Generalized Variational Principles for Convective Heat Transfer and Irreversible Thermodynamics

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Abstract. Variational principles for convective heat transfer are extended to nonhomogeneous fluids and to fluids with thermal expansion. The results apply to nonlinear problems with temperature dependent properties. The context is restricted to heat transfer but the derivation and a discussion of the physics brings out the general validity of the variational principles for a large category of irreversible processes.

1. Introduction. Variational methods in heat transfer for both linear and non-linear problems were obtained as an extension of general thermodynamic principles [1] [2]. The method is applicable to convective heat transfer in a fluid. *For the fluid with constant properties a variational principle was derived* from the classical linear equations for the temperature field [3]. It was shown that an approach based on thermodynamic concepts provides a very general form of the variational principle which point to its validity in a large class of dissipative phenomena and is applicable to the non-linear problem of convective heat transfer in a fluid with temperature-dependent properties [4]. The aforementioned results were derived for an incompressible homogeneous fluid. We will extend the variational method to fluids composed of heterogeneous particles and to a fluid with thermal expansion. This generalization introduces the concept of thermal potential of an individual fluid particle. The derivation is obtained in a concise form which brings out the mathematical structure and the physical significance of the results. In particular we have discussed the analogy with the treatment of holonomic systems in classical mechanics, the potential development of the method in general thermodynamics as well as applications to turbulent flow, internal heat generation and mixed fluid-solid systems such as porous media.

The derivation is based on a simple but unconventional formulation. Its equivalence to the more familiar equation for convective phenomena is clarified in the last paragraph.

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2. Thermal potential of a fluid particle. Consider an heterogeneous fluid composed of incompressible fluid particles. The motion of the fluid is assumed to be known. We identify the particles by their initial coordinates X_i at the time $t = 0$. At the time t the coordinates of a particle become

$$x_i = x_i(X, t), \tag{1}$$

where X denotes the three initial coordinates.

The velocity components v_i of the fluid at any instant are

$$v_i = \frac{\partial}{\partial t} x_i(X, t). \tag{2}$$

Since the fluid is heterogeneous each particle is characterized by a heat capacity c *per unit volume* which depends not only on the temperature θ but on the physical nature of the particular fluid particle. This is expressed by writing

$$c = c(X, \theta). \tag{3}$$

For a given fluid particle we now define the *heat content per unit volume* as

$$h = \int_0^\theta c(X, \theta)\, d\theta. \tag{4}$$

The integration is performed with respect to θ and for constant values of X_i.

We further define the *thermal potential* of a given fluid particle as

$$F = \int_0^\theta \theta\, dh. \tag{5}$$

The integration is again carried out with respect to θ and for constant values of X. Hence we may write the heat content and thermal potential of a particle as

$$\begin{aligned} h &= h(X, \theta), \\ F &= F(X, \theta). \end{aligned} \tag{6}$$

In the following derivation we shall express the vector and scalars defined above in terms of the time t and the fixed coordinates x_i. Therefore we solve equations (1) for the initial coordinates X_i and write

$$X_i = X_i(x, t). \tag{7}$$

This equation gives the initial coordinates of a particle flowing through the fixed point x at a particular instant t. By substituting the values (7) of X_i into expressions (2), (3) and (6) we obtain

$$\begin{aligned} v_i &= v_i(x, t), \\ c &= c(x, t, \theta), \\ h &= h(x, t, \theta), \\ F &= F(x, t, \theta). \end{aligned} \tag{8}$$

3. Basic equations. The physics of the heat transfer is governed by two basic equations which express the conservation and rate of flow of heat.

Consider a vector field

$$J_i = J_i(x, t), \tag{9}$$

which represents the instantaneous rate of heat flow due to thermal conduction and the local temperature gradient. The vector J_i measures the rate of heat flow per unit area through a surface element normal to J_i and attached to the fluid particle.

Conservation of thermal energy is expressed by the following equation

$$\iiint_\tau \dot{h}\, d\tau + \iint_A (J_i + v_i h) n_i \, dA = 0, \tag{10}$$

with the functions (8) and (9) of x_i, t, and θ. We have used the notation

$$\dot{h} = \partial h / \partial t.$$

The integrations are extended to an arbitrary volume τ and its boundary A of outward unit normal n_i. By Green's theorem equation (10) is equivalent to

$$\dot{h} + \frac{\partial}{\partial x_i} (J_i + v_i h) = 0. \tag{11}$$

In the paragraph at the end of this paper we have also derived equation (11) by a conventional but more elaborate procedure.

One essential feature of the author's variational method is to describe the thermal flow by means of a vector field $H_i(x, t)$ and to define h and J_i by the expressions.

$$\begin{aligned} h &= -\frac{\partial H_i}{\partial x_i}, \\ J_i &= \dot{H}_i - v_i h, \end{aligned} \tag{12}$$

with the notation

$$\dot{H}_i = \partial H_i / \partial t.$$

As a result the conservation equation (11) is satisfied *identically.*

Note the physical significance of the vector

$$\dot{H}_i = J_i + v_i h. \tag{13}$$

It represents the total conductive and convective heat flow per unit area through a surface *fixed in space* and normal to $\dot{H}_i$.

The second basic equation is the following relation between the heat flow and the temperature gradient.

$$\frac{\partial \theta}{\partial x_i} = -\lambda_{ij} J_j . \tag{14}$$

The tensor λ_{ij} is the thermal resistivity. Due to *Onsager's relations* the resistivity tensor is symmetric

$$\lambda_{ij} = \lambda_{ji} \,. \tag{15}$$

The matrix $[\lambda_{ij}]$ is by definition the inverse of the thermal conductivity matrix $[k_{ij}]$. For isotropic conduction the resistivity tensor becomes

$$\lambda_{ij} = \frac{1}{k}\,\delta_{ij}\,, \tag{16}$$

where k is the thermal conductivity and δ_{ij} is the Kronecker symbol. In this case Onsager's relations are a direct consequence of the property of isotropy.

Note that the thermal resistivity of a given fluid particle may be assumed a function of both time and temperature. Hence

$$\lambda_{ij} = \lambda_{ij}(X, t, \theta). \tag{17}$$

This is a functional dependence which is more general than for h and F in equations (6). By introducing the value (7) of X_i the resistivity matrix becomes a function $\lambda_{ij}(x, t, \theta)$.

4. Total thermal potential and dissipation function. Variational principles and Lagrangian equations are obtained by considering a total thermal potential V and a dissipation function D whose definitions are formally the same as in previous papers [1] [2]. We have referred to expression (5) as the thermal potential of a particle per unit volume. The total thermal potential of the fluid in a volume τ is defined by

$$V = \iiint_\tau F\,d\tau. \tag{18}$$

The integral is (18) extended to any *arbitrary volume* τ of space. Similarly a dissipation function is defined as

$$D = \frac{1}{2}\iiint_\tau \lambda_{ij}J_iJ_j\,d\tau. \tag{19}$$

Note that D is expressed in terms of the flow field J_i due to thermal conduction only.

5. Variational principle. With the foregoing definitions the derivation of variational principles follows the same procedure as in a previous paper [4]. It is therefore not necessary to repeat the details. We write the variational equation

$$\left(\frac{\partial\theta}{\partial x_i} + \lambda_{ij}J_j\right)\delta H_i = 0. \tag{20}$$

For arbitrary variations of the field H_i this equation is equivalent to the law of heat flow (14).

Equation (20) is integrated over an arbitrary volume. The first term is integrated by parts. Using the relations

$$\delta h = -\frac{\partial}{\partial x_i}\,\delta H_i\,, \qquad \delta F = \theta\,\delta h, \tag{21}$$

derived from equations (5) and (12) we obtain

$$\delta V + \iiint_\tau \lambda_{ij} J_j\,\delta H_i = -\iint_A \theta n_i\,\delta H_i\,dA. \tag{22}$$

The surface integral is extended to the boundary A of the volume τ and the unit outward normal is denoted by n_i.

6. Generalized coordinates and Lagrangian equations. The previously introduced formulation [1] [4] by means of generalized coordinates is applicable. The field H_i is written as a function of n parameters q_i considered as generalized coordinates which are unknown functions of time

$$H_i = H_i(q_1 q_2 \cdots q_n x_1 x_2 x_3 t). \tag{23}$$

The variation δH_i are due entirely to the variations δq_i

$$\delta H_i = \frac{\partial H_i}{\partial q_j}\,\delta q_j\,. \tag{24}$$

Also

$$\dot H_i = \frac{\partial H_i}{\partial q_j}\,\dot q_j + \frac{\partial H_i}{\partial t}. \tag{25}$$

Hence

$$\frac{\partial \dot H_i}{\partial \dot q_j} = \frac{\partial H_i}{\partial q_j}\,, \tag{26}$$

and the variation (24) is also written as

$$\delta H_i = \frac{\partial \dot H_i}{\partial \dot q_j}\,\delta q_j\,. \tag{27}$$

Expressions (24) and (27) for δH_i are substituted respectively in the surface and volume integrals of equation (22). Taking into account the symmetry property $\lambda_{ij} = \lambda_{ji}$ we derive

$$\frac{\partial V}{\partial q_i} + \frac{\partial D}{\partial \dot q_i} = Q_i\,. \tag{28}$$

The generalized thermal force at the boundary is

$$Q_i = -\iint_A \theta n_j \frac{\partial H_j}{\partial q_i}\,dA. \tag{29}$$

7. Arbitrary choice of the domain of integration and physical significance of the equations. No restriction is implied in the derivation regarding the choice of the domain of integration τ for the definition of the total thermal potential (18) and the dissipation function (19). The domain is chosen arbitrarily to suit the problem and may be time-dependent. For example, the domain may be attached to a flowing mass of fluid. This is understandable physically if we remember that the Lagrangian equations (28) simply express the law of instantaneous heat flow for a given temperature field at any particular instant. For the case of heat conduction in a solid this property has been used in the solution of ablation problems with melting boundaries [5] [6].

8. Internal heat sources. In many problems it is necessary to take into account internal generation of heat in the fluid. For example, the heat may be generated internally by viscous friction, chemical reactions, nuclear reactions or radiation absorption.

A general procedure to include the effect of thermal sources has already been outlined in previous papers [2] [4]. We assume the rate of heat generation w per unit volume to be a given function of x_i and t

$$w = w(x, t). \tag{30}$$

The conservation equation in this case is obtained by adding this term into equation (11). It becomes

$$\dot{h} + \frac{\partial}{\partial x_i}(J_i + v_i h) = w. \tag{31}$$

This equation will be satisfied *identically* by putting

$$\begin{aligned} h &= -\frac{\partial H_i}{\partial x_i}, \\ J_i &= \dot{H}_i + \dot{H}_i^* - v_i h, \end{aligned} \tag{32}$$

where the field $H_i^*(x\ t)$ is a known function of x_i and t chosen so that it satisfies the relation

$$\frac{\partial H_i^*}{\partial x_i} = \int_0^t w\, dt. \tag{33}$$

The vector field H_i^* is not defined uniquely by this equation since it is also satisfied by adding any arbitrary divergence-free field. In practice the choice may be dictated by considerations of convenience.

With these definitions the foregoing derivation of the variational principle and Lagrangian equations is applicable.

9. Homogeneous fluid. The particular case of an homogeneous incompressible fluid was considered previously (4). In this case all the fluid particles are the same and the heat capacity c per unit volume is the same function of the temperature for all particles. Hence

$$
\begin{aligned}
c &= c(\theta), \\
h &= h(\theta), \qquad (34)\\
F &= F(\theta).
\end{aligned}
$$

10. Turbulent flow. As already pointed out in a previous paper [4] equations (28) are applicable to an incompressible homogeneous fluid in turbulent flow. In this case we consider the tensor

$$K_{ij} = k_{ij} + c\epsilon_{ij} \,, \tag{35}$$

where k_{ij} is the thermal conductivity and ϵ_{ij} the turbulent diffusivity. The effect of turbulence on the heat transfer is taken into account by introducing a resistivity tensor λ_{ij} whose matrix is

$$[\lambda_{ij}] = [K_{ij}]^{-1} \tag{36}$$

The right side represents the inverse matrix of K_{ij}.

11. Fluid with thermal expansion. The foregoing analysis assumes the fluid to be incompressible. If the fluid viscosity is independent of the temperature the fluid motion is not influenced by the heat transfer. This is not the case if the volume expansion of the fluid with temperature is taken into account. However, in a restricted sense it is still possible to extend the variational method to this case by introducing some special assumptions.

Consider a homogeneous fluid and let us assume that it flows under conditions such that pressure variations may be neglected. In this case the density $\rho(\theta)$ depends only on the temperature θ. A coupling will occur between the temperature and velocity fields through the condition of conservation of mass,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0. \tag{37}$$

It is possible to introduce an unknown velocity field

$$v_i = v_i(q_1 q_2 \cdots q_n x_1 x_2 x_3 t), \tag{38}$$

which depends on the generalized coordinates q_i of the temperature field and such that the mass conservation equation (37) is satisfied identically. In many problems the velocity field will satisfy additional conditions resulting from the geometry. For example, the streamlines may be known approximately.

We may also extend the concept of thermal potential to a fluid with thermal expansion. Consider the heat capacity $\bar{c}(\theta)$ per unit mass. We define the heat content per unit mass as

$$\bar{h}(\theta) = \int_0^\theta \bar{c}(\theta)\, d\theta. \tag{39}$$

The heat content per unit volume is

$$h(\theta) = \rho(\theta)\bar{h}(\theta). \tag{40}$$

The thermal potential $F(\theta)$ is defined as before by

$$F(\theta) = \int_0^\theta \theta \, dh. \tag{41}$$

The heat content h satisfies the same conservation equation (11). This may be further verified by writing equation (11) in the more familiar form (46) discussed in the last paragraph, and putting $c = \bar{c}\rho$. In this case the derivation requires that relation (42) be replaced by the mass conservation equation (37).

With these definitions and assumptions the variational principle (22) and the Lagrangian equations (28) are valid for a fluid with thermal expansion. Note that in this case the velocity field (38), which appears in the dissipation function, is not given, but is a function of the generalized coordinates q_i.

12. Application to mixed solid-fluid systems. Attention should be called to a category of problems where the present results are particularly useful. The Lagrangian equations are applicable to a mixed system composed of solids and moving fluids. The domain of integration may contain both. In the solid portion the velocity v_i is put equal to zero and λ_{ij} represents the thermal resistivity of the solid. Problems including simultaneous heat conduction and convection may then be treated from the viewpoint of a unified single system.

The method seems particularly well suited for problems of "sweat cooling" and heat transfer in a porous medium containing a moving fluid. A numerical application of the variational method to such problems has recently been given [7].

13. Relation to the thermodynamics of irreversible processes. The author has shown that equations (28) govern a large class of irreversible processes in the range of linear thermodynamics for systems in equilibrium and at rest in the initial state. In many cases it is possible to extend the theory to non-linear phenomena as already done in a previous treatment [1] [4].

The present case of convective heat transfer may be considered as a perturbation from an initial state of flow. Hence the unperturbed system is not at rest. Actually, the physics is not modified by this motion in any fundamental way. Onsager's relations are still valid locally and the dissipation function (19) is of the same form as if the system were at rest. However, as already shown [4], the reciprocity relations are not verified macroscopically. The significance of this fact becomes clear if we consider the heat conduction in a moving solid. When the heat transfer is referred to fixed axes the reciprocity properties are not maintained. The physics, of course, is the same, but the apparent behavior of the field has been modified by the time dependent change of coordinates. The case of convective heat transfer in a moving fluid is basically similar except for the fact that the frame of reference is also being deformed as a function of time.

This is analogous to what happens in mechanics when we consider perturbations of a state of motion which involve time dependent constraints and lead to gyroscopic forces. The reciprocity properties are not valid in this case. The effect is due entirely to the kinematics and does not add any physics beyond Newton's law. Another similarity with classical mechanics should be noted. In the author's variational formulation of heat transfer the condition of conservation of thermal energy has been satisfied automatically as if it were a holonomic constraint.

These considerations point to yet undeveloped potentialities of the Lagrangian equations (28) in the general thermodynamics of irreversible processes including nonlinear phenomena and convection.

14. Alternative formulation of the conservation equation (11). Equation (11) may be expressed in more familiar form. By taking into account the condition of incompressibility

$$\frac{\partial v_i}{\partial x_i} = 0, \tag{42}$$

equation (11) becomes

$$\frac{\partial h}{\partial t} + v_i \frac{\partial h}{\partial x_i} + \frac{\partial J_i}{\partial x_i} = 0. \tag{43}$$

The time derivative of h considered to be attached to a fluid particle is

$$\frac{Dh}{Dt} = \frac{\partial h}{\partial t} + v_i \frac{\partial h}{\partial x_i}. \tag{44}$$

From equations (4) we derive

$$\frac{Dh}{Dt} = c\frac{D\theta}{Dt} = c\left(\frac{\partial \theta}{\partial t} + v_i \frac{\partial \theta}{\partial x_i}\right). \tag{45}$$

With expressions (44) and (45) equation (43) becomes

$$c\frac{\partial \theta}{\partial t} = -\frac{\partial J_i}{\partial x_i} - cv_i \frac{\partial \theta}{\partial x_i}. \tag{46}$$

The flow rate equation (14) may also be written by using the thermal conductivity tensor k_{ij}

$$J_i = -k_{ij}\frac{\partial \theta}{\partial x_j}. \tag{47}$$

By introducing this expression into equation (46) we finally obtain

$$c\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial \theta}{\partial x_j}\right) - cv_i \frac{\partial \theta}{\partial x}. \tag{48}$$

This is the familiar differential equation for the temperature field in a fluid.

Because the fluid is nonhomogeneous the heat capacity $c(x, t, \theta)$ is a function of x_i, t and θ. However we must remember that this functional relationship is not arbitrary but results from substituting into expressions (3) the values (7) of the initial coordinates. Another way of stating this is to say that the dependence of c upon x_i and t is restricted to functions such that

$$\left(\frac{\partial}{\partial t} + v_i \frac{\partial}{\partial x_i}\right)c = 0, \tag{49}$$

when θ is assumed to be constant.

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