi_i} \left(\frac{\dot{M}_i}{\rho} \right). \quad (56)$$

The acceleration a_i is expressed by means of (3) with $v_i = \dot{M}_i/\rho$, while ρ is given by (26) and p, k, T and θ are known functions of ρ and \bar{s} .

The field equations (55) provide a novel form governing the coupled dynamics and convective heat transfer of a viscous compressible heat conducting fluid for Newtonian as well as non-Newtonian viscosity. The corresponding variational principle is expressed by Eq. (2). This generalizes the variational principle obtained earlier [4, 5, 6] for uncoupled convective heat transfer.

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