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A thermodynamic description of hydrodynamics

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1. Introduction

In hydrodynamics, two basic problems arise. The first is the establishment of the laws governing the processes, the second is the resolution of these equations. In this note, we consider the rather general problem of the flow of a multicomponent viscous compressible and isotropic fluid with r constituents between which there is diffusion and amongst which a chemical reaction is possible; the temperature and all the other properties of the systems are supposed to vary in time and space.

Such a flow obey the following local balance equations:

(1) $\dot{\varrho} = -\varrho \operatorname{div} \mathbf{v}$ (total mass conservation)

(1′) $\varrho \dot{c}^k = -\operatorname{div} \mathbf{j}^k + \Gamma^k$ (mass conservation of constituent k)

(2) $\varrho \dot{\mathbf{v}} = \operatorname{div} \boldsymbol{\sigma} + \varrho \mathbf{F}$ (momentum conservation)

(3) $\varrho \dot{u} = -\operatorname{div} \mathbf{q} + \widetilde{\boldsymbol{\sigma}} : \widetilde{\mathbf{v}} - p \operatorname{div} \mathbf{v} + \varrho r$ (energy conservation)

with

$\varrho^k(\mathbf{x}, t)$: density of constituent k

$\varrho(\mathbf{x}, t)$ total density $\left(\varrho = \sum_1^r \varrho^k\right)$

$c^k(\mathbf{x}, t)$: concentration of constituent k $\left(c^k = \frac{\varrho^k}{\varrho} \text{ and } \sum_1^r c^k = 1\right)$

$\mathbf{v}(\mathbf{x}, t)$: barycentric velocity vector

$\mathbf{v}^k(\mathbf{x}, t)$: velocity of constituent k

$\mathbf{j}^k = \varrho^k(\mathbf{v}^k - \mathbf{v})$: mass flux of constituent

ν^k: stoichiometric coefficient

$\dot{\xi}(\mathbf{x}, t)$: rate of advancement of the reaction

$\Gamma^k(\mathbf{x}, t)$: chemical source term $(\Gamma^k = \nu^k \dot{\xi})$

$\boldsymbol{\sigma}(\mathbf{x}, t)$: symmetric stress tensor

$\mathbf{F}(\mathbf{x}, t)$: body force per unit mass

$\mathbf{q}(\mathbf{x}, t)$: heat flux vector

$p(\mathbf{x}, t)$: thermodynamic pressure $\left(p = -\frac{1}{3} \operatorname{tr} \boldsymbol{\sigma}\right)$

$r(\mathbf{x}, t)$: energy source term
$\mathbf{v}(\mathbf{x}, t)$: rate of deformation tensor

A tilda means the deviatoric part of the tensor, in cartesian coordinates:

$$v_{ij}=\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)-\frac{1}{3}\frac{\partial v_k}{\partial x_k}\delta_{ij}$$

The balance laws (1) to (3) constitute a set of $4+r$ equations with $11+4r$ unknowns:

$$\varrho, \mathbf{c}^k, \mathbf{j}^k, \mathbf{v}, \tilde{\boldsymbol{\sigma}}, p, \mathbf{u}, \mathbf{q}, \dot{\xi}$$

(only $r-1$ of the c^k are independent since $\Sigma c^k=1$).

It is precisely the goal of thermodynamics to furnish the lacking $7+3r$ relations.

In thermodynamics several ways may be followed to derive those relations. Among the most important, let us mention those of Meixner [1], Truesdell [2] and Onsager [3], [4]. In this paper, we shall use Onsager's formalism because in author's opinion, it gives a very good and complete description of thermodynamic systems. Let us briefly recall the essential points of Onsager's theory.

2. Onsager's thermodynamic theory of irreversible processes

The theory rests on the following hypotheses:

1. local action. It is assumed that the behaviour of a system at a position $\mathbf{x}$, is only influenced by what happens in its direct vicinity.

2. determinism, in the sense that the behaviour of a system at time t is completely determined by the values taken by the state variables at that time. The actual state is therefore influenced neither by the future, nor the past.

3. local equilibrium. Locally, the system is supposed to be in equilibrium. It follows that all the quantities which have been defined in equilibrium (like temperature, pressure, entropy...) keep their definition out of equilibrium. Moreover all the relations between the thermodynamic variables remain true at the condition to formulate these relations locally. In particular, Gibbs equation remains valid. For a multicomponents fluid system, it takes the form

$$du=Tds-pdv+\Sigma\mu^k dc^k \tag{4}$$

all the quantities are measured per unit mass, T is the temperature, s the entropy, v the specific volume ($v=\varrho^{-1}$), μ^k the chemical potential of component k.

Locally the entropy obeys the balance relation

$$\varrho\dot{s}=-\operatorname{div}\mathbf{j}^s+\sigma, \tag{5}$$

where $\mathbf{j}^s$ represents the entropy flux and σ the entropy production per unit volume. According to the second principle of thermodynamics, it is a positive definite quantity:

$$\sigma\geq 0. \tag{6}$$

To derive an explicit expression for σ, one eliminates the internal energy between the expression of the energy balance law (3) and the Gibbs equation. Using also (1) and (2), one obtains

$$\varrho\dot{s}=-\operatorname{div}\frac{1}{T}(\mathbf{q}-\Sigma\mu^k\mathbf{j}^k)+\mathbf{q}\,.\,\operatorname{grad}\,T^{-1}-\sum_{k=1}^{r-1}\mathbf{j}^k\cdot\operatorname{grad}\frac{\mu^k-\mu^r}{T}+\frac{1}{T}\,\tilde{\boldsymbol{\sigma}}:\tilde{\mathbf{v}}+A\dot{\xi}, \tag{7}$$

where A is the affinity of the chemical function ($A=-\Sigma\nu^k\mu^k$). By comparison with the balance law (5) it is seen that

$$\mathbf{j}^s=\frac{1}{T}\,(\mathbf{q}-\Sigma\mu^k\,\mathbf{j}^k) \tag{8}$$

$$\sigma=\mathbf{q}\,.\,\operatorname{grad}\,T^{-1}-\sum_{k=1}^{r-1}\mathbf{j}^k\,.\,\operatorname{grad}\frac{(\mu^k-\mu^r)}{T}+\frac{1}{T}\,\tilde{\boldsymbol{\sigma}}:\tilde{v}+A\dot{\xi}. \tag{9}$$

Expression (9) has the structure of a bilinear form in fluxes like $\mathbf{q}$, $\mathbf{j}^k$, $\dot{\xi}$, $\tilde{\boldsymbol{\sigma}}$ and terms like grad T^{-1}, grad $\frac{\mu^k-\mu^r}{T}$ which measure the deviation with respect to equilibrium. The former terms are called thermodynamic fluxes J^α and the latter, thermodynamic forces X^α. In whole generality, σ takes the form

$$\sigma=\sum_{\alpha=1}^{n}J^\alpha X^\alpha\geq 0. \tag{10}$$

The fluxes and the forces are related by so-called phenomenological relations which, in the vicinity of equilibrium are linear;

$$J^\alpha=\Sigma L^{\alpha\beta}X^\beta \tag{11}$$

$L^{\alpha\beta}$ are the phenomenological relations. If moreover the system is *isotropic*, one derives from general considerations on isotropic tensors that it is forbidden to couple fluxes and forces of different tensorial character. Such a law is frequently referred in the literature as *Curie's law.*

The linear phenomenological laws of our problem are

$$\mathbf{q}=L^{qq}\,\operatorname{grad}\,T^{-1}-\sum_{k=1}^{r-1}L^{qk}\,\operatorname{grad}\frac{\mu^k-\mu^r}{T} \tag{12}$$

$$\mathbf{j}^k=L^{kq}\,\operatorname{grad}\,T^{-1}-\sum_{j=1}^{r-1}L^{kj}\,\operatorname{grad}\frac{\mu^j-\mu^r}{T}\,(k=1,\ldots r-1) \tag{13}$$

$$\tilde{\boldsymbol{\sigma}}=\frac{\eta}{T}\,\tilde{\mathbf{v}} \tag{14}$$

$$\dot{\xi}=eA. \tag{15}$$

The first and the second relations (12) and (13) generalize respectively Fourier's and Fick's law, (14) is nothing but the Stokes — Newton law while (15) relates the chemical degree of advancement with the affinity.

The phenomenological coefficients are submitted to restrictions arising from the second law of thermodynamics. By substitution of (11) in (10), one obtains

$$\sigma=\Sigma L^{\alpha\beta}X^\alpha X^\beta\geq 0,$$

from which follows that

(16) $$L^{\alpha\alpha}>0 \quad L^{\alpha\alpha}L^{\beta\beta}\geq\frac{1}{4}(L^{\alpha\beta}+L^{\beta\alpha})^2,$$

As a consequence the heat conductivity coefficient which is related to L^{qq} by

(17) $$\lambda=\frac{L^{qq}}{T^2}$$

and the shear viscosity $\mu=\frac{\eta}{T}$ must always be positive.

Finally, Onsager has shown that the phenomenological coefficients are either symmetric or anti-symmetric, according that one couples processes which have the same parity or not with respect to the time reversal:

(18) $$L^{\alpha\beta}=\pm L^{\beta\alpha}.$$

These relations, although contested by Truesdell's school, have received many experimental confirmations, especially in the field of thermo-electricity.

Let us now go back to our problem of closing our set of equations. The phenomenological laws (12) to (15) gives $9+3(r-1)$ supplementary relations but they introduce additional unknowns T and μ^k. The remaining equations are obtained from the Gibbs equation from which one derives the following state equations:

$$u=u(T, \varrho, c^k)$$

$$p=p(T, \varrho, c^k)$$

$$\mu^k=\mu^k(T, \varrho, c^k) \quad k=1 \ldots r.$$

We have thus established the complete set of equations for the $12+5r$ unknowns; of course, the above equations must be supplemented by the adequate initial and boundary conditions.

3. Variational criterion for a one-component fluid flow

Practically, it is very difficult to solve this system of non-linear partial differential equations. An analytic solution is excluded, except in some particular situations. The most common attitude is to solve the problem by finite difference or the finite elements techniques. Another possibility is to construct a variational principle whose Euler-Lagrange equations are the set of equations to be solved. If a variational principle exists, one can use variational methods like Rayleigh—Ritz's, Kantorovitch's or an iteration procedure to obtain approximate solutions.

Many variational criteria have been presented. All of them present the common characteristic to be restricted principles which means that, during the variational procedure, some variables have to be kept constant. Among the best known variational principles in fluid mechanics, let us mention the criteria of Herival, Bateman which are "exact" ones but their range of applicability is limited to perfect fluids. For viscous fluids, only Rayleigh—Helmholtz principle is an exact one but it applies only to incompressible and isothermal fluids in slow motion. All the other principles like Gyarmathi's (6), Vujanovics' (7), Glansdorff-Prigogine's (8) are restricted ones.

Here we propose a new variational criterion which is more general than those of Vujanović and Gyarmathi which present some shortcomings as mentioned in refs. (9) and (10). Compared to Glansdorff-Prigogine local potential,

our formulation is, in our opinion, more systematic and there is no need like in Glansdorff-Prigogine's formalism to construct the principle for each new problem.

We shall limit our analysis to a one component Newtonian fluid. The more general case of a multi-components chemically active system is treated in ref. (5). Substituting the phenomenological laws in the conservation equations, one obtains the following set:

$$\frac{\partial \varrho}{\partial t} = -\nabla . (\varrho \mathbf{v}) \quad \text{(mass balance law)} \tag{19}$$

$$\varrho \dot{\mathbf{v}} = -\nabla_p p \nabla . (\mu \tilde{\mathbf{v}}) \quad \text{(Navier-Stokes equation)} \tag{20}$$

$$\varrho \dot{u} = \nabla . (\lambda \nabla T) - p \nabla . \mathbf{v} + \tilde{\mu \mathbf{v}} : \tilde{\mathbf{v}} \quad \text{(energy equation).} \tag{21}$$

We have neglected body forces and the energy source term. The heat conductivity coefficients λ and the shear viscosity may eventually depend on the temperature. When the state equations

$$u = u(T, \varrho)$$

$$p = p(T, \varrho)$$

are given, the expressions (19) to (21) constitute a set of 5 equations for the five unknowns, ϱ, $\mathbf{v}$ and T.

a. Heat conduction

In order to show the way of building up the principle, consider firstly the simple problem of heat conduction in a rigid body of volume Ω whose temperature is prescribed at the boundary and at the initial time. The heat transfer is governed by the energy equation

$$\dot{u}_v = -\nabla . \mathbf{q}, \tag{22}$$

where u_v is the internal energy per unit volume: one has

$$\dot{u}_v = c \dot{T}, \tag{23}$$

where c is the heat capacity per unit volume, the heat flux $\mathbf{q}$ is assumed to be related to ∇T by

$$\mathbf{q} = -\frac{L}{T} \nabla T.$$

It is easily seen that the dissipation energy function defined by

$$\psi = \frac{1}{2} T \sigma$$

is given by

$$\psi = -\frac{1}{2T^2} L (\nabla T)^2. \tag{24}$$

Introduce now the functional

$$I(T) = \int_{\Omega t_0}^{t} \int F(T) d\Omega dt = \int_{\Omega t_0}^{t} \int (\dot{f}_v - \psi) d\Omega dt. \tag{25}$$

where f_v is the Helmholtz free energy function

$$f_v = u_v - Ts_v, \dot{f}v = -s_v\dot{T}.$$

Our principle states that

$$\delta_t I(T) = 0 \tag{26}$$

underscript t means that the time variation of the variable submitted to variation, i. e. the temperature, must be held constant during variation. Of course, if the exact expression of $\dot{T}$ is known, the principle is an exact one. The Euler - Lagrange equation corresponding to (26) is

$$\frac{\partial F}{\partial T} - \nabla \cdot \frac{\partial F}{\partial(\nabla T)} = 0, \tag{27}$$

which is verified to be identical with (22), if L is constant. If L depends on the temperature, L must be kept constant during variation. From (25) it is seen that the quantity which determines the evolution of the process is the difference between the thermodynamic energy f_v and the heat dissipated during the time interval $t_0 - t$.

In the stationary case, criterion (25) reduces to the minimum dissipated energy criterion proposed by Prigogine

$$\delta \int \psi d\Omega = 0. \tag{28}$$

If L is constant, this principle is an exact one: no quantities are frozen.

b. Hydrodynamics

The above criterion may be generalized to include convective processes like fluids flows. Before formulating the definite form of the principle, let us introduce some notation. The kinetic energy per unit volume being given by

$$k_v = \frac{1}{2} \varrho \, \mathbf{v} \cdot \mathbf{v},$$

we define a function L, by

$$L = k_v + p. \tag{29}$$

The dissipation function is now expressed by

$$\psi = \frac{1}{2}\left(-\mathbf{q} \cdot \frac{1}{T} \nabla T + \tilde{\boldsymbol{\sigma}} : \tilde{\mathbf{v}}\right) = \frac{1}{2} T^{-2}(L(\nabla T)^2 + \eta \tilde{\mathbf{v}} : \tilde{\mathbf{v}}). \tag{30}$$

If Ω represents a fixed volume through with the fluid flows, the principle takes the general form

$$\delta_t \int_{t_0}^{t} \int_{\Omega} \frac{\partial L}{\partial t} d\Omega dt + \delta_x \int_{t_0}^{t} \int_{\Omega} \operatorname{grad}(L\,\mathbf{v}) d\Omega dt + \delta \int_{t_0}^{t} \int_{\Omega} (\psi + k_v \operatorname{div} \mathbf{v}) \, d\Omega dt = 0. \tag{31}$$

By analogy with δ_t, δ_x means that the spatial derivatives are frozen during variation.

It has been verified (12) that one recovers as Euler - Lagrange corresponding to arbitrary variations of μ, $\mathbf{v}$ and T respectively the mass, the Navier - Stokes and the energy laws.

In the particular case of an incompressible fluid in stationary motion, expression (28) takes the simpler form

$$\delta_x \int_\Omega \mathbf{v} \cdot \nabla L d\Omega - \delta \int_\Omega (\psi - \lambda \nabla \cdot \mathbf{v}) d\Omega = 0, \tag{32}$$

where λ is a Lagrange multiplier.

For the slow motion of an incompressible fluid at uniform temperature, the first term in the l. h. s. of (32) is of the order v^3 and therefore negligeable while ψ is given, at constant T, by

$$\psi = \frac{1}{2} \eta \tilde{\mathbf{v}} : \tilde{\mathbf{v}}.$$

It follows that one recovers Helmholtz minimum dissipation energy principle

$$\delta \int (\eta \tilde{\mathbf{v}} : \tilde{\mathbf{v}} - \lambda \nabla \cdot \mathbf{v}) d\Omega = 0. \tag{33}$$

The criterion (31) has also been applied to study the stability with respect to small perturbations of several fluid flows (13). Other applications of the principle may be found in (10), (11), (15). They concern heat transfer problems in rigid body and in fluid systems as well as the determination of velocity and temperature profiles in laminar boundary layers. Generally, Rayleigh -Ritz or Kantorovitch partial integration methods are used as variational methods.

In our opinion, the advantages of variational techniques are threefold. Firstly, the numerical methods involved are very simple. Secondly, the time duration of the calculation are appreciably shorter than with finite difference or finite elements techniques and thirdly, the approximated solutions are given in an analytic form, which permits easier manipulations.

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