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Formulation of some homogeneous thermodynamic processes as variational inequality

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THE aim of this paper is to show how for the basic problem of the thermodynamics of homogeneous processes there exists a formulation which takes an alternative collocation in relation to the results of COLEMAN and NOLL (1963, [1]). We prove the existence of a class of processes which are thermodynamically incompatible according to the theory of COLEMAN and NOLL, but are neverthless a solution of the variational problem.

Zadaniem obecnej pracy jest wykazanie, że podstawowy problem termodynamiki procesów jednorodnych ma alternatywne sformułowanie do propozycji COLEMANA i NOLLA (1963, [1]). Udowodniono istnienie klasy procesów, które są termodynamicznie niezgodne z teorią COLEMANA i NOLLA, ale pomimo to są rozwiązaniem zagadnienia wariacyjnego.

Целью данной работы является формулировка основных понятий термодинамики однородных процессов, отличающаяся от предложений Колемана и Нолла (1963, [1]). Доказано существование класса процессов, которые согласно теории Колемана и Нолла являются терминамически несовместимыми, тем не менее являются решениями некоторых вариационных задач.

1. Introduction

THE MAIN aim of this note is to show how for the basic problem of the thermodynamics of homogeneous processes, there exists a formulation which takes an alternative collocation in relation to the results of COLEMAN & NOLL [1963, 1].

Indeed, while the method of COLEMAN & NOLL(1) gives the restrictions on the response functionals in such a way that the reduced dissipation inequality holds for every process, a different presentation of the problem in the form of variational inequality (when this is possible) enables simultaneous consideration of equations and inequalities (2), avoiding the necessity to introduce the potentials in the constitutive equations, and modifying also the actual concept of solution.

For reasons of simplicity and clarity, only the problem of the thermomechanic equilibrium of a particular homogeneous simple process with one grade of freedom is considered. This choice, apart from the advantage of utilizing certain results already systematized in the theory, is sufficiently general to examplify the principal features of the present approach and its connections with the classic one.

(1) Successively extended to non-homogeneous materials with memory (cf. COLEMAN [1964, 2]).

(2) We shall make systematic reference to the paper by STAMPACCHIA [1968, 1] as regards the general theory, and specific use of certain results by LIONS [1969, 8].

In fact, we prove the existence of a class of processes which are thermodynamically incompatible according to the theory of COLEMAN and NOLL, but are nevertheless a solution of the variational problem.

2. The differential problem and its formulation as a variational inequality

Let $\Upsilon(t)$, $\theta(t)$ be a pair of functions defining a given thermokinetic process: $\Upsilon(t)$ characterizes the place occupied by the system and $\theta(t)$ $(\theta > 0)$ is the absolute temperature, both being assumed continuously differentiable functions of the time t. The dependence of Υ, θ on t expres es the *homogeneity* of the system, while the possibility of describing it with only one scalar function $\Upsilon(t)$ means that one is the number of the *degrees of freedom* (3).

Assuming that the material is *simple*, the following quantities are defined in terms of the primitives:

$$
\begin{aligned}
\omega &= \hat{\omega}(\Upsilon), && \textit{thermodynamic force}, \\
\varepsilon &= \hat{\varepsilon}(\Upsilon, \theta), && \textit{internal energy}, \\
\eta &= \hat{\eta}(\Upsilon, \theta), && \textit{entropy},
\end{aligned}
\tag{2.1}
$$

and the *free energy*, given by

$$
\psi = \varepsilon - \eta\theta. \tag{2.2}
$$

All are assumed continuously differentiable with respect to their arguments, and the thermodynamic force is assumed as depending only on $\Upsilon(t)$ (4).

Thus, if $B(t)$ and $\theta(t)$ are the *external force* and the *heating* applied to the system (both continuous functions of t), its evolution in time is ruled by the *equilibrium* equation:

$$
\ddot{\Upsilon} - \omega = B(t), \tag{2.3}
$$

and the *balance* equation:

$$
\dot{\varepsilon} + \omega\dot{\Upsilon} = Q(t), \tag{2.4}
$$

together with the boundary conditions, which are assumed in the following form (5):

$$
\Upsilon(0) = \Upsilon(T) = 0, \quad \theta(0) = \theta_0 > 0. \tag{2.5}
$$

In addition to the conservation Eqs. (2.3), (2.4), $\Upsilon(t)$ and $\theta(t)$ are ruled by two thermodynamic restrictions — that is, the Clausius-Duhem inequality

$$
\dot{\psi} + \omega\ddot{\Upsilon} + \eta\theta \leqslant 0, \tag{2.6}
$$

and the strict positivity of the absolute temperature — that is, $\theta(t) > 0$.

(3) For the symbols and the definitions see TRUESDELL [1969, 7].

(4) This somewhat strong assumption is suggested by reasons of mathematical simplicity in the application of the theory.

(5) We suppose that the boundary conditions on $\Upsilon(t)$ are homogeneous and of Dirichlet type. For the extension to different boundary conditions see LIONS [1969, 8].

The assumed dependence of ω on the only $\Upsilon(t)$ makes possible to put the problem in another form. To this aim, we introduce a function $\Omega(\Upsilon)$ such that

$$\Omega(\Upsilon) = \int_0^t \omega \dot{} \, d\tau$$

whence, integrating the Eq. (2.4) with respect to the time, we obtain

$$\varepsilon - \varepsilon_0 + \Omega(\Upsilon) = \int_0^t Q(\tau) d\tau, \tag{2.7}$$

where

$$\varepsilon_0 = \hat{\varepsilon}(0, \theta_0).$$

Then, since (2.7) defines implicitly $\theta(t)$ as a function of $\Upsilon(t)$, assuming that for each t on $[0, T]$ the hypotheses of the Dini theorem are satisfied, we can make $\theta(t)$ explicit in terms of $\Upsilon(t)$ in the form:

$$\theta(t) = \Theta[Y(t), t], \tag{2.8}$$

while its partial derivative with respect to Υ is

$$\Theta_{,\Upsilon} = -\frac{\varepsilon_{,\Upsilon} + \omega}{\varepsilon_{,\theta}}, \tag{2.9}$$

being of course $\varepsilon_{,\theta} \neq 0$, for each t on $[0, T]$.

Then, substituting (2.8) in (2.3) and (2.6), we reduce the thermomechanical problem to search for a function $\Upsilon(t)$ such that the Eq. (2.3) holds with the boundary conditions (2.5) and the inequality (2.6).

But, as an alternative to the differential form, this problem can be formulated in the form of a variational inequality [6]. In fact, let V be the reflexive Banach space constituted by the functions with the first derivative of the square summable on the interval $(0, T)$, endowed with the norm

$$||\Upsilon||_V^2 = \int_0^T [\Upsilon^2(\tau) + \dot{\Upsilon}^2(\tau)] d\tau, \tag{2.10}$$

and let V' be its dual. By V_0, we indicate the linear subspace of V described by the members of V satisfying $(2.5)_1$ and let K be a convex subset of V_0 formed by the functions $\Upsilon^*(t)$ such that

$$\dot{\psi}^* + \omega^* \dot{\Upsilon}^* + \eta^* \dot{\theta}^* \leqslant 0,$$

having denoted by $\psi^*, \omega^*, \theta^*$ the values of (2.1) when $\Upsilon = \Upsilon^*$ and $\theta^* = \Theta[\Upsilon^*(t), t]$. With these statements, we call solution of the variational inequality a function $\Upsilon(t)$, for which:

$$\int_0^T (-\ddot{\Upsilon} + \omega)(\Upsilon^* - \Upsilon) dt \geqslant -\int_0^T B(\Upsilon^* - \Upsilon) dt, \quad \forall \Upsilon^* \in K, \tag{2.11}$$

with B belonging to V' [7].

[6] For non-linear variational inequalities see STAMPACCHIA [1968, 6].

[7] In order that the formulation (2.11) be consistent, it is also necessary to postulate that ω belongs to V' (see LIONS [1969, 8,7]).

Since the existence of a solution of the problem (2.11) is based on the *strict monotonicity* of the operator (2.3) and the *convexity* of the subset K, some rather general criteria implying these properties will be discussed below.

3. Conditions of monotonicity

According to definition (STAMPACCHIA [1968, 3]), the operator (2.3) is said to be *strictly monotone* if, for each pair Υ and Υ^* in K, the inequality

$$\int_0^T [(-\ddot{\Upsilon}^*+\omega^*)-(-\ddot{\Upsilon}+\omega)](\Upsilon^*-\Upsilon)dt > 0 \tag{3.1}$$

holds. But, since ω is assumed a continuously differentiable function of $\Upsilon(t)$, it is possible to impose some restrictions ensuring *a fortiori* the monotonicity.

In fact, by the mean value theorem, we can write

$$\omega^*-\omega = \overline{\omega}_{,\Upsilon}(\Upsilon^*-\Upsilon),$$

where

$$\overline{\omega}_{,\Upsilon} = \hat{\omega}_{,\Upsilon}(\overline{\Upsilon}),$$

with $\overline{\Upsilon}$ suitable determination of the argument between Υ^* and Υ (8).

Therefore, the condition (3.1) assumes the form

$$\int_0^T [(\dot{\Upsilon}^*-\dot{\Upsilon})^2+\overline{\omega}_{,\Upsilon}(\Upsilon^*-\Upsilon)^2]dt > 0, \tag{3.2}$$

which by Wirtinger's inequality can be further modified into the simpler condition

$$\left(\frac{\pi^2}{T^2}+m\right)\int_0^T (\Upsilon^*-\Upsilon)^2\,dt > 0,$$

with

$$m = \inf_{\Upsilon} \omega_{,\Upsilon},$$

so that we may immediately conclude that if

$$\frac{\pi^2}{T^2}+m \geqslant \alpha, \tag{3.3}$$

with $\alpha > 0$, the first member of (3.2) is always positive and the operator (2.3) is strictly monotone (9).

Since the validity of (3.3) is essential for the correct formulation of the problem (2.11), and in particular for the uniqueness of solution (STAMPACCHIA [1968, 6]), we state as a postulate that *on the constitutive equations all the restrictions, ensuring* (3.3), *hold.*

(8) In more precise form: $\overline{\Upsilon} = \Upsilon+\varepsilon(\Upsilon^*-\Upsilon)$, with $0 < \varepsilon < 1$.

(9) It may be of interest to remark that the condition (3.3) is always satisfied with thermodynamical forces ω monotone with Υ, while, if ω is anitone with Υ, as it happens when ω is a restoring force, the monotonicity is ensured only below the first proper frequency of a certain problem of free vibration.

4. Conditions of convexity

A second set of restrictions on ω and η derives from the necessity that the surface

$$(\psi_{,\Upsilon}+\omega)\dot{\Upsilon}+(\psi_{,\theta}+\eta)\dot{\theta} = 0 \tag{4.1}$$

be convex in the space of the variables Υ, $\dot{\Upsilon}$. In (4.1), θ and $\dot{\theta}$ are understood as functions of Υ and $\dot{\Upsilon}$. The explicit form of (4.1) is obtained resolving (2.4) with respect to $\dot{\theta}$ and substituting in (4.1) — that is,

$$\left[\psi_{,\Upsilon}+\omega-\frac{1}{\varepsilon_{,\theta}}(\psi_{,\theta}+\eta)(\varepsilon_{,\Upsilon}+\omega)\right]\dot{\Upsilon}+\frac{1}{\varepsilon_{,\theta}}(\psi_{,\theta}+\eta)Q = 0.$$

But, since this is linear on $\dot{\Upsilon}$ and Q, the same definition of convexity implies that *necessary and sufficient* (10) *condition of convexity is the existence of two constants* K_1, K_2 *such that*:

$$\begin{aligned}\psi_{,\Upsilon}+\omega-\frac{1}{\varepsilon_{,\theta}}(\psi_{,\theta}+\eta)(\varepsilon_{,\Upsilon}+\omega) &= K_1,\\ \frac{1}{\varepsilon_{,\theta}}(\psi_{,\theta}+\eta) &= K_2.\end{aligned} \tag{4.2}$$

In geometrical terms, the conditions (4.2) require that K be a half plane, while, from the mechanical point of view, they prove that *the thermodynamic force and the entropy are not determined from the free-energy as a potential, but satisfy certain not simple identities involving the partial derivatives of the functions of state.* Of course, the situation considered by the theorem of COLEMAN and NOLL, where every admissible process of a simple material is reversible (see TRUESDELL [1966, 5, 26]), happens when $K_1 = K_2 = 0$.

5. Solution of (2.11)

In these hypotheses it is known that the solution of the unconstrained problem, that is without the inequality (2.6), plays an important role in the individualization of the solution. In fact, applying the results of the general theory (see STAMPACCHIA [1968, 6]), three situations are possible:

a) If Υ^0, θ^0 is the solution of the unconstrained problem, and Υ^0, θ^0 belong to K, then Υ^0, θ^0 itself is the (unique) solution of the variational inequality.

b) If Υ^0, θ^0 is external to K, the solution necessarily lies on the boundary of K.

c) In the special case, where K_1 and K_2 are zero, K is the whole plane, so every pair Υ^0, θ^0 is a solution.

According to the definition that a process is reversible when the constraint (2.6) holds as an inequality, we can classify as *irreversible* a process described by the case (a), while the cases (b), (c) define *reversible* processes.

A further specification of the solution can be given in the particular case when

$$\omega = \gamma\Upsilon, \tag{5.2}$$

(10) The proof of this property is postponed to Appendix.

where γ is a constant $> -\pi^2/T^2$, for the Eq. (2.3) becomes linear on the only function Υ. Therefore, it is known that we can associate with the operator a bilinear form:

$$a(\Upsilon, \Upsilon^*) = \int_0^T (\dot{\Upsilon}\dot{\Upsilon}^* + \gamma\Upsilon\Upsilon^*)\,dt, \tag{5.2}$$

having the properties of a scalar product in a Hilbert space with norm (2.10).

In this situation, the solution of the variational inequality is the canonical projection of B on the convex K (11).

Appendix

The proof of the result quoted in Sec. 4 is essentially contained in the following:

LEMMA 1. *Necessary and sufficient condition in order that the surface* (12)

$$f(y)x + g(y)z = 0 \tag{A.1}$$

be convex, is the existence of two constants K_1, K_2 such that:

$$f(y) \equiv K_1, \quad g(y) \equiv K_2. \tag{A.2}$$

While the sufficiency is obvious, the necessity derives from the fact that, if (x_1, y_1, z_1), (x_2, y_2, z_2) are belonging to the surface (A.1), the pair $(-x_1, y_1, -z_1)$, $(-x_2, y_2, -z_2)$ satisfies the same property. Therefore, if we make the provision that a convex combination of the first two points is not external to the surface (A.1) — that is,

$$f[ty_1 + (1-t)y_2]\,[tx_1 + (1-t)x_2] + g[ty_1 + (1-t)y_2]\,[tz_1 + (1-t)z_2] \leqslant 0, \tag{A.3}$$

with $0 \leqslant t \leqslant 1$, this condition cannot hold for the second pair of points. This only situation permitting the (weak) convexity of (A.1) is the existence of (A.2).

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(11) See STAMPACCHIA [1964, 2]. Since K is a half plane, the construction of this projection can be effected by elementary operations.

(12) Defined in the three-dimensional space.