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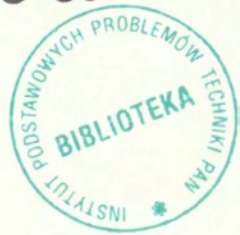
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# On non-equilibrium entropy in continuum thermodynamics of materials with memory <sup>(1)</sup>

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BASED ON PREVIOUS WORKS of the author, the fundamentals of some basic concepts and methods currently used in the formulation of constitutive equations for linear or non-linear dissipative materials are revisited. The principles of the local state – or local equilibrium state – frequently used as the basis of Thermodynamics of Irreversible Processes in connection with the problem of the definition of a non-equilibrium entropy – are discussed, with emphasis laid on materials with memory exhibiting – as in linear or non-linear viscoelasticity – a delayed response to a constant loading. An adiabatic relaxation experiment is defined, from which it is shown that the usual formulation of the local state principle is too strong, since the set of relations which holds in equilibrium, and which makes use of macroscopic variables only, can never be applied without modification out of equilibrium. The same holds for the non-equilibrium Gibbs equation generally associated with the corresponding formalism when written with the real stress and temperature involved in the process. For dissipative behaviour of the differential type of order one, called also Markovian behaviour, a non-equilibrium entropy can be defined and some of the equilibrium relations can be applied to non-equilibrium situations. From this, a basic thermodynamic classification of rheological behaviour is obtained. In the non-Markovian case, the results are applied to the method of internal variables. A criterion for identifying suitable internal variables is obtained. They should correspond to Markovian behaviour when directly stimulated.

## 1. Introduction

EXPERIMENTAL EVIDENCE concerning the delayed response of most real materials and its coupling with physical and chemical effects, has been obtained since the pioneering experiments of BUFFON [10] in the eighteenth century with the delayed fracture of wood, those of VICAT [88] (the discoverer of the fundamentals of the hardening of cement) with the creep of iron, and a few years later the study of the creep of silk, glass, and silver threads by other authors. Since that time, it has been found that such effects can appear, with magnitudes depending on each specific case and environment, in all materials. Formulation in a realistic and consistent fashion of the corresponding three-dimensional constitutive equations and criteria, and evaluation of the risk of deterioration under long term evolution, still

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<sup>(1)</sup>The paper partly develops an invited lecture given to the 31th Solid Mechanics Conference in Mierki, Poland, in September 1996 [57].

remains a widely open problem, while the need is continuously increasing with the development of new techniques and new materials [4, 43, 47, 48, 50]. This is also needed in the development and application of numerical simulations techniques taking into account the real microstructure of the material and the interactions with the climatic and chemical changes in the framework of statistical continuum micro-mechanics [58, 45, 46, 48–51, 81]. From this viewpoint, the usefulness of Thermodynamics in providing a consistent framework for constitutive laws has been emphasized many times.

The thermomechanical aspects of material behaviour is often considered in the framework of Continuum Thermodynamics – also called Rational Thermodynamics. The latter was mainly developed in the fifties and sixties by NOLL, TRUESDELL *et al.* [71, 83–85], COLEMAN [16, 17], BRUN [8, 9], DAY [18] and others, through an approach directly derived from the works of CLAUSIUS [14, 15], MASSIEU [65] and DUHEM [23, 24] in a rather axiomatic form. In this approach, use is made of macroscopic variables for which the memory effects can be dealt with in the form of functionals of the history, first introduced by BOLTZMANN [6], and then developed by VOLTERRA [89–91], FRÉCHET [25] and others. In particular, the use of such history functionals is well adapted to materials endowed by experimental evidence with continuous spectra of response times, as experimentally found on many real materials devoid of aging [34–36, 2, 3, 32, 26, 78] (also adressed using fractional calculus [1, 82]) or with aging due to chemical reactions occuring under load as in the case of cement concrete [3, 4]. In this approach by functionals, the existence of various thermodynamic functions is postulated, the justification being left to the consequences of the theory.

By contrast, the chemical and physical phenomena are most often considered in the framework of the Thermodynamics of Irreversible Processes (TIP) [59], itself being based on the efforts performed in the forties and fifties [66, 73–75] to extend the powerful formalism elaborated by GIBBS [30] for Equilibrium Thermodynamics. In TIP, it is accepted only as an approximation to take as non-equilibrium thermodynamic functions the very ones already defined for the case of equilibrium and/or reversible processes, this expressing the so-called “principle of local equilibrium”, or “principle of the local state”, in which the use of the so-called Gibbs equation plays a central role. From this, the range of validity of the approach is considered limited to the case qualified as “sufficiently near equilibrium”, for which linear complementary equations are derived through a Taylor expansion limited to the first order [73–75, 59], the theory being extended to history-dependent behaviour through the use of internal or hidden variables [5, 2, 79, 57].

Thus, in order to include the chemical and physical aspects in the continuum-thermomechanics theory, one may have to combine theoretical formalisms of various origins based on seemingly incompatible statements. Some of the associated

problems and discussions were presented in specialised symposia [22, 56]. This paper considers some of these problems on the basis of our previous attempts to ensure compatibility [37–42, 44]. For the sake of clarity and self-containment, Section 2 to 4 below recall the fundamental features of these two approaches. Section 5 comes back to discussing the principle of the local state by providing, for the case of finite deformations, a refined version of the derivations first presented in [37, 39]. From this, Section 6 provides a status of the non-equilibrium entropy for a specific class of behaviour called Markovian and provides a full thermodynamic theory for this class. Section 7 applies the obtained results to the method of internal variables frequently used for approximating non-Markovian behaviour, providing a criterion for the choice of internal variables. Section 8 compares the approach used in the paper with those used for the same problem by two other authors. The results are recapitulated in Section 9, which provides an exhaustive thermodynamic classification of material behaviour and proposes a physical interpretation.

## 2. Universal relationships of Continuum Thermodynamics

### 2.1. Conservation equations in global form

Continuum Thermodynamics starts by stating a set of universal relationships, valid for every materials and bodies, and which express conservation equations for mass, momentum, moment of momentum and energy. Their original form is a global one which relates mechanical and physical variables defined on any finite part of the body to its environment. We consider an open domain  $D$  with mass  $M$ , momentum  $B$ , moment of momentum  $L$  and the total (internal plus kinetic) energy  $E$ , and which may experience a movement relatively to matter, or for which some matter may flow across its boundary  $\partial D$ . Denoting by  $x$  the coordinates of a material point,  $\nu$  its velocity  $\dot{x}$ , and  $\nu_\Sigma$  the velocity of the corresponding geometric point on the moving boundary  $\partial D$ , the global conservation equations at time  $t$  are:

$$(2.1) \quad M' \equiv \frac{\delta M}{\delta t} = \int_{\partial D} \rho(\nu - \nu_\Sigma) \cdot n d\Sigma,$$

$$(2.2) \quad B' \equiv \frac{\delta B}{\delta t} = \int_D F^d dV + \int_{\partial D} \{P + \rho\nu(\nu_\Sigma - \nu) \cdot n\} d\Sigma,$$

$$(2.3) \quad L' \equiv \frac{\delta L}{\delta t} = \int_D x \wedge F^d dV + \int_{\partial D} x \wedge \{P + \rho\nu(\nu_\Sigma - \nu) \cdot n\} d\Sigma,$$

$$(2.4) \quad U' + C' = \int_D (F^d \cdot \nu + r) dV + \int_{\partial D} \{P \cdot \nu + h + (\rho u + \rho \nu \cdot \nu)(\nu_\Sigma - \nu) \cdot n\} d\Sigma.$$

In these equations,

$$(2.5) \quad G' = \frac{\delta D}{\delta t} = \frac{\partial G}{\partial t} + \nu_\Sigma \cdot \text{grad } G.$$

denotes the total time derivative of any quantity  $G$  in any material or immaterial movement of the domain,  $(\cdot)$  the once contracted tensor product,  $\wedge$  the vector product,  $U$  and  $C$  the total internal and kinetic energies, respectively. The volume and surface densities  $F^d, P, r, h$  denote the – assumed to be regular – external volume forces, surface tractions, non-mechanical volume and surface energy supplies (heat), respectively. The above equations are valid either for the whole body, or for every subdomain inside it, or still for every superdomain including the body and a part of its environment. For a closed body or domain with boundary impervious to matter or following its movement, the time derivatives involved in this equations become the material derivative:

$$(2.6) \quad \dot{G} = \frac{dG}{dt} = \frac{\partial G}{\partial t} + \nu \cdot \text{grad } G.$$

The above conservation equations are then supplemented by additional relationships expressing the second Principle of Thermodynamics and involving additional physical variables, temperature and entropy.

## 2.2. Global Clausius inequality and entropy

Historically, the Second Principle of Thermodynamics – or Carnot-Clausius Principle – was, from the work of CARNOT [13] and after acceptance of the energy conservation principle now known as the First Principle, originally expressed by CLAUSIUS [14, 15] in his own notation, as the following weak inequality, globally valid for any system in every evolution forming a closed cycle of the control variables:

$$(2.7) \quad \oint \frac{dQ}{T} \leq 0.$$

Here  $dQ$  is the increment of heat provided to the body during the time interval  $dt$  while  $T$  denotes the empirical temperature at time  $t$ . The equality to zero is obtained for reversible processes or behaviour, while the inequality is strict for

all other cases, characterised by irreversible processes or behaviour. After some delay, this led CLAUSIUS [15] to introduce a new physical quantity, which he called the entropy  $S$ , having the property that, for *reversible* processes or behaviour in a closed cycle of the controlled variables, the above inequality becomes the equality:

$$(2.8) \quad \oint \frac{dQ}{T} = \oint dS = 0,$$

making thus entropy a function of state (understood as the set of controlled variables), this giving, for every reversible evolution between the initial state 0 and the present state 1:

$$(2.9) \quad \int_0^1 \frac{dQ}{T} = S - S_0.$$

For irreversible evolutions between the two states, CLAUSIUS writes, Eq. (71) of his original 1865 memoir [15], denoted (C71) in the following:

$$(C71) \quad N = S - S_0 - \int_0^1 \frac{dQ}{T},$$

where  $N$  is a quantity which should be positive for every irreversible process or behaviour, and which vanish for all reversible processes. It is thus the total amount of entropy produced within the body during its irreversible evolution. Of course, the above equation can also be written:

$$(2.10) \quad S = S_0 + \int_0^1 \frac{dQ}{T} + N,$$

This relationship (C71) was derived from a modified form of the Carnot principle by considering that there exists at least one reversible process through which the body can be brought back from its present state to its initial state. Considering the closed cycle thus obtained, Clausius wrote:

$$(2.11) \quad \int_0^1 \frac{dQ}{T} = -N < 0,$$

which is consistent with the first inequality written above.

Clausius obtained from this his Eq. (C71) by taking account of the vanishing of the entropy production during the reversible return process. The necessity of having such a reversible path led most physicists to state that entropy is not



defined – strictly speaking – in non-equilibrium situations. On the other hand, some physicists and most continuum mechanicians consider that the thermodynamic quantities, and in particular entropy, can be taken as primitive quantities of the theory, *a priori* defined also in non-equilibrium situations [11, 85, 83]. This has been questioned especially for entropy, seemingly without achieving mutual agreement up to now, see for instance [59].

In fact, taking the time derivative of Eq. (2.10) gives:

$$(2.12) \quad \dot{S} = \frac{d}{dt} \left( \int_0^1 \frac{dQ}{T} \right) + \frac{dN}{dt},$$

showing that the original equation (C71) of Clausius can be considered as the first historical expression – in an integrated form – of an entropy balance equation if the existence of a non equilibrium entropy is to be accepted.

### 2.3. Local forms of the universal balance equations at regular points

For subdomains devoid of non-integrable singularities in the mechanical or physical variables, it is possible to express  $M, B, L, U$ , and  $S$  through the integrals of the corresponding local densities, denoted, per unit mass,  $\rho, \nu, u$  and  $s$ , respectively. For the entropy produced in an irreversible change between times 0 and, one may write:

$$(2.13) \quad N = \int_0^1 Z(u) du,$$

$Z$  being the global entropy production rate, expressed in terms of the local density one  $\zeta$  by:

$$(2.14) \quad Z = \int_D \zeta dV,$$

this expressing the additivity property of the entropy production. The balance equation (2.12) then becomes:

$$(2.15) \quad \dot{S} = \int_D \left( \zeta + \frac{r}{T} \right) dV + \int_{\partial D} \frac{h}{T} d\Sigma.$$

This, together with the global forms of Subsec. 2.1 and the use of the classical divergence and transport theorems makes it possible to obtain the classical local forms of the universal balance equations at every regular point inside the body

through a localisation procedure based on the consideration of a dense family of homogeneous domains around a given material point. Denoting the specific volume by  $\tau = 1/\rho$ , the universal balance equations in local form reduce eventually, in Euler variables, to:

$$(2.16) \quad \rho \dot{\tau} = \operatorname{div} \nu,$$

$$(2.17) \quad \rho \dot{\nu} = F^d + \operatorname{div} \sigma,$$

$$(2.18) \quad \sigma^T = \sigma,$$

$$(2.19) \quad \rho \dot{u} = \sigma : d + r - \operatorname{div} q,$$

$$(2.20) \quad \rho \dot{s} = \zeta + \frac{r}{T} - \operatorname{div} \frac{q}{T}.$$

In the above expressions, all densities are functions of  $x$  and  $t$ . A similar localisation procedure applied to subdomains involving interfaces leads to a corresponding set of jump relationships at every point of an interface, see for instance [27, 51]. Considering that Clausius inequality must remain valid for every domain with vanishing volume around a given point, it is postulated in addition that the density of the entropy production rate  $\zeta$  is non-negative at all times, giving:

$$(2.21) \quad \zeta \geq 0,$$

the inequality being strict for all irreversible processes or behaviour and the equality to zero for reversible transitions or behaviour only.

Most often (the formalism proposed in [39–42] being one of the exceptions), the entropy balance (2.20) is not directly used as a general field equation of the problem, temperature and entropy being involved at the level of constitutive equations only. After appropriate transformation, Clausius inequality is used as providing restrictions on the possible forms that can be taken by these constitutive equations.

#### 2.4. Universal expressions for the entropy production and dissipation densities

Entropy balance equation (2.20) may be considered as providing a universal expression for the entropy production rate  $\zeta$ :

$$(2.22) \quad \zeta = \rho \dot{s} - \frac{r}{T} + \operatorname{div} \frac{q}{T}.$$

Developing the divergence of the quotient in the R.H.S. of Eq. (2.22) makes it possible to split this expression for into two parts:

$$(2.23) \quad \zeta = \rho \dot{s} - \frac{r}{T} + \operatorname{div} q + q \cdot \operatorname{grad} \frac{1}{T} \equiv \zeta_M + \zeta_T,$$

with

$$(2.24) \quad \zeta_T = q \cdot \operatorname{grad} \frac{1}{T}$$

and

$$(2.25) \quad \zeta_M = \rho \dot{s} - \frac{1}{T}(r - \operatorname{div} q).$$

It is generally postulated that  $\zeta_T$  and  $\zeta_M$  are non-negative separately.

Eliminating the heat supply between Eqs. (2.18) and (2.25) provides us with universal expressions for the mechanical part  $\zeta_M$  of the entropy production and for Clausius inequality,

$$(2.26) \quad \zeta_M = \rho \dot{s} - \frac{1}{T}(\rho \dot{u} - \sigma : \dot{\epsilon}) \geq 0.$$

In Lagrange variables, valid for finite deformations as well as for small strains, it reads, in terms of the entropy density per unit initial volume, as:

$$(2.27) \quad \zeta_M = \dot{S} - \frac{1}{T}\dot{U} + \frac{\Pi}{T} : \dot{\Delta} \geq 0.$$

Defining as usual the local dissipated power  $\mathcal{D}$  per unit volume, also called *dissipation*, as:

$$(2.28) \quad \mathcal{D} = T\zeta_M,$$

and taking account of Eq. (2.27), provides us with an universal expressions for the dissipation together with a corresponding form of the local Clausius-Duhem inequality in terms of the internal energy. In Lagrange variables, it becomes:

$$(2.29) \quad \mathcal{D} = -(\dot{U} - T\dot{S} - \Pi : \dot{\Delta}) \geq 0.$$

The relationships (2.27) and (2.29) are not constitutive properties: derived from the universal balance equations, they are valid for every material and every behaviour, dissipative or not, once entropy has been defined for non-equilibrium situations.

### 3. Constitutive equations in the Equilibrium Thermodynamics Formalism

#### 3.1. Extended Gibbs space and Gibbs equilibrium surface

In all classical formalisms of continuum thermomechanics, the constitutive equations are a set of equations by which the set of universal equations must be supplemented in order to determine the whole thermomechanical behaviour, namely displacements and stress distribution with their time evolution, of a body of finite size under external loadings and appropriate boundary conditions. In contradistinction to the conservation equations, that hold for every materials, these constitutive equations are not universal, but are specific to the material from which the body is made.

Considering perfect fluids with mechanical variables limited to volume  $V$  and pressure  $p$ , GIBBS [29, 30] showed that all the constitutive equations of a homogeneous medium in its various states of thermodynamic equilibrium can be represented by the geometric properties of a hypersurface in an affine hyperspace.

For a material which can be solid, the mechanical variables are the strain tensor  $\Delta$ , which corresponds to the scalar variable  $V$ , and the stress tensor  $\Pi$ , which corresponds to the scalar variable  $(-p)$ . When the materials contains  $n$  chemical constituents involving thermal, mechanical and chemical phenomena only, we get an extended Gibbs hyperspace with  $8+n$  dimensions. The properties at thermodynamic equilibrium are fully determined by a hypersurface, which is a  $7+n$ - dimensional manifold when the symmetry of the tensor  $\Delta$  is taken into account. This hypersurface may be called the equilibrium surface or the extended Gibbs surface and is denoted  $\Sigma$  in the sequel. It is defined by a fundamental equation expressing the entropy as a function of the strain tensor  $\Delta$ , the internal energy  $U$  per unit volume and the number of moles  $N_k$  of each constituent  $k$ :

$$(3.1) \quad S = \underset{\sim}{S} (\Delta, U, N_1, \dots, N_n).$$

The fact that the thermal gradient has not to be involved in the thermodynamic functions when the temperature is not uniform has been shown by various authors [16, 18, 83, 85].

#### 3.2. Properties of entropy at equilibrium and in reversible changes

As is known, in case of elastic materials without chemical changes expressed in the entropy representation, the properties of entropy at equilibrium or in reversible changes can be recapitulated as follows:

i) Entropy is a state function of  $\Delta$  and  $U$ , that is, possible states in the extended Gibbs space  $(\Delta, U, S)$  lie on a surface of this space (equilibrium surface property);

ii) the whole (thermo-elastic) behaviour is completely determined by the explicit knowledge of the fundamental equation expressing the specific entropy  $S$  in terms of the set  $(\Delta, U)$  of independent variables;

$$(3.2) \quad S = \tilde{S}(\Delta, U);$$

iii) entropy is a potential for  $1/T$  and  $-\Pi/T$ :

$$(3.3) \quad -\frac{\Pi}{T} = \frac{\partial \tilde{S}}{\partial \Delta},$$

$$(3.4) \quad \frac{1}{T} = \frac{\partial \tilde{S}}{\partial U};$$

iv) a Gibbs equation holds in macroscopic variables, that is:

$$(3.5) \quad \dot{S} = \frac{1}{T} \dot{U} - \frac{\Pi}{T} : \dot{\Delta};$$

v) various reciprocity relations, analogous to the well known Maxwell relations of the classical thermodynamics of homogeneous fluid phases and expressing in fact the Schwarz theorem on the crossed second partial derivatives hold;

vi) reversible accessibility from one state (one point on the equilibrium surface in the extended Gibbs space) to another state holds;

vii) the second differential of  $S$  in terms of  $(\Delta, U)$  is negative definite;

viii) sets of independent variables can be interchanged and give equivalent formalisms by means of duality, involving various Legendre transforms.

In the reversible case, the constitutive equations are equations of state, relating for instance  $\Pi$  to  $(\Delta, U)$ , and which should be distinguished from the fundamental equation. When the set of derived equations of state is incomplete, there are usually many compatible ways of completing it, giving some freedom of expression for the missing equations of state and thus for the choice of the fundamental equation. The converse is not true: when the fundamental equation is given explicitly, the equations of state are fully defined and may be written in one way only. When a system evolves from one equilibrium state to another, the entire set of total variations of the different thermodynamic quantities experienced by the system at the end of the evolution is completely well defined if the equilibrium surface is assumed to be known. This is the case whether the evolution is reversible or not, provided that the initial and final states are both equilibrium states.

However, the equilibrium surface in the space  $(\Delta, U, S)$  is generally considered to be not able to provide information about phenomena which occur during an irreversible evolution, nor does it indicate which (perhaps new) quantities could be defined to describe these phenomena. In particular, if entropy is not to be defined in out-of-equilibrium situations in terms of the variables  $(\Delta, U)$ , there is no way to describe the process in the extended Gibbs space  $(\Delta, U, S)$ . This may make rather paradoxical the classical statement, already proposed by CLAUSIUS [15], that the entropy of an isolated system – i.e. with constant  $(\Delta, U)$  – tends towards a maximum which is obtained when the equilibrium is reached:

*“Energie der Welt ist constant. Entropie der Welt strebt einem Maximum zu!”*

Which entropy of the Universe Clausius had in view if it is not defined in an isolated system out of equilibrium? This was already questioned by Meixner, who stated that the use made by Clausius of the entropy concept for non-equilibrium situations was without justification [67].

We shall see below that this question can in fact be directly answered for a wide class of behaviour containing most classical models without or with internal variables. Before doing this, we consider the significance and limits of two frequently invoked corner stones of TIP: the local state principle and the fundamental Gibbs equation.

## 4. The basic concepts of the TIP formalism

### 4.1. The Local State Principle

In order to be able to make use of thermodynamics in non-equilibrium situations, the viewpoint adopted in the Thermodynamics of Irreversible Processes is that a medium in non-uniform conditions must be considered as the union of a number of subdomains in homogeneous condition, and the various possible exchanges or interactions between these must be examined, each subdomain being itself supposed to be in a homogeneous state which is governed by the laws of thermodynamics for equilibrium states, see [66, 73–75, 31, 21, 33, 53, 59] and others.

In case of non-uniform conditions, each of these subdomains is considered as the infinitesimal volume element. Each infinitesimal volume element is taken to be in a homogeneous state, so that, since the necessary condition for thermodynamic equilibrium is thus satisfied, it can be considered, at least heuristically, as a homogeneous element in thermodynamic equilibrium governed by the laws of classical thermodynamics and their associated concepts, magnitudes and equations. It is then examined how these elements react between themselves by considering the irreversible processes which appear within the system as resulting from (thermodynamic) mutual imbalance.

These irreversible phenomena generally take the form of flux – i.e. transfer of measurable quantities – passing through the surfaces surrounding the element of volume considered and tending to re-establish mutual equilibrium. They appear in connection with gradients expressing the difference of state between two adjacent elements: temperature gradient for thermal conduction, potential difference for electric conduction, concentration gradient for the diffusion of a gas, to cite the simplest cases. Then, the tools of Equilibrium Thermodynamics are used for these situations thanks to introducing a set of additional assumptions [74, 75, 21, 31, 53, 59] generally expressed as follows:

For a system which is not in equilibrium, it is assumed (or postulated or supposed) that:

1. locally the same quantities and thermodynamic functions (internal energy, entropy, temperature, free energy, ...) exist as those defined in the system in thermodynamic equilibrium;
2. these quantities are expressed in the same way as if the system were locally in equilibrium;
3. in particular, thermodynamic functions such as internal energy, entropy, free energy, ..., so defined, are independent of the rate of the transformation.

While its original authors named this set of statements the “local equilibrium hypothesis”, some authors have named it more recently the “Principle of the local state”, see [53], p. 211 of the 1979th issue, [27, 28]. The origin of this terminology is perhaps to be found in the memoir by PRIGOGINE [74], p.18 of the French translation [75] where it is mentioned that the “local” expression for the Second Principle has to be opposed to its “global” expression, used in classical Thermodynamics, due to the fact that the coupling between the irreversible processes is possible only when they intervene in the same region of the system. This statement of locality is then said to be the central postulate on which the whole book is based. But, what is visible from the localisation procedure used in Continuum Thermodynamics, this does not imply the assumptions 1, 2, 3 presented above.

#### 4.2. The fundamental Gibbs equation

Another basic ingredient of TIP is the use of the Gibbs equation, validity of which is postulated even for non-equilibrium conditions. In p. 103 of the memoir by PRIGOGINE [75], this is expressed in the following fashion (re-translated from the French):

*“The main concern of Irreversible Thermodynamics is to assess the entropy production from the Gibbs equation. ... (This) constitutes a new postulate, on which the whole TIP is based”.*

*“The physical significance of this basic formula is that, even in non-equilibrium*

situations, entropy depends on the same variables as those which characterise an equilibrium process."

"This is certainly not true anymore far from equilibrium".

For fluid systems with constant chemical composition under uniform pressure  $p$  and temperature  $T$ , the Gibbs equation is written as for the equilibrium case, Eq. (3.8) p. 19 of [75]:

$$(4.1) \quad dS = \frac{1}{T}dU + \frac{p}{T}dV,$$

which, taking as usual positive sign for tension stress, would have the following form for solids in three dimensions:

$$(4.2) \quad \dot{S} = \frac{1}{T}\dot{U} - \frac{\Pi}{T} : \dot{\Delta}.$$

Then, the consideration of two subsystems at different temperatures in diathermal contact leads to the conclusion that the rate of entropy production is a bilinear form in the heat flow rate and the temperature difference, a conclusion similar to the one obtained for  $\zeta_T$  in the Rational Thermodynamics approach when passing from the finite difference to a gradient. The same approach is used for systems with chemical reactions for which the Gibbs equation is postulated in the form:

$$(4.3) \quad dS = \frac{1}{T}dU + \frac{p}{T}dV - \sum_{\gamma} \frac{\mu_{\gamma}}{T}dN_{\gamma},$$

where  $N_{\gamma}$  is the mole number of constituent  $\gamma$  ( $\gamma = 1, \dots, m$ ) and  $\mu_{\gamma}$  its chemical potential defined, according to GIBBS [30] and DE DONDER [19] by:

$$(4.4) \quad \mu_{\gamma} = -T \frac{\partial S}{\partial N_{\gamma}} = \frac{\partial U}{\partial N_{\gamma}}.$$

On the other hand, the entropy production increment is introduced in terms of the chemical reaction increment  $d\xi_C$  and the chemical affinity  $A$  in the form [19]:

$$(4.5) \quad d_i S = \frac{1}{T} A d\xi_C > 0,$$

$d\xi_C$  being itself defined as the degree of growth of the reaction, linked to the stoichiometric coefficients  $\nu_{\gamma}$  by

$$(4.6) \quad dN_{\gamma} = \nu_{\gamma} d\xi_c.$$



Then it is stated that the affinity  $A$  is a function of the state expressed in terms of the chemical potentials  $\mu_\gamma$  by

$$(4.7) \quad A = - \sum_{\gamma} \nu_{\gamma} \mu_{\gamma} ,$$

with the property that it should be zero at equilibrium.

Of course, postulating a Gibbs equation in the form (4.3) for non-equilibrium situations implies that existence of non-equilibrium entropy has also been postulated since it is involved in the Gibbs equation, assumed to be still valid in such situations. Since no other definition has been given to entropy in non-equilibrium situations, this means that, in TIP, entropy is considered as a primitive quantity, just as in Rational Thermodynamics. Thus, the non-equilibrium entropy has the same postulated status in both approaches.

## 5. A criterion of validity for the local state principle: the adiabatic relaxation experiment

### 5.1. The adiabatic relaxation experiment in macroscopic variables

If the local state principle is considered to be valid, it should be checked first in the case for which macroscopic variables are used only. We consider here the simplest situation, in which no change in the chemical composition of the body is involved. Using the entropy representation, the equilibrium fundamental equation is Eq. (3.2). In the right-hand side of this equation, the set of arguments  $(\Delta, U)$  can be controlled experimentally, not only in the case of equilibrium but in every situation, including the irreversible ones, since:

- the deformation  $\Delta$  can be imposed by a mechanical system;
- the heat flow inwards or outwards can also be controlled (by more or less insulating wall and heating devices), which determines  $U$  when  $\Delta$  is fixed.

In addition, if the set  $(\Delta, U)$  is fixed at a certain time (which implies adiabaticity from this time onwards), the system will tend spontaneously towards internal equilibrium if it has not already reached this state. This is an adiabatic relaxation experiment.

Since, for fixed chemical composition,  $U$  and  $\Delta$  can be controlled at will, it can be said that the internal energy and the deformation are meaningful thermodynamical quantities even out of equilibrium.

Moreover, during the relaxation experiment, they have the same meaning and numerical values out of equilibrium as they have once the relaxed thermodynamic equilibrium is reached at the end of the adiabatic relaxation process. Entropy, however, is different.

## 5.2. The growth of entropy in delayed adiabatic relaxation

Let us consider again, in the extended Gibbs space  $(\Delta, U, S)$ , the extended hypersurface  $\Sigma$  of equilibrium states, or fundamental surface, discussed in Sec. 3. If, during a change from one equilibrium state to another, the value of the set of governing independent variables  $(\Delta, U)$  changes from  $(\Delta_1, U_1)$  to  $(\Delta_2, U_2)$ ,  $S$  varies between two equilibrium values  $S_1$  and  $S_2$  which depend only on  $(\Delta_1, U_1)$  and  $(\Delta_2, U_2)$ , and not on the path taken in the  $(\Delta, U)$ -space to travel from  $(U_1, \Delta_1)$  to  $(U_2, \Delta_2)$ . When the path is reversible,  $S$  is defined all along the path and its representative point in the  $(\Delta, U, S)$  space has its trajectory necessarily contained in the equilibrium surface  $\Sigma$  during the whole process. In the traditional approach, this requires in addition the path to be covered at an infinitely slow speed.

However, the path in the  $(\Delta, U)$ -space may also correspond to an irreversible process, during which the representative point in the  $(\Delta, U, S)$ -space may – at least as a provisional working assumption – leave from the equilibrium surface  $\Sigma$  if we assume the entropy being still defined during this process, for instance through a functional of the history of  $(\Delta, U)$  [16, 18]. Then, it is clear that the properties defined by the equations in Subsec. 3.2 above, being geometrical properties of the  $\Sigma$  surface, will no longer hold for such functionals, which jeopardizes the validity of the principle of local state as stated in Subsec. 4.1 above.

Let us consider now that some process takes the point  $M$  representing entropy in the  $(\Delta, U, S)$ -space, from an initial equilibrium state  $(\Delta_0, U_0, S_0)$  on the equilibrium surface to a point  $(\Delta_1, U_1, S_1)$  outside this surface. Then, let us perform an adiabatic relaxation from the point  $(\Delta_1, U_1, S_1)$ . From this point onwards, the system is thermodynamically insulated. Its entropy can only increase as the system tends towards thermodynamic equilibrium defined by the point with coordinates  $(\Delta_1, U_1, S_1^{eq})$  on the equilibrium surface  $\Sigma$ . Final thermodynamic equilibrium means that all the variables that can be defined on the system, including stress and temperature, do not change anymore, which is not the case, by definition, in retarded relaxation. Since entropy production is the only possible change of entropy during adiabatic relaxation, and since it should be strictly positive in the retarded relaxation, the point  $M$  is really outside  $\Sigma$  if the relaxation is retarded. Moreover, all points outside the surface  $\Sigma$  which are accessible from any initial point  $(\Delta_0, U_0, S_0)$  are necessarily on one and the same side relatively to it.

A point like  $(\Delta_1, U_1, S_1)$ , being situated outside the equilibrium surface, is inaccessible by a reversible path (which might be used as a return path if it would exist), contrarily to the requirement stated by Clausius for defining entropy in non-equilibrium situations. This is a version of the BRIDGMAN paradox [7] underlined several times by KESTIN [55] for the case of plasticity.

### 5.3. A necessary condition of validity for the local state principle in macroscopic variables

Conversely, a necessary condition for the principle of local state, as enunciated in Subsec. 4.1, to be valid in macroscopic variables is that  $S = S_1^{eq} = S^{eq}(\Delta_1, U_1)$  at all times during the adiabatic relaxation, i.e. that the adiabatic relaxation is isentropic. Since an adiabatic relaxation can be introduced at any time and at any point of a non-equilibrium process, a necessary and sufficient condition for this relaxation to be isentropic is that the dissipative evolution occurs within the equilibrium surface  $\Sigma$  in the extended Gibbs space  $\Delta, U, S$ . However, since it has just been admitted that this cannot happen if the adiabatic relaxation is retarded, an instantaneous relaxation is a *necessary* condition for having an isentropic adiabatic relaxation. It must be noted that this last condition is *not*, *a priori*, sufficient to ensure that the instantaneous adiabatic relaxation is isentropic: it is quite possible at first sight to envisage an instantaneous adiabatic relaxation showing an instantaneous jump in entropy from  $(\Delta_1, U_1, S_1)$  out of  $\Sigma$  to  $(\Delta_1, U_1, S_1^{eq})$  on  $\Sigma$ . This important point will be especially examined in Subsec. 6.1. To summarize, adiabatic relaxation provides three conditions, each of which is sufficient to invalidate the local state principle:

*A material does not obey the principle of local state in macroscopic variables if at least one of the following conditions is true:*

- *the adiabatic relaxation is not isentropic;*
- *some trajectories representing the process in the extended Gibbs space may take place outside the equilibrium surface;*
- *the adiabatic relaxation is not instantaneous.*

### 5.4. Non-equilibrium Gibbs equation in macroscopic variables and the two Principles of Thermodynamics

For irreversible processes, the Clausius-Duhem inequality is strict and has, from Eq. (2.27) of Sec. 2, the form:

$$(5.1) \quad \frac{1}{T} \dot{U} - \frac{\Pi}{T} : \dot{\Delta} < \dot{S},$$

for all irreversible processes, i.e for all  $\dot{U}$  and  $\dot{\Delta}$ , independently of the fact that it would take place on the equilibrium surface or not. For reversible processes, the inequality becomes an equality which reads:

$$(5.2) \quad \frac{1}{T} \dot{U} - \frac{\Pi}{T} : \dot{\Delta} = \dot{S}.$$

From Subsec. 3.2, this coincides with the Gibbs equation when written in the entropic representation in macroscopic variables.

The two relationships (5.1) and (5.2) are incompatible. Thus, when using the strain and internal energy only as macroscopic independent variables, a Gibbs equation written in the same form as in equilibrium cannot hold for dissipative solids, using the real non-equilibrium values of stress and temperature involved in the irreversible process. Hence, TIP cannot be based on the whole set of statements recalled in Subsecs. 4.1 and 4.2 above when these variables are used. At least one of these statements have to be relaxed or modified in order to have a consistent theory.

## 6. A status for the non-equilibrium entropy

### 6.1. Instantaneous entropy recovery and 2nd Principle for materials of the Markovian type

From a purely mechanical point of view, a material which can relax instantaneously at constant temperature is one for which the stress at the time  $t$  can only be a function of the present values at the same time  $t$  of the governing variables and their rates, and perhaps – as in the RIVLIN-ERICKSEN behaviour models [77] – of its right-time derivatives of higher order up to some finite one:

$$(6.1) \quad \Pi = \underset{\sim}{\Pi} (\Delta; \dot{\Delta}; \ddot{\Delta}; \dots; \Delta^{(n)}; T).$$

In this subsection, we consider that the time derivatives of the first order only are involved in the dependence of  $\Pi$  and  $T$  upon the governing variables. Taking the latter as  $(\Delta, U)$ , we consider the class of materials for which the stress tensor and the temperature are of the form, at every instant  $t$ :

$$(6.2) \quad \Pi = \underset{\sim}{\Pi} (\Delta, U; \dot{\Delta}, \dot{U}),$$

$$(6.3) \quad T = \underset{\sim}{T} (\Delta, U; \dot{\Delta}, \dot{U}).$$

To avoid any possible confusion, attention is drawn to the fact that such constitutive equations are not proposed here as substitutes for other modes of representation of the behaviour of real materials, as the ones that we shall consider later on in Subsec. 6.2 and Sec. 7.

Materials with stress expressed by Eq. (6.1) are called materials of the differential type [85, 18]. Materials with behaviour defined by Eqs. (6.2) and (6.3) are materials of the differential type in some extended sense on the one hand, since the dependence upon the time derivatives of  $U$  is also involved, and more restricted on the other hand since the rate dependence is limited to the order one. All along this paper, we refer more briefly to the class of behaviour defined by Eqs. (6.2) and (6.3) as *Markovian behaviour*, an expression borrowed

from CALLEN [11] (we used this terminology without the order one restriction in [37, 38, 39, 40]).

For example, classical models of Markovian behaviour are the viscous and Kelvin models of linear viscoelasticity, the rigid-plastic, Bingham and Norton-Hoff models of viscoplasticity and the Eyring model of chemical kinetics (see for instance [47, 48]). In particular, the rigid-plastic behaviour is indeed Markovian since the stress is a homogeneous function of order zero in terms of the strain rate.

Markovian behaviour exhibits instantaneous relaxation: at some instant of  $t$  an irreversible evolution corresponding to non-zero values of the time derivatives of  $\Delta$  and  $U$ ,  $\Pi$  and  $T$  differ from their equilibrium value at this time. If  $\Delta$  and  $U$  are then kept fixed at their value already reached at time  $t$  – so that their first and higher right derivatives are set to zero (adiabatic relaxation experiment) – there is a sudden change from the values  $\Pi(t^-), T(t^-)$  of  $\Pi$  and  $T$  to their values  $\Pi(t^+), T(t^+)$ , with:

$$(6.4) \quad \Pi(t^+) = \underset{\sim}{\Pi}(\Delta, U, 0, 0) = \underset{\sim}{\Pi}^{eq}(\Delta, U),$$

$$(6.5) \quad T(t^+) = \underset{\sim}{T}(\Delta, U, 0, 0) = \underset{\sim}{T}^{eq}(\Delta, U).$$

Since the equilibrium values of  $\Pi$  and  $T$  are reached instantaneously, the same must hold for the entropy, assumed to exist in non-equilibrium, and which, at the worse, must be thus of the form:

$$(6.6) \quad S = \underset{\sim}{S}(\Delta, U; \dot{\Delta}, \dot{U}; \ddot{\Delta}, \ddot{U}; \dots; \Delta^{(p)}, U^{(q)}),$$

with the orders  $p$  and  $q$  of the highest-order derivatives being finite and with the equilibrium value given by:

$$(6.7) \quad S(t^+) = \underset{\sim}{S}(\Delta, U; 0, 0; 0, 0; \dots; 0, 0) = S^{eq}(\Delta, U).$$

We make use now of a classical argument due to COLEMAN [16] and previously to DEFAY [20, 76]. From Eq. (6.6), the time derivative of the entropy has the form:

$$(6.8) \quad \dot{S} = \frac{\partial \underset{\sim}{S}}{\partial \Delta} : \dot{\Delta} + \frac{\partial \underset{\sim}{S}}{\partial \dot{\Delta}} : \ddot{\Delta} + \dots + \frac{\partial \underset{\sim}{S}}{\partial \Delta^{(p)}} : \Delta^{(p+1)} \\ + \frac{\partial \underset{\sim}{S}}{\partial U} \dot{U} + \frac{\partial \underset{\sim}{S}}{\partial \dot{U}} \ddot{U} + \dots + \frac{\partial \underset{\sim}{S}}{\partial U^{(q)}} U^{(q+1)}.$$

Substitution of Eq. (6.8) in the Clausius-Duhem Inequality (2.27) rewritten in its strict form gives:

$$(6.9) \quad \left( \frac{\partial \tilde{S}}{\partial \Delta} + \frac{\Pi}{T} \right) : \dot{\Delta} + \frac{\partial \tilde{S}}{\partial \dot{\Delta}} : \ddot{\Delta} + \dots + \frac{\partial \tilde{S}}{\partial \Delta^{(p)}} : \Delta^{(p+1)} \\ + \left( \frac{\partial \tilde{S}}{\partial U} - \frac{1}{T} \right) \dot{U} + \frac{\partial \tilde{S}}{\partial \dot{U}} \ddot{U} + \dots + \frac{\partial \tilde{S}}{\partial U^{(q)}} U^{(q+1)} > 0.$$

Since, by hypothesis, the entropy  $S$  is independent of  $\Delta^{(p+1)}$  and  $U^{(q+1)}$ , which are independent right-derivatives, the first member of Inequality (6.9) is a linear form in  $\Delta^{(p+1)}$  and  $U^{(q+1)}$  which cannot remain non-negative for any values of these quantities unless their coefficients are zero. Thus the entropy  $S$  is independent of  $\Delta^{(p)}$  and  $U^{(q)}$ . Since, from Eqs. (6.2) and (6.3),  $\Pi$  and  $T$  are assumed to be independent of  $\Delta^{(p)}$  and  $U^{(q)}$  for all  $p$  and  $q$  bigger than 1, the argument can be repeated for these latter variables. Working backwards to the terms in  $\ddot{\Delta}$  and  $\ddot{U}$ , it is seen that  $S$  does not depend on any of the present derivatives of  $\Delta$  and  $U$ . The expression (6.6) for the entropy out of equilibrium is thus reduced to:

$$(6.10) \quad S = \tilde{S}(\Delta, U).$$

This means that, for Markovian behaviour, the entropy is dependent only on the present values of  $\Delta$  and  $U$ , whatever their previous history may be, and whatever values their time derivatives may take. However, when the adiabatic relaxation is over, the entropy reaches its equilibrium value  $S = \tilde{S}^{eq}(\Delta, U)$ , so that, for consistency, the entropy out of equilibrium should be identified with its equilibrium value, for all values the rates  $\dot{\Delta}, \dot{U}$  and of the governing independent variables may take in the process and how far from the equilibrium one may be:

$$(6.11) \quad S = \tilde{S}(\Delta, U) \equiv \tilde{S}^{eq}(\Delta, U).$$

Hence, there can be no instantaneous jump in entropy for this behaviour, contrary to the provisional assumption made in Subsec. 5.3. All the processes related to a material with stress and temperature in the form of Eqs. (6.2), (6.3) must of necessarily take place, in the extended Gibbs space  $\Delta, U, S$ , on the equilibrium surface  $\Sigma$ . This happens even if the path is runned at a *finite rate* of the governing independent variables  $\Delta$  and  $U$ . Conversely, the problem of defining entropy out of equilibrium can now be solved in a precise way for Markovian behaviour:

*For materials with Markovian behaviour, a non-equilibrium entropy  $S$  **may always** be defined. It **must** be taken as the same function of the strain tensor and internal energy as the equilibrium entropy  $S^{eq}$ .*

**6.2. General case of the instantaneous adiabatic relaxation followed by delayed relaxation**

When the stress and temperature depend not only on the present values of  $\Delta$  and  $U$  and their right time first derivatives, but also on their past history  $H^-(\Delta, U)$ , being of the form:

$$(6.12) \quad \Pi = \underset{\approx}{\Pi} \left[ \Delta, U; \dot{\Delta}, \dot{U}; H^-(\Delta, U) \right],$$

$$(6.13) \quad T = \underset{\approx}{T} \left[ \Delta, U; \dot{\Delta}, \dot{U}; H^-(\Delta, U) \right],$$

the assumed defined non-equilibrium entropy  $S$  should be *a priori* – not only a function of the present values of  $\Delta$  and  $U$  and their time derivatives, but also a history functional of  $\Delta$  and  $U$ . Therefore, in this case  $S$  should *a priori* be written as:

$$(6.14) \quad S = \underset{\approx}{S} \left[ \Delta, U; \dot{\Delta}, \dot{U}; \ddot{\Delta}, \ddot{U}; \dots; \Delta^{(p)}; \dots; U^{(q)} H^-(\Delta, U) \right].$$

Taking the time derivative gives:

$$(6.15) \quad \dot{S} = \frac{\partial \underset{\approx}{S}}{\partial \Delta} : \dot{\Delta} + \frac{\partial \underset{\approx}{S}}{\partial \dot{\Delta}} : \ddot{\Delta} + \dots + \frac{\partial \underset{\approx}{S}}{\partial \Delta^{(p)}} : \Delta^{(p+1)} \\ + \frac{\partial \underset{\approx}{S}}{\partial U} \dot{U} + \frac{\partial \underset{\approx}{S}}{\partial \dot{U}} \ddot{U} + \dots + \frac{\partial \underset{\approx}{S}}{\partial U^{(q)}} U^{(q+1)} + \underset{\approx}{\dot{S}}_{\Delta U},$$

where  $\underset{\approx}{\dot{S}}_{\Delta U}$  is the continuation functional expressing the rate of variation of  $S$  from the moment when  $\Delta$  and  $U$  are kept constant (i.e. during an adiabatic relaxation). Thus, by the same line of reasoning as in Subsec. 6.1, cannot depend on the time derivatives of  $\Delta$  and  $U$  and must take the form:

$$(6.16) \quad S = \underset{\approx}{S} \left[ \Delta, U; H^-(\Delta, U) \right],$$

meaning that, if it exists, it should reduce to a function of the present values of  $\Delta$  and  $U$  and a functional of their previous history. Remark that, as explained for instance in [51], the partial derivatives involved in Eq. (6.15) are not the gradient involved in the Gateaux differential of the functional  $\underset{\approx}{S}$ , but only the instantaneous partial derivatives, given by the value of this gradient at time  $t$ .

### 6.3. Consequences for the potential properties

From Eq. (6.16), the fundamental inequality reduces to

$$(6.17) \quad \left( \frac{\partial S}{\partial \Delta} \approx + \frac{\Pi}{T} \right) : \dot{\Delta} + \left( \frac{\partial S}{\partial U} \approx - \frac{1}{T} \right) \dot{U} + \dot{S}_{\Delta U} \approx > 0,$$

where  $\Pi$  and  $T$  are history functionals of  $\Delta$  and  $U$ , and may or may not also depend on the present values of the rates  $\dot{\Delta}$  and  $\dot{U}$ .

If  $\Pi$  and  $T$  do not depend upon these rates, being simply of the form:

$$(6.18) \quad \Pi = \Pi \approx [\Delta, U; H^-(\Delta, U)],$$

$$(6.19) \quad T = T \approx [\Delta, U; H^-(\Delta, U)],$$

(as is the case when instantaneous elasticity exists), then by re-applying the same argument, one obtains:

$$(6.20) \quad \frac{\Pi}{T} = - \frac{\partial S}{\partial \Delta} \approx ; \quad \frac{1}{T} = \frac{\partial S}{\partial U} \approx ; \quad S \neq S^{eq} ; \quad \dot{S}_{\Delta U} \approx > 0,$$

where the first two equations correspond to the main result of COLEMAN in [16], see also [83]. For this reason, the class of behaviour defined by constitutive equations of the form (6.18), (6.19) has been named *Colemanian* [37–39].

However, if  $\Pi$  depends upon  $\dot{\Delta}$  and  $T$  upon  $\dot{U}$ , then, taking into account the fact that  $\frac{\partial S}{\partial \Delta} \approx$  and  $\frac{\partial S}{\partial U} \approx$  cannot depend on these derivatives since  $S$  itself does not, one has:

$$(6.21) \quad \frac{\Pi}{T} \neq - \frac{\partial S}{\partial \Delta} \approx = \frac{\Pi^{eq}}{T^{eq}} ; \quad \frac{1}{T} \neq \frac{\partial S}{\partial U} \approx = \frac{1}{T^{eq}} ; \quad S \neq S^{eq} ; \quad \dot{S}_{\Delta U} \approx > 0.$$

That the potential properties expressed by Eqs. (6.20) are not of general validity, but correspond to a specific class of behaviour, was shown by MANDEL [61–64], and independently by HUET [37–39].

By contrast, for a Markovian behaviour, the relations (6.21) become:

$$(6.22) \quad \frac{\Pi}{T} \neq - \frac{\partial S}{\partial \Delta} \approx = \frac{\Pi^{eq}}{T^{eq}} ; \quad \frac{1}{T} \neq \frac{\partial S}{\partial U} \approx = \frac{1}{T^{eq}} ; \quad S = S^{eq} ; \quad \dot{S}_{\Delta U} \approx = 0$$

showing that entropy is not a potential for the non-equilibrium stress and temperature in this case despite the fact that  $S$  and  $S^{eq}$  are equal. However, the first



two equations of (6.22) follow trivially from the third since, from Eq. (6.11), one has:

$$(6.23) \quad \dot{S} = \frac{\partial S}{\partial \Delta} \dot{\Delta} + \frac{\partial S}{\partial U} \dot{U} = -\frac{\Pi^{eq}}{T^{eq}} \dot{\Delta} + \frac{1}{T^{eq}} \dot{U} = \dot{S}^{eq},$$

so that they neither require nor express any new principle. Remark that the last Eq. (6.23) is the equilibrium Gibbs equation, always valid at equilibrium.

Consequently, from the results obtained in Subsecs. 6.1 and 6.2, *there is no non-equilibrium behaviour* each of which satisfies the *complete set* of rules given in Subsec. 4.1 to define the local state principle. It is possible to find various special classes of behaviour which each, in out of equilibrium conditions, satisfy some relation which was originally established within equilibrium, but these cases are mutually exclusive: for example, a class which satisfies (6.20) does not satisfy (6.22) and *vice versa*.

There are also certain types of dissipative behaviour, such as those defined by (6.17), which satisfy none of the characteristic relations of thermodynamic equilibrium in macroscopic variables: entropy is not a function of the present value of  $\Delta$  and  $U$  (but depends also on their whole history), and the entropy is not a potential for the stress and temperature. To express the stress and the temperature, some additional terms have to be added to the entropy gradient in the  $(\Delta, U)$  space, similar to what is done for instance in [51] using the free energy in the  $(\Delta, T)$  space. Of course, the use of the latter presupposes the existence of the non-equilibrium entropy which is in discussion here.

## 7. Reducing hereditary behaviour to Markovian ones

### 7.1. The internal variables approach

Of course, the class of Markovian behaviour is not large enough to encompass all the classes of behaviour that can be observed in real materials. When macroscopic variables only are considered in the constitutive equations for materials with delayed response, history functionals are needed in order to express the stress in finite terms. However, except in the case of linear viscoelasticity without aging, the practical identification of these functionals rises many practical problems, and leads most often to unstable results. On the other hand, in order to extend the equilibrium thermodynamics formalism to the irreversible behaviour of solids, a powerful method has been progressively elaborated since about fifty years through the use of the so-called *internal variables* or *hidden variables* [66–68, 5, 79, 80, 53–55, 28, 63, 86, 87, 69, 70]. Initially, this method was based on the Thermodynamics of Irreversible Processes. In the entropy representation we are using here, it involves, in addition to the internal energy  $U$  and

the strain tensor  $\Delta$ , a set  $a = \{a_1, a_2, \dots, a_k, \dots, a_N\}$  of internal variables, that do not appear in the universal balance equations. Sometimes they are introduced through an appropriate analogy, the most well known being rheological models based on mechanical and electrical systems [79, 72]. The introduction of these internal variables is generally associated with a set of constitutive assumptions. For instance it is assumed that the stress tensor  $\Pi$  at time  $t$  is an ordinary function of the present values of  $(\Delta, U, a)$  at the same instant  $t$ , but not of the rates. Furtherly it is supposed that the entropy  $S$  exists in non-equilibrium situations and that the function relating  $S$  to  $(\Delta, U, a)$  is again the same as for equilibrium. In some cases, it is assumed that a Gibbs equation is still valid with this extended set of variables. From these assumptions, it is generally obtained that the entropy is again a potential for the stress divided by the temperature (this result coming from the most often assumed independence of  $\Pi$  on  $\dot{\Delta}$ , and thus being limited to the case with instantaneous elasticity as seen in Sec. 6.2 above). Finally, it is stated that the set of equations thus obtained must be complemented by a set of – linear or non-linear – rate equations on which, again, no other information is provided.

## 7.2. A criterion for the internal variables

From the discussion of the preceding sections, it follows that in the internal variables method, the entropy may be – without *a priori* assumption – given a meaning out of equilibrium by appropriately choosing the set of internal variables. To yield realistic results, the latter have to be obtained by identifying the involved dissipative mechanisms and relating them in a way satisfying the characteristics of the experimental response and/or of the observed dissipative mechanisms identified in the microstructure of the material. Together with non-dissipative ones, these dissipative mechanisms can be considered as forming the elements of a system representing its macroscopic behaviour. Let us assume that they can be chosen in such a way that each of them is Markovian when disconnected from the others and directly stimulated. Then, from the results obtained in the above sections, entropy is well defined for each dissipative mechanism *even when they are under irreversible evolution at finite rate*. Moreover, it depends neither on the rates nor on the history of the involved variables, but only on their present values. Thus, using the additivity property of entropy, it can be stated [37, 40, 44] that the overall entropy density of the material is well defined and is a simple function of the present values of the governing set of variables  $(\Delta, U, a)$  involving the macroscopic variables  $(\Delta, U)$  and the set  $a$  of the internal variables:

$$(7.1) \quad S = \underset{\sim}{S}(\Delta, U, a).$$

This means that all the transformations – including those performed at a

finite rate – take place in the equilibrium surface of the space  $(\Delta, U, a, S)$  while the continuation functional of  $S$  corresponding here to the one considered in Sec. 6.2 vanishes:

$$(7.2) \quad \dot{S}_{\Delta U a} \equiv 0.$$

Therefore, the preceding results supply a rule to ensure that the decomposition of the behaviour into internal mechanisms has been taken far enough to make possible the definition of an out of equilibrium entropy. For this, it is necessary and sufficient that the identified mechanisms have either reversible or Markovian behaviour when directly stimulated.

It can be verified from the literature that, even in the non-linear case (including plasticity, viscoplasticity and chemical kinetics), the dissipative mechanisms that are used in practice when applying this method are Markovian when directly stimulated. Although not explicitly formulated in general, this may explain why the internal variables approach has been found so successful.

In the adiabatic relaxation performed on the macroscopic variables as defined in Sec. 5.1, the internal variables only are allowed to change. Thus, in the macroscopic Gibbs space  $(\Delta, U, S)$ , each combination of fixed values taken by the internal variables define a hypersurface  $\Sigma'(a)$ . All these surfaces are situated on one and the same side of the equilibrium surface  $\Sigma$ .

## 8. Comparison with other approaches

### 8.1. The Kestin method of the Accompanying Equilibrium State

In view of providing a consistent thermodynamic theory – exempted of a postulated non-equilibrium entropy – for the study of irreversible systems out of equilibrium, a variant of TIP has been constructed by KESTIN [53–55] in the framework of the internal variables approach. In this theory, the Gibbs equation is still considered fundamental and taken as a starting point, but the idea that entropy and temperature are really defined out of equilibrium is rejected. The Principle of *local equilibrium*, or of *local state* is made more precise than in classical TIP by specifying that the considered equilibrium is some appropriately defined accompanying equilibrium state (AES) corresponding to *frozen values* of the internal variables. Then, the accompanying equilibrium state is used in order to define the *accompanying entropy* and the *accompanying temperature* of the system when the latter is not in thermodynamic equilibrium, i.e. when the internal variables at least are evolving at a finite rate. This is performed by assuming that entropy and temperature are taken as the ones defined on the AES. Corresponding reversible processes are defined. They are considered as occurring in a virtual *Gibbsian state space*, and not on the so-called “physical space” [55]. For Kestin, the Gibbsian state space is the space with dimensions

$(\varepsilon, U, a)$ , which in Lagrange coordinates needed for finite strains becomes here  $(\Delta, U, a)$ . It is then stated that the non-equilibrium states are defined in a wider space admitting the Gibbsian space as a subspace forming a base manifold of the former. It is emphasised that the *dependent* physical variables *differ* from the ones associated to the AES. It is also emphasised that the entropy is calculated by integration on the Gibbsian state space and not on the physical space (for the sake of clarity, it should be noted that the name “Gibbsian state space” of Kestin differs from the “extended Gibbs space” that we used in Sec. 3.2 above, since the latter includes the entropy while Kestin’s Gibbsian state space does not).

In addition to the above assumptions, the Gibbs equation is again written, *but only for the values of the dependent variables involved in the accompanying equilibrium state*. Hence, this avoids the problem of defining the entropy of the body in non-equilibrium situation. This equilibrium Gibbs equation is then used in order to obtain an explicit expression for the entropy production by elimination of the internal energy rate between the Gibbs equation of the AES and the energy balance equation. Here again, it is stated that the set of equations thus obtained must be complemented by a set of – linear or non-linear – rate equations, on which no other information is provided.

It is clear from the above description that Kestin’s AES is the one obtained at the end of an adiabatic relaxation experiment performed, not only on the macroscopic variables, but also on the dissipative mechanisms corresponding to the internal variables supposed to be directly stimulated (which in fact modifies the system itself since then the subsystems become disconnected and the internal distribution of stresses is changed: for example, it is impossible to maintain the same stress in the two components of a Maxwell model if the partial strains in each component, taken as the internal variables, are frozen from some later instant). Thus, the Gibbs equation used is again an equilibrium one, and not an out of equilibrium one. Moreover, if Kestin’s relaxation of internal variables would involve production of entropy, the calculated entropy production would not be the one really involved in the non-equilibrium process, but a greater one.

But, as seen in the above Subsection, when all the internal dissipative mechanisms are supposed to be Markovian, a non-equilibrium entropy can really be defined for the whole system when the independent variables, including the internal ones, are experiencing evolutions at finite rates. This can be done without having to state that the internal variables are frozen. Moreover, the dissipation can then be directly evaluated without having to invoke the Gibbs equation, neither the detour of an Accompanying Equilibrium State: it is simply the sum of the dissipations of all the dissipative mechanisms.

## 8.2. The Valanis-Caratheodory method based on integrability of the first law

Another approach addressing the existence of entropy in the internal variables formalism has been used by VALANIS [86, 87] who extends to this case the non-accessibility theorem obtained by CARATHEODORY [12] for reversible processes. Caratheodory's theorem can be expressed by the fact that, when the supply of heat to a reversible system is prevented (adiabatic process), the previously chosen *independent* variables  $(\Delta, U)$  of the reversible case cannot remain independent. This defines an hypersurface in the  $(\Delta, U)$ -space and yields the integrability of the first law for reversible behaviour in adiabatic conditions (as shown in [86], Appendix II to Sec. 3). Therefore, adiabatic access to points outside this hypersurface of the  $(\Delta, U)$ -space are forbidden. Moreover, the converse is also true.

In the extension to the non-reversible case made by Valanis, adiabatic processes with frozen internal variables are again considered, as in the work of Kestin mentioned above. Valanis considers the space  $(U, \Delta, a)$  of the governing independent variables, which he calls the *thermodynamic state space*, which thus coincides in fact with the Gibbsian state space of Kestin, but not with our extended Gibbs space  $(U, \Delta, a, S)$ . As a basic axiom of the theory and a – somewhat restrictive – definition of irreversible behaviour, it is postulated that the stress tensor is a state function of  $(U, \Delta, a)$  (and thus is independent of the rates). The integrability of the first law in this space is then proven when the internal variables are kept frozen, which gives both a definition of entropy and temperature as in the Caratheodory treatment of the reversible case. Potential properties, due again to the basic axiom of the theory postulating independence of  $\Pi$  from the rates of  $(\Delta, U)$ , are also obtained. The Carnot-Clausius Principle on the positive production of entropy is replaced by – and in fact deduced from – a postulate on the behaviour of the free energy in an isothermal relaxation experiment.

The problem of defining an entropy remaining meaningful during a real process is addressed, in the approach by Valanis, through the concept of *partial integrability* of the first law which, in fact, reduces again to keeping frozen the internal variables, the system becoming reversible in this situation (Sec. 4 of [87]).

By choosing explicitly the internal variables as relating to dissipative mechanisms that are Markovian, it seems possible to relax the restriction of frozen internal variables, making the entropy defined by Valanis also having a meaning when the internal variables are changing at finite rates, i.e. in every real process. Moreover, it suggests it might be possible to extend the basic axiom and mathematical derivations of the Caratheodory-Valanis theory to the case where the stress depends explicitly on the strain and internal energy rates in addition to the dependence upon the present values of  $(U, \Delta, a)$ , i.e. to materials devoid of instantaneous elasticity, providing thus, in the same framework, a direct definition of entropy for more general cases. But this is still an open question needing further research.

## 9. Conclusion

From the derivations performed in this paper, it can be stated that, depending on the form taken by the response to the adiabatic relaxation experiment, materials behaviour with delayed response falls into four mutually exclusive categories when using macroscopic variables only:

1. *Reversible behaviour which exhibits no adiabatic relaxation.*
2. *Markovian dissipative behaviour, for which the adiabatic relaxation is instantaneous.*
3. *Colemanian dissipative behaviour in which there is a delayed relaxation, either of the stress, or of temperature, or of both, but no instantaneous one.*
4. *General hereditary dissipative behaviour, where there is an instantaneous relaxation, either of the stress, or of temperature, or of both, followed by a delayed one.*

Reversible behaviour is governed by the classical thermodynamics of equilibrium and all its classical relationships. For some types of dissipative behaviour, it is possible to apply some of the equilibrium relations to some cases out of equilibrium, but then there are always other relations which cannot be directly applied.

For Markovian behaviour, a fundamental result is that *not only the reversible evolutions of a Markovian system take place on the equilibrium surface in the extended Gibbs space  $(\Delta, U, S)$ , but also their irreversible ones, whatever the magnitude of the rates – and thus whatever the distance reached from equilibrium – might be.*

In the non-Markovian case, the power of the method of internal variables with their mechanical or electrical analogs – appears to be connected with the fact that it is often possible to obtain a reduction to Markovian behaviour by introducing a sufficient number of suitable supplementary – “internal” or “hidden” – variables. *But the behaviour of a suitable internal variable must itself be reversible or Markovian when directly stimulated.*

From this, it appears possible to relax some restrictive assumptions and to enlarge the domain of validity of some of the theories using the internal variables approach while addressing also the problem of the existence of entropy in dissipative processes.

It has to be remarked that the above fundamental result concerning the dependence of entropy upon the macroscopic variables  $\Delta$  and  $U$  only, as found for Markovian behaviour, means that instantaneous adiabatic relaxation – which corresponds to a change of mechanical state and is thus a real process – must be considered a reversible one. Effectively, since there is no change in the entropy and no supply of entropy from the exterior, there is no production of entropy

in the instantaneous adiabatic relaxation for Markovian behaviour. Thus the question arises if this can be given a direct physical meaning.

In fact, the above remark is consistent with the observation that every adiabatic *unloading* of a perfectly rigid body can itself be considered a reversible process, devoid of any dissipation since it involves neither expense nor release of work, and thus nothing to be converted into heat. Indeed, no deformation is associated with the instantaneous finite unloading of a body with Markovian behaviour, for instance of the viscous, Kelvin, Bingham or rigid-plastic types. Thus, every Markovian body appears as perfectly rigid under any finite instantaneous unloading, making non-dissipative the instantaneous relaxation process. Since all points of the equilibrium surface are connected by reversible paths, this provides the reversible return process required by Clausius in its original definition of entropy. This physically justifies the choice made in Secs. 6 and 7 of this paper for the definition of the non-equilibrium entropy for Markovian behaviour and answers the question raised at the end of Sec. 3.

Other consequences of the above discussion and other aspects of the thermodynamic theory of real materials dealt with by the author may be found in [40–52].

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## References

1. R. L. BAGLEY, P. J. TORVIK, *On the fractional calculus of viscoelastic behaviour*, *J. Rheology*, **30**, 133–155, 1986.
2. Z. P. BAZANT, *Theory of creep and shrinkage of concrete, a precis of recent developments*, [In:] S. NEMAT-NASSER [Ed.], *Mechanics Today*, **2**, Pergamon, 1975.
3. Z. P. BAZANT [Ed.], *Mathematical modeling of creep and shrinkage of concrete*, Wiley, 1988.
4. Z. P. BAZANT, F. KAPLAN [Eds.], *Concrete at high temperature: material properties and mathematical models*, Longman, 1996.
5. M. A. BIOT, *Theory of stress-strain relation in anisotropic viscoelasticity and relaxation phenomena*, *J. Appl. Phys.*, **25**, 11, 1385–1391, 1954.
6. L. BOLTZMANN, *Zur Theorie der elastischen Nachwirkungen*, *Sitzungsber. Kaiserlich Akad. Wiss., Wien, Math. Naturwiss. Klasse.* **70** (II), 275, 1874.
7. P. W. BRIDGMAN, *The thermodynamics of plastic deformation and generalized entropy*, *Rev. Modern Physics*, **22**, 1, 56–63, 1950.
8. L. BRUN, *Thermodynamique et viscoélasticité*, *Cahiers du Groupe Français de Rhéologie*, **I**, 4, SEDOCAR, Paris, 191–202, 1967.

9. L. BRUN, *Méthodes énergétiques dans les systèmes évolutifs linéaires*, J. Mécanique, **8**, 125–166, 1969.
10. G. L. BUFFON, LE CLERC, Comte de, *Expériences sur la force du bois*, L'Académie Royale des Sciences, Histoire et mémoires, Paris, 453–467, 1740.
11. H. R. CALLEN, *Thermodynamics*, John Wiley and Sons, 6th Ed., New-York 1966.
12. CARATHEODORY, *Untersuchungen über die Grundlagen der Thermodynamik*, Math. Annalen, **67**, 355–, 1909.
13. S. CARNOT, *Réflexions sur la puissance motrice du feu et sur les machines propres à développer cette puissance*, Bachelier, Paris 1824.
14. R. CLAUDIUS, *On another form of the Second Principle of the mechanical theory of Heat*, Pogg. Ann., December 1854, French translation by R. Folie, in: "R. Clausius, Théorie Mécanique de la Chaleur", Mémoire IV, Lacroix, Paris 1865, 131–160.
15. R. CLAUDIUS, *Sur diverses formes des équations fondamentales de la théorie mécanique de la chaleur qui sont commodes dans l'application*, Journ. de Liouville, 2, X, 361 [In:] "R. CLAUDIUS, Théorie Mécanique de la Chaleur", Mémoire IX, Lacroix, Paris 1865, 377–420.
16. B. N. COLEMAN, *Thermodynamics of materials with memory*, Arch. Rational Mech. Anal., **17**, 1–46, 1964.
17. B. N. COLEMAN, V. J. MIZEL, *Existence of caloric equations of state in thermodynamics*, J. Chem. Phys., **40**, 1116–1125, 1964.
18. W. A. DAY, *The Thermodynamics of simple materials with fading memory*, Springer-Verlag, Berlin 1972.
19. TH. DE DONDER, *L'Affinité*, Gauthier-Villars, Paris 1931.
20. R. DEFAY, Bull. Ac. Roy. Belg. (Cl. Sc.), 347, 1938.
21. S. R. DE GROOT, P. MAZUR, *Non-equilibrium thermodynamics*, North-Holland, Amsterdam 1962.
22. J. J. D. DOMINGOS, M. N. R. NINA, J. H. WHITELAW (Eds), *Foundations of continuum thermodynamics*, MacMillan, London 1974.
23. P. DUHEM, *Le potentiel thermodynamique et ses applications à la mécanique chimique et à l'étude des phénomènes électriques*, Hermann, Paris 1886.
24. P. DUHEM, *Traité d'énergétique ou de thermodynamique générale*, 2 volumes, Gauthier-Villars, Paris 1911.
25. M. FRÉCHET, *Sur les fonctionnelles continues*, Ann. Sc., Paris, **27**, 3, 193–216, 1910.
26. C. FRIEDRICH, H. BRAUN, *Generalized Cole-Cole behaviour and its rheological relevance*, Rheologica Acta, **31**, 309–322, 1992.
27. P. GERMAIN, *Mécanique des milieux continus*, Masson, Paris 1973.
28. P. GERMAIN, *The role of thermodynamics in continuum mechanics*, [In:] J. J. D. DOMINGOS et al. [Eds.], *Foundations of Continuum Thermodynamics*, Mc Millan, London 1974, 317–333.
29. J. W. GIBBS, *A method of geometrical representation of the thermodynamic properties of substances by means of surfaces*. Trans. Connecticut Academy, **II**, 382–404, 1873.
30. J. W. GIBBS, *On the equilibrium of heterogeneous substances*. Trans. Connecticut Academy, **III**, 108–248 and 343–524, 1875.
31. P. GLANSDORF, I. PRIGOGINE, *Structure, stabilité et fluctuations*, Masson, Paris 1971.
32. P. GRESSEL, *Prediction of long term deformation behavior from short term creep experiments*, Holz als Roh-und Werkstoff, **42**, 8, 293–301, 1984.
33. E. A. GUGGENHEIM, *Thermodynamics*, North-Holland, Amsterdam 1967.
34. C. HUET, *Comportement viscoélastique d'un matériau hydrocarboné*, C. R. Ac. Sc. Paris, **257**, 1438–1442, 1963.



35. C. HUET, *Etude par une méthode d'impédance du comportement viscoélastique des matériaux hydrocarbonnés*, Annales des Ponts et Chaussées, Paris, **6**, 373–429, 1965.
36. C. HUET, *Représentation des modules et complaisances complexes dans les plans complexes arithmétique et logarithmique*, Cahiers du Groupe Français de Rhéologie, **1**, 5, 237–58, 1967.
37. C. HUET, *Sur la notion d'état local en rhéologie*, Sciences et Techniques de l'Armement, Paris, **53**, 4, 611–651, 1979.
38. C. HUET, *Topics in thermodynamics of rheological behaviour*, Rheologica Acta, **21**, 360–365, 1982.
39. C. HUET, *Thermodynamique des comportements rhéologiques en variables naturelles*, Rheologica Acta, **22**, 245–259, 1983.
40. C. HUET, *Macroscopic rheology without functionals: the natural variables formalism*, [In:] B. MENA *et al.* [Eds.], *Advances in Rheology*, Mexico University Press 1984, 497–507.
41. C. HUET, *A new approach for the thermodynamics of materials with delayed response*, [In:] H. D. BUI, Q. S. NGUYEN [Eds.], *Thermomechanical Coupling in Solids*, North-Holland, Amsterdam 1987, 37–42.
42. C. HUET, *Application of the natural variables formalism to classical rheological models*, [In:] P. H. T. UHLHERR [Ed.] *Proc. Xth Int. Congress in Rheology*, Sydney, Australia, vol. 1, 419–421, 1988.
43. C. HUET, *Modeling the kinetics of the thermo-hygro-viscoelastic behaviour of wood under constant climatic conditions*, [In:] R. ITANI [Ed.], *Proc. International Conference on Timber Engineering*, FPRS, Madison 1988, 395–401.
44. C. HUET, *Definition of the out of equilibrium entropy through the use of markoffian variables and the example of elasto-visco-plastic mechanical models*, [In:] J. KESTIN AND TH. LEHMAN [Eds.] "What is the Correct Form of the Gibbs Equation for Inelastic Deformations in Solid Bodies", Universität Bochum, 1988.
45. C. HUET, *An integrated approach of concrete micromechanics*, [In:] C. HUET [Ed.], *Micromechanics of Concrete and Cementitious Composites*, Presses Polytechniques et Universitaires Romandes, Lausanne 1993, 117–146.
46. C. HUET [Ed.], *Micromechanics of concrete and cementitious materials*, Presses Polytechniques et Universitaires Romandes, Lausanne 1993.
47. C. HUET, *Some basic tools and pending problems in the development of constitutive equations for the delayed behaviour of concrete*, [In:] Z. P. BAZANT AND I. CAROL [Eds.], *Creep and Shrinkage of concrete*, Spon, London 1993, 189–200.
48. C. HUET, *Recent advances in the long term deformation and deterioration behaviour of structural materials and components through the integrated micromechanics and thermodynamics of solids approach*, [In:] A. GERDES [Ed.] *Advances in building materials*, Aedificatio, Freiburg 1996, 161–196.
49. C. HUET, *Hybrid continuum thermodynamics framework and numerical simulations examples for the delayed micromechanical behaviour of heterogeneous materials with chemical, climatic and defects sensitivity*, [In:] Q. S. NGUYEN AND V. D. NGUYEN [Eds.], *Engineering Mechanics Today*, University of Hanoi 1995, 170–184.
50. C. HUET, *Continuum thermodynamics and microstructure-creep couplings in heterogeneous and/or microcracked materials: some recent general results and examples of application*, [In:] A. JAKOWLUK [Ed.], *Creep and coupled processes*, Bialystock Technical University Publishers, 1996.
51. C. HUET, *An integrated micromechanics and statistical continuum thermodynamics approach for studying the fracture behaviour of microcracked heterogeneous materials with delayed response*, *Engineering Fracture Mechanics*, **58**, 5–6, 459–556, 1997.

52. C. HUET and P. NAVI, *Multiparabolic multitransition model for thermo-viscoelastic behaviour of wood*, [In:] ASME [Ed.] *Mechanics of Woods and Paper Materials*, Dallas, Texas. 17–24, 1990.
53. J. KESTIN, *A course in Thermodynamics*, Hemisphere Publishing Comp., New-York; 2 vols., 1979.
54. J. KESTIN, *Entropy and entropy production; discussion paper*, [In:] J. J. D. DOMINGOS, M. N. R. NINA AND J. H. WHITELAW [Eds.]. *Foundations of Continuum Thermodynamics*, Mc Millan, London 1974, 143–158.
55. J. KESTIN, *Local-equilibrium formalism applied to mechanics of solids*, *Int. J. Solids Structures*, 29, 14/15, 1827–1836, 1992.
56. J. KESTIN and TH. LEHMAN, [Eds.], “*What is the correct form of the Gibbs equation for inelastic deformations in solid bodies*”, *Symposium Proceedings*, Universität Bochum, 1988.
57. W. KOSINSKI, R. DE BOER, D. GROSS [Eds.], *Problems of environmental and damage mechanics*, *Proceedings of the 31st Polish Solid Mechanics Conference*, Mierki, IPPT, Warsaw 1996.
58. E. KRÖNER, *Statistical continuum mechanics*, Springer-Verlag, Vienna 1972.
59. D. C. KUIKEN, *Thermodynamics of irreversible processes: Applications to diffusion and rheology*, Wiley, 1994.
60. J. MANDEL, *Cours de mécanique des milieux continus*, Gauthier-Villars, Paris, 2 vols. 1966.
61. J. MANDEL, *Application de la thermodynamique aux milieux viscoélastiques à élasticité nulle ou restreinte*, *Comptes-rendus Ac. Sc. Paris*, **264**, 133–134, 1967.
62. J. MANDEL, *Introduction à la mécanique des milieux continus déformables*, Editions Scientifiques de Pologne, Warsaw 1974.
63. J. MANDEL, *Variables cachées. Puissance dissipée. Dissipativité normale*, *Sciences et techniques de l’armement*, Paris 1979, **210**, 4, 525–538.
64. J. MANDEL, L. BRUN, *Thermodynamique et ondes dans les milieux viscoélastiques*, *J. Mech. Phys. Solids*, **16**, 33–58, 1967.
65. F. MASSIEU, *Sur les fonctions caractéristiques des divers fluides*. *C. R. Acad. Sc., Paris*, **69**, 858–862, 1869.
66. J. MEIXNER, *Zur Thermodynamik der irreversiblen Prozesse in Gasen mit chemisch reagierenden, dissozierenden und anregbaren Komponenten*, *Annalen der Physik*, **5**, 43, 244–270, 1943.
67. J. MEIXNER, *Entropy and entropy production*, [In:] J. J. D. DOMINGOS *et al.* [Eds.] *Foundations of Continuum Thermodynamics*, Mc Millan, London 1974, 129–142.
68. J. MEIXNER, H. G. REIK, *Thermodynamik der irreversiblen Prozesse*, [In:] S. FLÜGGE [Ed.], *Encyclopedia of Physics*, III/2, 23B, Springer, 413–523, 1959.
69. S. NEMAT-NASSER, *On non-equilibrium thermodynamics of viscoelasticity and viscoplasticity*, [In:] J. J. D. DOMINGOS *et al.* [Eds.], *Foundations of Continuum Thermodynamics*, Mc Millan, London 1974, 259–282.
70. S. NEMAT-NASSER, *On non-equilibrium thermodynamics of continua*, [In:] S. NEMAT-NASSER [Ed.], *Mechanics Today*, Pergamon, 2, 94–158, 1975.
71. W. NOLL, *A mathematical theory of the mechanical behaviour of continuous media*, *Arch. Rational Mech. Anal.* **2**, 197–226, 1958.
72. B. PERSOZ, *Modeles non-linéaires*, [In:] B. PERSOZ [Ed.], *La Rhéologie*, Masson, Paris 1969.
73. I. PRIGOGINE, *Etude thermodynamique des phénomènes irréversibles*, Desoer, Liege, Dunod, Paris 1947.

74. I. PRIGOGINE, *Introduction to thermodynamics of irreversible processes*, Wiley, 1962.
75. I. PRIGOGINE, *Introduction a la thermodynamique des processus irreversibles*, Dunod, Paris 1962.
76. I. PRIGOGINE, R. DEFAY, *Thermodynamique chimique*, Desoer, Liège 1950.
77. R. S. RIVLIN, J. L. ERICKSEN, *Stress-deformation relations for isotropic materials*, J. Rational Mech. Anal. **4**, 323–425, 1955.
78. N. RUDDOCK, P. W. JAMES, T. E. R. JONES, *Modelling the viscoelasticity of unfilled and carbon black elastomers*, Rheol. Acta, **32**, 286–292, 1993.
79. A. J. STAVERMAN, P. SCHWARZL, *Thermodynamics of viscoelastic behaviour (model theory)*, Proc. Acad. Sc., The Netherlands, **55**, 474–485, 1952.
80. A. J. STAVERMAN, P. SCHWARZL, *Non-equilibrium thermodynamics of visco-elastic behaviour*, Proc. Acad. Sc., The Netherlands, **55**, 486–492, 1952.
81. H. SUNDERLAND, A. TOLOU, C. HUET, *Multilevel numerical microscopy and tri-dimensional reconstruction of concrete microstructure*, [In:] C. HUET [Ed.] *Micromechanics of Concrete and Cementitious Composites*, Presses Polytechniques et Universitaires Romandes, Lausanne 1993, 171–180.
82. P. J. TORVIK, R. L. BAGLEY, *On the appearance of the fractional derivative in the behaviour of real materials*, J. Appl. Mech., **51**, 294–298, 1984.
83. C. TRUESDELL, *Rational thermodynamics*, Mac Graw Hill, New-York, 1969.
84. C. TRUESDELL, R. TOUPIN, *The classical field theories of mechanics*, [In:] S. FLÜGGE [Ed.] *Encyclopedia of Physics*, vol. III/1 Springer-Verlag (Berlin 1960).
85. C. TRUESDELL, W. NOLL, *The non-linear field theories of mechanics*, [In:] S. FLÜGGE [Ed.], *Encyclopedia of Physics*, vol. III/3, Springer-Verlag, 1965.
86. K. C. VALANIS, *Irreversibility and existence of entropy*, Int. J. Non-Linear Mechanics, **6**, 337–360, 1971.
87. K. C. VALANIS, *Partial integrability as a basis for the existence of entropy in irreversible systems*, ZAMM, **63**, 73–80, 1983.
88. L. J. VICAT, *Note sur l'allongement progressif du fil de fer soumis a diverses tensions*, Annales de Chimie et de Physique, Paris, **54**, 35–40, 1833.
89. V. VOLTERRA, *Sopra le funzioni che dipendono da altre funzioni*, R. C. Accad. Lincei, **4**, 3, 97–105, 1887.
90. V. VOLTERRA, *La théorie des fonctionnelles appliquées aux phénomènes héréditaires*, Rev. Gén. Sci. pur. appl., **41**, 197–206, 1930.
91. V. VOLTERRA, *Theory of functionals and of integral and integro-differential equations*, 1925 Madrid Lectures, Dover, New-York 1959.

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## Transverse Stokes flow through regular arrays of cylinders

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THE PAPER PRESENTS RESULTS of calculations of the Stokes flow through square and triangular arrays of parallel cylinders. The results were derived using the method of singular force distributions [1]. The results are obtained to  $O(f^7)$  for a square and to  $O(f^8)$  for a triangular array, where  $f$  is the reduced volume fraction. They are compared with the results of previous authors. The new expressions for the drag force and the permeability coefficient valid in the whole range of  $f$  are also derived, using Padé approximation technique.

### 1. Introduction

THE STOKES FLOW through a square array of parallel cylinders was recently the subject of the paper [1] where the problem was studied by means the method of singular force distribution proposed by HASIMOTO [2]. In the present paper we extend the study to the array of triangular geometry and derive new results of higher order approximation than in the previous papers, for both the square and triangular arrays.

We treat here the array of cylinders as a porous medium where mean velocity  $U$  and mean pressure gradient  $\nabla p$  are related by the linear Darcy's law [3]

$$(1.1) \quad U = -K \cdot \tau_0 \cdot \frac{l^2}{\mu} \cdot \nabla p.$$

Here  $\mu$  denotes dynamic viscosity,  $\tau_0$  is a non-dimensional cross-sectional area of a unit cell and  $l$  is the distance between axes of cylinders within the unit cell. The symbol  $K$  denotes a non-dimensional permeability coefficient which may be presented by the following general expression:

$$(1.2) \quad K(a) = \frac{1}{8\pi} \cdot [\ln 1/a^2 - C_0 + 2\beta(a)] ,$$

where

$$(1.3) \quad \beta(a) = \sum_{i=1}^N C_i \cdot a^{2i} ,$$

$a$  being the cylinder radius non-dimensionalized with the distance  $l$  and  $C_i$  are

coefficients of expansion. The radius  $a$  and the volume fraction of cylinders  $\varphi$  are related as follows

$$(1.4) \quad \varphi = \pi a^2 / \tau_0,$$

where  $\tau_0$  is a non-dimensional cross-sectional area of a unit cell.

HASIMOTO [2] obtained the result (1.3) to  $N = 1$  for square arrays. The method of Hasimoto was then developed by SANGANI and ACRIVOS [4] who got expansions to  $N = 3$  for the both square and triangular arrays. DRUMMOND and TAHIR [5] made calculations applying the method of singularities using a different analytical technique than that of Hasimoto. They obtained expansions (1.3) to  $N = 4$  for square arrays and to  $N = 6$  for triangular arrays. All these results have been collected in a monograph by ADLER [3]. Recently the present author the extended calculations to  $N = 5$  for square arrays [1].

The theoretical research of the Stokes flow through spatially periodic systems of particles found several technological applications. The approach of HASIMOTO [2] inspired DAVIS and JAMES [6] to calculate the Stokes flow through a periodic array of thin rings. These results appeared to be important in mathematical modelling of paper formation processes. Another application of the Stokes flow calculations for periodic systems in industrial practice is mathematical modelling of hydrodynamic processes in man-made fiber formation. This problem was first studied by SZANIAWSKI and ZACHARA [7] who treated a bundle of fibers as a porous medium using the transverse and parallel permeability coefficients according to HAPPEL and BRENNER [8]. This approach was then used to study fiber formation in various conditions of manufacturing (see ZACHARA [9]). Recently this method was modified and applied by OCKENDON and TERRILL [10] to mathematical modelling of various aspects of wet-spinning processes. They used permeability coefficients according to DRUMMOND and TAHIR [5].

The present paper follows the approach of HASIMOTO [2] and SANGANI and ACRIVOS [4]. This approach was modified by the present author [1] where a new functional basis has been derived. It allowed to obtain explicit expressions for matrix elements of the system of linear algebraic equations. The solution of the truncated system could be then derived using the symbolic computations of *Mathematica* [11] and the analytical expression for the permeability coefficient (1.2) was obtained. This expression has been expanded to  $N = 7$  for square and to  $N = 8$  for a triangular arrays. It covered a wide range of the volume fraction  $\varphi$  with the exception of  $\varphi$  close to  $\varphi_{\max}$ , corresponding to densely packed cylinders. However, making use of the asymptotic solution of KELLER [12], valid in the range  $\varphi \rightarrow \varphi_{\max}$ , and the solutions obtained in this paper, we have derived the new expressions for the permeability coefficient  $K$  valid in the full range of the volume fraction. These expressions have been obtained using the multipoint Padé approximants technique [13]. The results of calculations derived in various orders

of approximation have been compared with the numerical results of SANGANI and ACRIVOS [14].

## 2. Calculation of the permeability coefficient

The calculation method, based on the approach of HASIMOTO [2] and SANGANI and ACRIVOS [4], has been derived in the previous paper [1]. We do not repeat here details of the analytical procedure which can be found in [1] but instead, we present new results of calculations which enable higher order approximation of the permeability coefficient  $K(a)$  (1.2) for square and triangular arrays of cylinders. The quantity  $\beta$  which appears in (1.2) is defined as

$$(2.1) \quad \beta = \frac{1}{Y_1},$$

with  $Y_1$  being the component of the vector  $\mathbf{Y}$  which fulfils the algebraic system of equations

$$(2.2) \quad W_{ij}Y_j = \delta_{i1}.$$

The matrix elements  $W_{ij}$  are presented by the expressions (2.4)–(2.6). These expressions are different for odd and even subscripts  $j$  corresponding to the matrix columns. The elements of the first column  $W_{i1}$  are here excluded to simplify the odd columns expression. Thus the matrix elements may be presented as follows:

– for  $j = 1$ :

$$(2.3) \quad W_{i1} = \frac{\pi a^2}{2\tau_o} \cdot \delta_{i1} + \frac{1}{2} \cdot \left(1 - \frac{\pi a^2}{2\tau_o}\right) (\delta_{i3} - \delta_{i2}) + A_{i-1} \cdot a^{i-1} \\ - (i+1) \cdot \left[ \frac{1}{2} A_{i+1} \cdot a^2 + i \cdot B_{i+1} \right] \cdot a^{i-1} \\ + (i+2) \cdot \left[ \frac{1}{2} A_{i+2} \cdot a^2 + (i+1) \cdot B_{i+2} \right] \cdot a^i,$$

– for other odd subscripts  $j = 3, 5, 7, \dots$ :

$$(2.4) \quad W_{ij} = \frac{\pi}{2\tau_o} \cdot \delta_{i1} \delta_{j3} + \frac{(j-1)!}{2a^{j-1}} \cdot (\delta_{i,j+2} - \delta_{i,j+1} + \delta_{i,j-1}) \\ - \frac{(j-1)(j-2)!}{2 \cdot a^{j-1}} \cdot \delta_{ij} - \frac{(j-3)(i+j-2)!}{2 \cdot (i-1)!} A_{i+j-2} \cdot a^{i-1}$$

$$\begin{aligned}
& - \frac{(j-1)(i+j-1)!}{2i!} \cdot A_{i+j-1} \cdot a^i - \frac{(i+j)!}{i!} \cdot \left[ \frac{1}{2} \cdot A_{i+j} \cdot a^2 + i \cdot B_{i+j} \right] \cdot a^{i-1} \\
& - \frac{(i+j+1)!}{(i+1)!} \cdot \left[ \frac{1}{2} \cdot A_{i+j+1} \cdot a^2 + (i+1) \cdot B_{i+j+1} \right] \cdot a^i,
\end{aligned}$$

– for even subscripts  $j = 2, 4, 6, \dots$ :

$$\begin{aligned}
(2.5) \quad W_{ij} = & -\frac{2\pi}{\tau_0} \cdot \delta_{i1} \delta_{j2} + \frac{2 \cdot (j-1)!}{a^j} \cdot (\delta_{i,j+1} - \delta_{ij}) \\
& + \frac{2 \cdot (i+j-1)!}{(i-1)!} \cdot A_{i+j-1} \cdot a^{i-1} + \frac{2 \cdot (i+1)!}{i!} \cdot A_{i+j} \cdot a^i.
\end{aligned}$$

The system (2.2) has been truncated to the size  $9 \times 9$  and solved using the symbolic computations *Mathematica*. As a result, the expansions of  $\beta(a)$  (1.3) were obtained with  $N = 7$  for a square array and  $N = 8$  for a triangular array. The calculated coefficients  $C_i$  from (1.3) are as follows:

– for a square array:

$$\begin{aligned}
C_1 &= \pi/\tau_0, \quad C_2 = -[(\pi/\tau_0)^2/4 + 576 \cdot B_4^2], \quad C_3 = -768 \cdot A_4 B_4, \\
C_4 &= 288 \cdot \pi/\tau_0 \cdot A_4 B_4 - 260 \cdot A_4^2, \quad C_5 = 192 \cdot \pi/\tau_0 \cdot A_4^2, \\
C_6 &= -12 \cdot (3 \cdot (\pi/\tau_0)^2 \cdot A_4^2 + 6912 \cdot A_4^2 B_4^2 - 26880 \cdot A_4 B_4 B_8 + 3136 \cdot B_8^2), \\
C_7 &= 768 \cdot (-288 \cdot A_4^3 B_4 + 224 \cdot A_4 B_4 A_8 + 560 \cdot A_4^2 B_8 - 105 \cdot A_8 B_8),
\end{aligned}$$

– for a triangular array:

$$\begin{aligned}
C_1 &= \pi/\tau_0, \quad C_2 = -(\pi/\tau_0)^2/4, \quad C_3 = 0, \\
C_4 &= -7200 \cdot B_6^2, \quad C_5 = -17280 \cdot A_6 B_6, \\
C_6 &= 6A_6 \cdot (600 \cdot \pi/\tau_0 \cdot B_6 - 433 \cdot A_6), \\
C_7 &= 2160 \cdot \pi/\tau_0 \cdot A_6^2, \quad C_8 = -450 \cdot (\pi/\tau_0)^2 \cdot A_6^2.
\end{aligned}$$

The coefficients  $C_1, C_2, C_3$  for a square and a triangular array are fully equivalent to those obtained by SANGANI and ACRIVOS [4]. The coefficient  $C_4$  for a square array and the coefficients  $C_4, C_5, C_6$  for a triangular array were derived by DRUMMOND and TAHIR [5] with the calculation technique different from ours

hence the corresponding expressions cannot be directly compared. Instead we can compare their numerical values. To this aim we take the numerical values of  $A_4, B_4, A_8, B_8, C_0$  evaluated for a square array [1] and calculate the numerical values of  $A_6, B_6, C_0$  for a triangular array using procedures given by SANGANI and ACRIVOS [4] or ZACHARA [1].

Hence for a square array we have:

$$\begin{aligned} A_4 &= 7.878030005 \cdot 10^{-1}, & B_4 &= -1.044856181 \cdot 10^{-1}, \\ A_8 &= 5.319716294 \cdot 10^{-1}, & B_8 &= -4.031710210 \cdot 10^{-2}, \\ C_0 &= 2.621065852, \end{aligned}$$

and for a triangular array:

$$\begin{aligned} A_6 &= 9.771719489 \cdot 10^{-1}, & B_6 &= -9.428004796 \cdot 10^{-2}, \\ C_0 &= 2.786075894. \end{aligned}$$

In the case of a square array  $\tau_0 = 1$ , and of a triangular array  $\tau_0 = \sqrt{3}/2$ .

**Table 1. Expansion coefficients in the expression (1.2) for a square and a triangular array.**

$i$	$C_i$ (square)	$C_i$ (triangle)
0	1.310532926	1.393037947
1	$\pi$	3.627598728
2	-8.755733869	-3.289868134
3	$6.321721609 \cdot 10^1$	0
4	$-2.358407557 \cdot 10^2$	$-6.399883760 \cdot 10^1$
5	$3.743573485 \cdot 10^2$	$7.959843494 \cdot 10^2$
6	$2.267883043 \cdot 10^2$	$-3.683869238 \cdot 10^3$
7	$-2.632730210 \cdot 10^3$	$7.481952988 \cdot 10^3$
8		$-5.654483988 \cdot 10^3$

Inserting all these data to the expressions for  $C_i$  we obtain their numerical values which are collected in Table 1. The data of DRUMMOND and TAHIR [5] correspond to our data for  $i = 0 \div 4$  (square array) and for  $i = 0 \div 6$  (triangular array). The literature data for higher  $i$  are not known to the author. If we compare the results collected in Table 1 with the results of DRUMMOND and TAHIR we can see that they are equal at least to eight decimal places. The agreement is then excellent although these results were derived with the use of two different techniques.

It is convenient to present the permeability coefficient or the drag force as a function of a reduced volume fraction  $f$  which varies from 0 to 1



$$f = \varphi / \varphi_{\max},$$

where  $\varphi$  is the volume fraction of cylinders and  $\varphi_{\max}$  is the limiting volume fraction corresponding to the case of touching cylinders. In the case of a square array  $\varphi_{\max} = \pi/4$ , and in the case of triangular array  $\varphi_{\max} = \pi\sqrt{3}/6$ . It can be easily shown that the variable  $f$  is related to the radius of a cylinder  $a$  for both the square and triangular array as

$$(2.6) \quad f = 4a^2.$$

Substituting (2.6) to (1.2) we may present the coefficient  $K$  in the form

$$(2.7) \quad K(f) = \frac{1}{8\pi} \left[ \ln 1/f + \sum_{i=0}^N T_i \cdot f^i \right],$$

where the coefficients  $T_i$  are related to the coefficients  $C_i$  as follows:

$$(2.8) \quad T_0 = \ln 4 - C_0,$$

$$(2.9) \quad T_i = \frac{C_i}{4^i}, \quad \text{for } i > 0.$$

We obtain the new expressions for the permeability coefficient  $K$  (2.7). They are:

– for a square array

$$(2.10) \quad K(f) = \frac{1}{8\pi} \left[ \ln 1/f - 1.234771491 + \frac{\pi}{2} \cdot f \right. \\ \left. - 1.094466733 \cdot f^2 + 1.975538003 \cdot f^3 - 1.842505904 \cdot f^4 \right. \\ \left. + 0.7311666962 \cdot f^5 + 0.1107364767 \cdot f^6 - 0.3213781994 \cdot f^7 \right],$$

– for a triangular array

$$(2.11) \quad K(f) = \frac{1}{8\pi} \left[ \ln 1/f - 1.399781533 + 1.813799364 \cdot f \right. \\ \left. - 0.4112335167 \cdot f^2 - 0.4999909187 \cdot f^4 + 1.554656932 \cdot f^5 \right. \\ \left. - 1.798764276 \cdot f^6 + 0.9133243394 \cdot f^7 - 0.1725611569 \cdot f^8 \right].$$

The results obtained are presented in Fig. 1 for a square array and in Fig. 2 for a triangular array, in a form  $F(f) = K^{-1}$ , where  $F$  is a drag force per unit

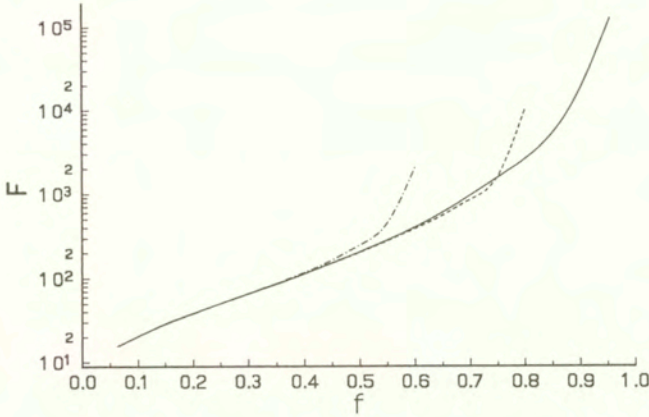


FIG. 1. Drag force  $F(f) = K^{-1}(f)$  for a square array calculated from (2.10) at various truncations: - · - · -  $O(f^4)$  [5]; - - -  $O(f^7)$  present results; ——— reference data [14].

length of the cylinder (see [1]). They are compared with the numerical results of SANGANI and ACRIVOS [14] derived in a wide range of the volume fraction from  $f = 0$  to  $f$  close to 1. It is seen that the present results evidently allowed to increase the accuracy of calculations. Thus the results are in agreement with the reference data [14] in a wide range of the volume fraction  $f$  up to about  $f = 0.8$ .

In the range of  $f$  close to 1 the coefficient  $K(f)$  is well approximated by the asymptotic relation of KELLER [12] obtained by means the theory of lubrication. For a square array this relation reads

$$(2.12) \quad K(f) = \frac{2\sqrt{2}}{9\pi} \cdot (1 - f^{1/2})^{5/2},$$

and for a triangular array

$$(2.13) \quad K(f) = \frac{4\sqrt{2}}{27\pi} \cdot (1 - f^{1/2})^{5/2}.$$

Thus we have two pairs of relations (2.10), (2.12) and (2.11), (2.13) for a square and triangular arrays, respectively. It would be however convenient to have only one expression  $K(f)$  for each geometry, which could cover the complete range of  $f$  with a good accuracy. To this aim we use the technique of multipoint Padé approximants [13]. This type of approximation often appears to be more convenient than polynomials since Padé approximants need in general much less terms to achieve a good accuracy. We seek the expression for the permeability coefficient in the following form:

$$(2.14) \quad K(f) = \frac{1}{8\pi} \left[ \ln 1/f - T_0 + [L/M] \right],$$

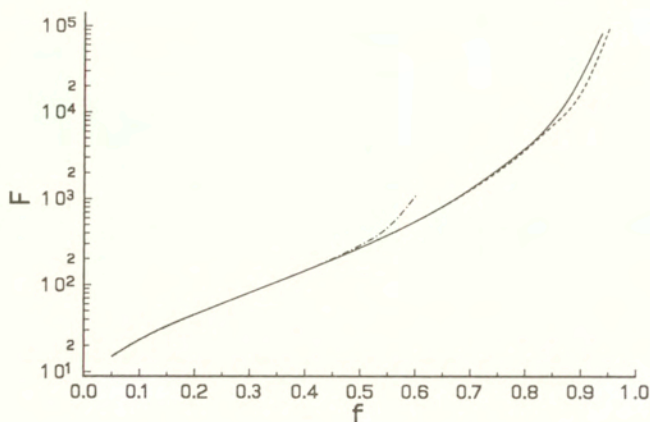


FIG. 2. Drag force  $F(f) = K^{-1}(f)$  for a triangular array calculated from (2.11) at various truncations.: - · - · -  $O(f^6)$  [5]; - - -  $O(f^8)$  present results; ——— reference data [14].

where

$$(2.15) \quad [L/M] = \frac{\sum_{i=1}^L a_i \cdot f^i}{1 + \sum_{i=1}^M b_i \cdot f^i},$$

is a Padé approximant. The coefficients  $a_i, b_i$  can be evaluated so that the expression (2.14) could take the values determined by (2.10) and (2.12) or by (2.11) and (2.13) for several selected values of  $f$ . We chose  $L = 3$  and  $M = 2$  and evaluated coefficients  $a_i, b_i$  which are presented in Table 2.

**Table 2. Coefficients of the Padé approximant (2.15) for a square and a triangular array.**

	Square array	Triangular array
$a_1$	1.556322044	1.823817915
$a_2$	4.462879026	-1.723614004
$a_3$	-3.117657159	0.174433692
$b_1$	3.689159025	-0.681877655
$b_2$	-2.339295968	-0.121922012

The coefficient  $K(f)$  (2.14) has been calculated and the results are presented in Fig. 3 for a square, and in Fig. 4 – for a triangular array. The results obtained from the power expansions (2.10), (2.11) and the Keller solutions (2.12), (2.13) are also included. The Padé approximants technique was also applied by DRUMMOND

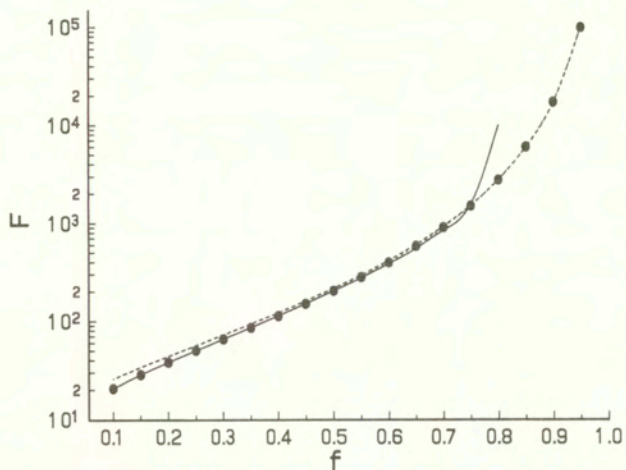


FIG. 3. Drag force  $F(f) = K^{-1}(f)$  for a square array; ———  $O(f^7)$ , present results; - - - Keller approximation calculated from (2.12); • • • Padé approximant calculated from (2.14) and Table 2.

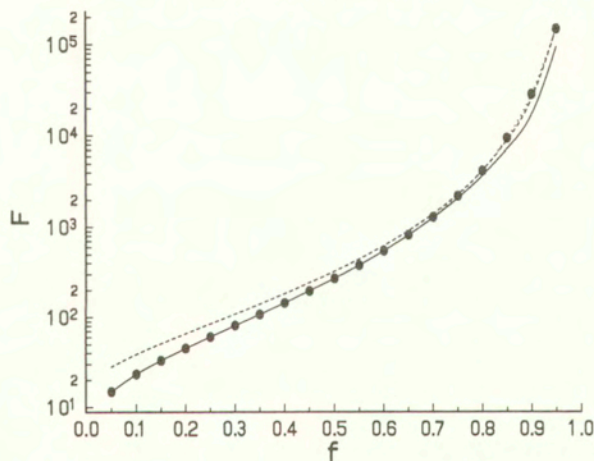


FIG. 4. Drag force  $F(f) = K^{-1}(f)$  for a triangular array; ———  $O(f^8)$ , present results; - - - Keller approximation calculated from (2.13); • • • Padé approximant calculated from (2.14) and Table 2.

and TAHIR [5], however their expressions in the Padé version were merely some correction of the expressions with power series expansions and did not cover the complete range of the volume fraction.

### 3. Conclusions

The Stokes flow through a square and triangular arrays of parallel cylinders was studied using the method based on the approach of HASIMOTO [2]. This

approach was modified and a new analytical technique was developed (see [1]). The solution of the governing equations has been derived with the aid of the functional basis which allowed to transform these equations into the system of linear algebraic equations with the matrix elements given in an explicit analytical form. It made possible to obtain the analytical expression for the permeability coefficient  $K$  or the drag force  $F$  using symbolic computations of *Mathematica* [11]. It is a meaningful advantage of the method since derivation of drag force expressions without computer assistance is very tedious even for quite a moderate order of approximation. The expressions for  $F$  derived in this paper are of a higher order of approximation than those previously obtained, i.e. to  $O(f^7)$  for a square and to  $O(f^8)$  for a triangular array.

It was of course possible to continue calculations and derive new expressions (2.7) of higher order. However these expressions, being more and more extended, would never cover the complete range of the volume fraction. For this reason the new expressions have been derived using the multipoint Padé approximants technique. These expressions, based on the results of the present paper and the asymptotic results of KELLER [12], allowed us to evaluate with a good accuracy the drag force  $F$  or, all the same, the permeability coefficient  $K$  in the full range of the reduced volume fraction  $f$  from 0 to 1.

## References

1. A. ZACHARA, *Transverse Stokes flow through a square array of cylinders*, Arch. Mech. **49**, 831–846, 1977.
2. H. HASIMOTO, *On the periodic fundamental solutions of the Stokes equations and their application to viscous flow past a cubic array of spheres*, J. Fluid Mech., **5**, 317–328, 1959.
3. P. M. ADLER, *Porous media: Geometry and transport*. Butterworth-Heinemann, 1992.
4. A. S. SANGANI and A. ACRIVOS, *Slow flow through a periodic array of spheres*, Int. J. Multiphase Flow, **8**, 343–360, 1982a.
5. J. E. DRUMMOND and M. I. TAHIR, *Laminar viscous flow through regular arrays of parallel solid cylinders*, Int. J. Multiphase Flow, **10**, 515–540, 1984.
6. A. M. J. DAVIS and D. F. JAMES, *Slow flow through a model fibrous porous medium*, Int. J. Multiphase Flow, **22**, 969–989, 1996.
7. A. SZANIAWSKI and A. ZACHARA, *Bath penetration into the solidification zone of a fibre bundle* [in Polish], Polimery, **19**, 143–146, 1974.
8. J. HAPPEL and H. BRENNER, *Low Reynolds number hydrodynamics*, Nordhoff International Publ., Leyden 1973.
9. A. ZACHARA, *How to estimate the flow characteristics in multifilament spinning*, ATI Fiber, World, Part I: May, 13–17; Part II: July, 52–60, 1987.
10. H. OCKENDON and E. L. TERRILL, *A mathematical model for the wet spinning process*, Euro. J. of Applied Mathematics, **4**, 341–360, 1993.
11. S. WOLFRAM, *Mathematica. A System for doing Mathematics by computer*, Addison-Wesley Publ. Co, 1991.
12. J. B. KELLER, *Viscous flow through a grating or lattice of cylinders*, J. Fluid Mech., **18**, 94–96, 1964.

13. G. A. BAKER and P. GRAVES-MORRIS, *Padé Approximants*. Cambridge University Press, 1996.
14. A. S. SANGANI and A. ACRIVOS, *Slow flow past periodic arrays of cylinders with application to heat transfer*, *Int. J. Multiphase Flow*, **8**, 93-206, 1982b.

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## Dusty plasma solitons in Vlasov plasmas

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VLASOV-GAUSS/AMPÈRE EQUATIONS for dust-ion-electron plasmas are considered. Dispersion relations are derived for longitudinal dusty plasma waves by use of linearized Vlasov equations. Assuming suitable equilibrium distributions for cold and hot charged particle/grain components, due to negligence of wave-particle interactions and assuming traveling the wave “far field” solutions, fully nonlinear ODE is obtained for SAGDEEV potentials. Examples of Sagdeev potentials and negative solitary waves associated with fully nonlinear dust-acoustic waves (DAW) and dust-ion acoustic waves (DIAW) are computed.

### 1. Introduction

DUST IS A COMMON COMPONENT of many space plasmas. Waves in dusty plasmas have recently been considered when the dust grains are negatively charged. Dusty plasma physics is of great importance with a number of applications. Recently, attention has been focused on planetary rings in which heavy micron-sized dust grains are charged to high degree voltage. In particular, in the F-ring of Saturn there is an extreme anomalous situation where the number density of free electrons is much smaller than the number density of ions. This could happen because the charged dust grains collect electrons from the background medium and the number density of free electrons is anomalously small. Recent Voyager 1 and 2 observations of Saturnian ring systems have started research interest in physics of dusty plasmas. Dust is rather ubiquitous in space; some well-known systems where the presence of dust has been established, are inter- and circumstellar clouds, solar system interplanetary dust, earth’s magnetosphere, comets and planetary rings. Also, dusty plasmas appear in laboratory system, e.g. rf plasmas used in the microelectronic processing industry, and it may also be present in the limiter regions of fusion plasmas due to the sputtering of carbon by energetic particles. We shall mainly discuss space dusty plasmas although many of the conclusions are valid for the laboratory plasmas as well. Grains are dielectric (ices, silicates...) or metallic (graphite, magnetite...), see [1]. We use the term “dusty plasma” when the number of grains in Debye sphere is greater than one, and “dust in a plasma” when the number density of grains is less than one. Usually, we have  $\lambda_D > Ro \gg a$  (dusty plasma), where  $\lambda_D$  is a plasma

Debye length,  $Ro$  is an average separation ( $Ro = (3/4N_{0d})^{1/3}$ , and “ $a$ ” is the grain radius.

After [1] and [2], we note the following typical data for dusty plasmas in:

- i) interstellar clouds, where  $a/\lambda_D \approx 10^{-8}$  and  $Ro/\lambda_D \approx 10^{-1}$ ,
- ii) ionosphere (80km), where  $a/\lambda_D \approx 10^{-6}$  and  $Ro/\lambda_D \approx 10^{-2}$ ,
- iii) rings, where  $a/\lambda_D \approx 10^{-6}$  and  $Ro/\lambda_D \approx 10^{-3}$ ,
- iv) comets, where  $a/\lambda_D \approx 10^{-6}$  and  $Ro/\lambda_D \approx 10 - 100$ ,
- v) magnetosphere, where  $a/\lambda_D \approx 10^{-6}$  and  $Ro/\lambda_D \approx 10 - 100$ .

The mechanism of dust grain charging due to plasma current, photoelectron and secondary emission currents can be found in [1] and [2]. Recently, see [3], it has been proved that *Vlasov description of dusty plasmas is valid not only in the usual weakly coupled plasma regime but also in the strong-coupling limit* for dusty plasmas. Deviations from both limits are to be expected for the intermediate range of coupling when Coulomb crystallization occurs.

The main objective of the paper is to determine asymptotic solutions to the initial-value conditions for Vlasov-Ampère equations, that is to find the “far field” solutions. Next, we determine dispersion relation for longitudinal waves (DAW and DIAW) by use of the linearized Vlasov equations. In case of simplified equilibrium velocity distributions but for fully nonlinear plasmas, we determine velocity distributions  $f_\alpha(u, \xi)$  where  $\xi = x - Ut$  as well as the Sagdeev potential equations and we compute the solitary waves for a set of dusty plasma parameters.

## 2. Statement of the problem

We investigate the Vlasov-Ampère/Gauss system of equations for multi-species plasmas, that is

$$(2.1) \quad \left[ \partial_t + u\partial_x + \frac{q_\alpha}{m_\alpha} E\partial_u \right] f_\alpha(u, x, t) = 0, \quad \partial_u \equiv \frac{\partial}{\partial u} \quad (\text{Vlasov}),$$

$$(2.2) \quad \epsilon_0 \partial_t E + \sum_\alpha q_\alpha \int u f_\alpha du = 0 \quad (\text{Ampère}),$$

$$(2.3) \quad \epsilon_0 \partial_x E = \int_{-\infty}^{\infty} f_\alpha du \equiv \sum_\alpha \rho_\alpha, \quad E = -\partial_x \phi \quad (\text{Gauss}),$$





where  $\xi = x - Ut$ ,

$$W_c(u, \xi) = (u - U) \left[ (1 + r)^{\frac{1}{2}} - 1 \right],$$

where

$$r = \frac{2q_c \phi(\xi)}{m_c (u - U)^2} \quad \text{and} \quad E(\xi) = -\partial_\xi \phi(\xi).$$

We note that  $W_c$  satisfies Eq. (2.7). The well-known “cold particle” number density can be obtained

$$(2.8) \quad n_c(\xi) = N_{0c} \int_{-\infty}^{\infty} \delta(u + W_c(u, \xi)) du = N_{0c} / \left[ 1 - \frac{2q_c \phi(\xi)}{m_c U^2} \right]^{\frac{1}{2}}.$$

In the case of “hot particles”, we accepted “square” equilibrium distribution

$$(2.9) \quad f_{oh}(u) = \frac{1}{2a_h} [H(u + a_h) - H(u - a_h)],$$

where  $H(\cdot)$  is a Heaviside function and

$$f_h(u, \xi) = \frac{1}{2a_h} [H(u + a_h + W_h(u, \xi)) - H(u - a_h + W_h(u, \xi))],$$

where  $\xi = x - Ut$  and (2.4) is convergent.

The hot particle number density takes the following form:

$$(2.10) \quad n_h(\xi) = N_{0h} \int_{-\infty}^{\infty} f_h(u, \xi) du = N_{0h} \frac{a_h + U}{2a_h} \left[ 1 - \frac{2q_h \phi(\xi)}{m_h (a_h + U)^2} \right]^{\frac{1}{2}} \\ + N_{0h} \frac{a_h - U}{2a_h} \left[ 1 - \frac{2q_h \phi(\xi)}{m_h (a_h - U)^2} \right]^{\frac{1}{2}}.$$

Assuming that  $U/a_h \ll 1$ , we have

$$(2.11) \quad n_h(\xi) \simeq N_{0h} \sqrt{1 - \frac{2q_h \phi(\xi)}{m_h a_h^2}}.$$

By use of  $n_c(\xi)$  and  $n_h(\xi)$ , we can determine the Sagdeev potentials and then calculate the dust-ion-sound solitary waves for fully nonlinear plasmas. We note that the results of “far field” solutions derived here, which are the asymptotic solutions to the initial value-problem, are strictly related to the results which can be obtained by use of the “water-bag” model, see [5], [6] and [7].

### 3. Dispersion relation for dusty plasmas

Assuming sufficiently small disturbances of plasma equilibrium, the solution of the linearized Vlasov-Ampère equations takes the form, see [4],

$$(3.1) \quad E(x, t) = E_0(x, t) + \int_0^t dt_1 \int_{-\infty}^{\infty} E(x - x_1, t - t_1) K(x_1, t_1) dx_1,$$

where

$$K(x, t) = - \sum_{\alpha} \omega_{\alpha}^2 f_{0\alpha} \left( \frac{x}{t} \right).$$

Let us consider three components of a dusty plasma having the following equilibrium distributions:

$$(3.2) \quad \begin{aligned} f_{0d}(u) &= \delta(u) && \text{(dust)}, \\ f_{0e}(u) &= \frac{1}{2a_e} [H(u + a_e) - H(u - a_e)] && \text{(hot electrons)}, \\ f_{0i}(u) &= \frac{1}{2a_i} [H(u + a_i) - H(u - a_i)] && \text{(hot ions)}, \end{aligned}$$

$\omega_{\alpha}^2 = N_0^{\alpha} q_{\alpha}^2 / \varepsilon_0 m_{\alpha}$  is the plasma  $\alpha$ -component frequency and  $a_{\alpha}$  is the thermal velocity. We take Fourier-Laplace transform of Eq. (3.1) to obtain:

$$E(k, s) = \frac{E_0(k, s)}{D(k, s)},$$

where  $D(k, s) \equiv 1 - K^e(k, s) - K^i(k, s) - K^d(k, s)$  and the dispersion relation for longitudinal plasma waves takes the form:

$$(3.3) \quad \omega^2 = \frac{\omega_e^2}{1 - \frac{k^2 a_e^2}{\omega^2}} + \frac{\omega_i^2}{1 - \frac{k^2 a_i^2}{\omega^2}} + \omega_d^2,$$

where  $s = -i\omega$ . Following the papers [8] and [9], we assume rather cold ions, that is  $\frac{k^2 a_i^2}{\omega^2} \ll 1$  and hot electrons  $\frac{k^2 a_e^2}{\omega^2} \gg 1$  to obtain the following dispersion relation for the dust-ion-acoustic waves (DIAW)

$$\omega^2 \simeq \frac{k^2 \lambda_{De}^2 (\omega_{oi}^2 + \omega_d^2)}{1 + k^2 \lambda_{De}^2}, \quad \text{where} \quad \lambda_{De} = \frac{a_e}{\omega_{0e}}.$$

If  $k^2 \lambda_{De}^2 \ll 1$ , (long wave approximation) and  $\omega_d^2 \ll \omega_{oi}^2$ , we have the dust-modified ion-acoustic speed

$$(3.4) \quad C_s^2 = \frac{\omega^2}{k^2} \simeq \frac{N_{0i}}{N_e} v_s^2, \quad \text{where} \quad v_s = a_e \left( \frac{m_e}{m_i} \right)^{\frac{1}{2}} \quad \text{and} \quad q_d = Z_d e.$$

The relation (3.4) is similar to the usual ion-sound wave spectrum for non-isothermal plasmas, that is  $m_i a_i^2 \ll m_e a_e^2$ . However in dusty plasmas, we usually have  $T_e \simeq T_i$ . The existence of new dust-acoustic waves, which occur as  $m_i a_i^2 \simeq m_e a_e^2$ , requires the presence of a very small amount of electrons in the background of the collisionless dusty plasma.

In virtue of (3.3), we have

$$\omega^2 \simeq \frac{\omega_d^2 k^2 \lambda_{De}}{1 + k^2 \lambda_{De} + \frac{N_{0i}}{N_{0e}}} \simeq \omega_d^2 k^2 \lambda_{De} \frac{N_{0e}}{N_{0i}},$$

since

$$\omega^2 \ll k^2 a_i^2 \ll k^2 a_e^2$$

and

$$\frac{\lambda_{De}^2}{\lambda_{Di}^2} = \frac{N_{0i}}{N_{0e}} \gg 1 + k^2 \lambda_{De}^2.$$

The frequency  $\omega$  of the dust-acoustic wave is very low and the dust-acoustic speed is

$$C_d \simeq \omega_d \lambda_{De} \sqrt{\frac{N_{0e}}{N_{0i}}}.$$

It is interesting to note, in the virtue of the conditions:  $a_i \ll \omega/k \ll a_e$  for DIAW as well as in view of the condition  $\omega/k \ll a_i \ll a_e$  for DAW, that the waves are subjected to insignificant electron and ion Landau damping. These waves should have some relevance to the low-frequency noise in the F-ring of Saturn.

#### 4. Calculation of Sagdeev potentials and solitons

In the view of (2.8), (2.10) and (2.11), we derive the following expressions for dust, ion and electron charge number densities:

$$\frac{n_d(\xi)}{N_{0i}} = \frac{S_d}{\left(1 + \frac{2y}{M^2}\right)^{\frac{1}{2}}},$$

$$\frac{n_i(\xi)}{N_{0i}} = \frac{1 + \nu_i}{2} \left(1 - \frac{2y}{(1 + \nu_i)^2}\right)^{\frac{1}{2}} + \frac{1 - \nu_i}{2} \left(1 - \frac{2y}{(1 - \nu_i)^2}\right)^{\frac{1}{2}}$$

(4.1)  $\simeq (1 - 2y)^{\frac{1}{2}}, \quad \text{if } \nu_i = \frac{U}{a_i} \ll 1,$

$$\frac{n_e(\xi)}{N_{0e}} = S_e \left[ \frac{1 + \nu_e}{2} \left(1 + \frac{2yR}{(1 + \nu_e)^2}\right)^{\frac{1}{2}} + \frac{1 - \nu_e}{2} \left(1 + \frac{2yR}{(1 - \nu_e)^2}\right)^{\frac{1}{2}} \right]$$

$\simeq S_e(1 + 2yR)^{\frac{1}{2}}, \quad \text{if } \nu_e = \frac{U}{a_e} \ll 1,$

where  $y = y(\xi) = q\phi(y)/m_i\alpha_i^2$ ,  $\xi$  is normalized with respect to  $\lambda_{Di} = \frac{a_i}{\omega_{0i}}$  – is the ion Debye length and,  $M = \frac{U}{a_i} \sqrt{\frac{m_d}{Z_d m_i}} = \frac{U}{c_s}$  – is the Mach number,  $c_s = a_i \sqrt{\frac{Z_d m_i}{m_d}}$  – is the dust-ion-acoustic speed and  $R = \frac{m_i a_i^2}{m_e a_e^2} = \frac{T_i}{T_e}$ . We assume global charge neutrality  $N_{0i} = Z_d N_{0d} + N_{0e}$  and  $S_d = S = \frac{Z_d N_{0d}}{N_{0i}}, S_e = S - 1 = \frac{N_{0e}}{N_{0i}}$ . We note that  $m_d \gg m_i \gg m_e, 0 \leq S \leq 1$ .

In view of Eq.(2.3), we have

$$(4.2) \quad \frac{\partial^2 y}{\partial \xi^2} + \frac{1}{\epsilon_0} \sum_{\alpha} \rho_{\alpha} = 0 \equiv \quad \text{and} \quad V'(y) = \frac{1}{\epsilon_0} \sum_{\alpha} \rho_{\alpha}, \alpha = e, i, d,$$

where  $V(y)$  is the *Sagdeev potential* [10]. The energy integral is

$$(4.3) \quad \frac{1}{2} \left(\frac{\partial y}{\partial \xi}\right)^2 + V(y) = 0,$$

where

$$V(y, M, S, R) = V_d(y, M, S) + V_i(y) + V_e(y, R)$$

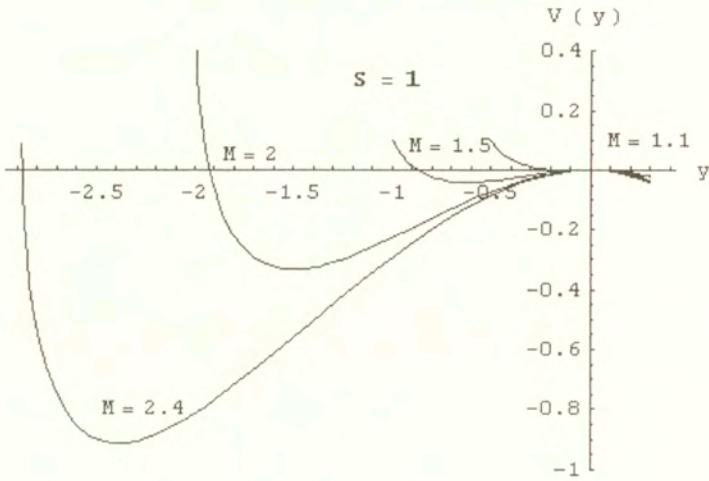


FIG. 1. Sagdeev potentials  $V(y)$  versus  $y$  for Mach numbers  $M = 1.1, 1.5, 2.0$  and  $2.4$  as  $S = 1$  (no electrons). Soliton amplitudes  $y_{\text{amp}}$  increase with increasing  $M$ .

and

$$V_d(y, M, S) = M^2 S \left( 1 - \left( 1 + \frac{2y}{M^2} \right)^{\frac{1}{2}} \right) > 0 \quad \text{for } y < 0,$$

$$V_i(y) = \frac{1}{3} \left( 1 - (1 - 2y)^{3/2} \right) < 0 \quad \text{for } y < 0,$$

$$V_e(y, S, R) = \frac{1 - S}{3R} \left( 1 - (1 + 2yR)^{3/2} \right) > 0 \quad \text{for } y < 0.$$

The inertial dust term for  $y < 0$  delivers the restoring force while thermal ions and electrons deliver wave pressures. We can expect negative potential solitons (rarefactive solitons, also called antisolitons). The case  $S = 1$  ( $S_e = 0$ ) represents the plasma where all the electrons are attached to the dust grains to form the two-component plasma. Whereas the case  $S = 0$  ( $S_e = 1$ ) is an electron-ion plasma.

The figures 1 to 4 show a number of Sagdeev potentials  $V(y, M, S, R)$  for a given set of parameters:  $M, S, R$ . The exhibited shape of  $V(y, \cdot)$  secures the existence of solitons.

The first figure depicts  $V(y, \cdot)$  for two-component dust-ion plasmas ( $S = 1$ ), when all electrons are collected by dust grains and the solitons exist in the anomalously large range of Mach number  $1 < M \leq 2.4$ . Soliton amplitudes increase with increasing  $M$  up to  $y_{\text{amp}} = 2.9$ .

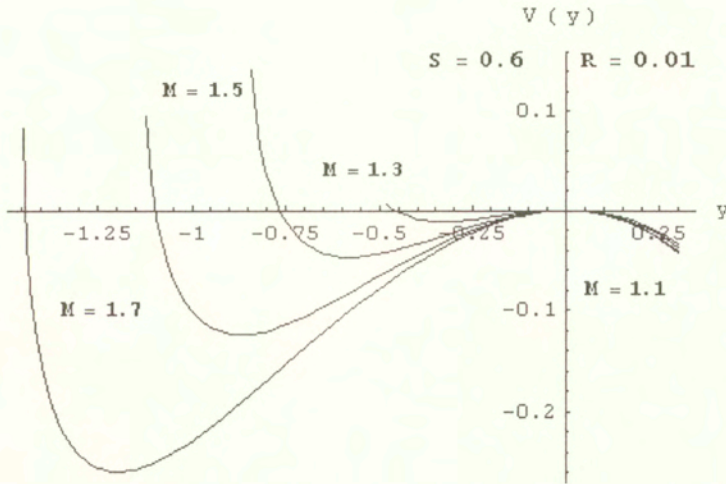


FIG. 2. Sagdeev potentials  $V(y)$  versus  $y$  for Mach numbers  $M = 1.1, 1.3$  and  $1.7$  as  $S = 0.6$ . Non-isothermal plasmas; hot electrons and cold ions  $R = T_i/T_e = 0.01$  (DIAW).

The case of three-component dusty plasmas with electron number  $S_e = 1 - S$ , where  $S = Z_d N_d / N_{0i} = 0.6$  and the low ion-electron temperature ratio  $R = T_i/T_e = 0.01$ , see Fig. 2, exhibits dust-ion-acoustic-wave (DIAW) solitons. The solitons exist in the Mach number range  $1 < M \leq 1.7$ .

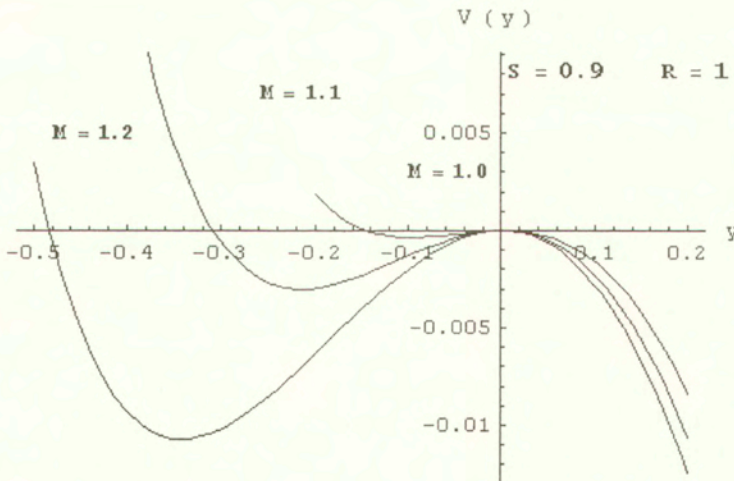


FIG. 3. Sagdeev potentials  $V(y)$  versus  $y$  for Mach numbers  $M = 1.0, 1.1$  and  $1.2$  as  $S = 0.9$ ,  $S_e = 0.1$ . Isothermal plasmas  $R = T_i/T_e = 1$  (DAW).

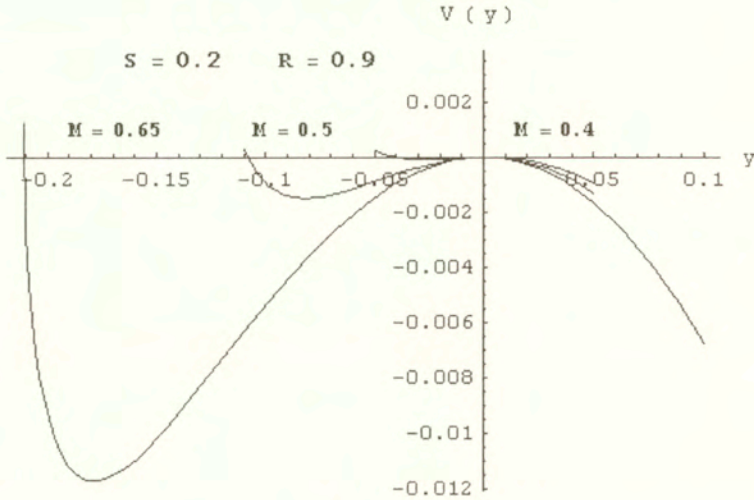


FIG. 4. Sagdeev potentials  $V(y)$  versus  $y$  for Mach numbers  $M = 0.4, 0.5$  and  $0.65$  as  $S = 0.2$ . Almost isothermal plasmas  $R = T_i/T_e = 0.9$  (DAW).

Dust-acoustic-wave (DAW) solitons for isothermal ions and electrons are shown in Fig. 3. The Mach number range of soliton existence is the smallest one and it amounts to  $M = 1 \div 1.2$ ,  $S = 0.9$ ,  $R = 1$ .

It is interesting to note that, if there are dusty plasmas with almost isothermal ions and electrons  $R = 0.9$  and the number density of dust is small enough  $S = S_d = 0.2$ , then solitons still exist but of smaller amplitudes and for  $M < 1$ , see Fig. 4. For such plasmas the Mach number is to be redefined. We conclude that even a small number density of dust  $Z_d N_d$  gives enough inertia to support negative solitons.

Figure 5 depicts the  $V(y)$ -insert, and the respective soliton  $y(\xi)$  in the case of three-component, non-isothermal plasma:  $M = 1.5$ ,  $S = 0.6$  and  $R = 0.01$  (DIAW). This soliton is computed on the basis of one of the Sagdeev potentials presented in Fig. 2. We note that if  $Z_d = 1000$  then for 3 dust grains, we would have 5000 ions and 2000 electrons — on the average. We can conclude that a small number of dust grains gives enough inertia to support negative solitons like in the case of isothermal plasmas.

Figure 6 exhibits the case of the rarefactive soliton for three-component plasma which is nearly isothermal  $R = 0.9$  (DAW),  $S = 0.2$  and  $M = 0.65$ . This soliton is computed on the basis of one of the Sagdeev potentials presented in Fig. 4. We note that if  $Z_d = 1000$  then for 1 dust grain, we would have 5000 ions and 4000 electrons — on the average.



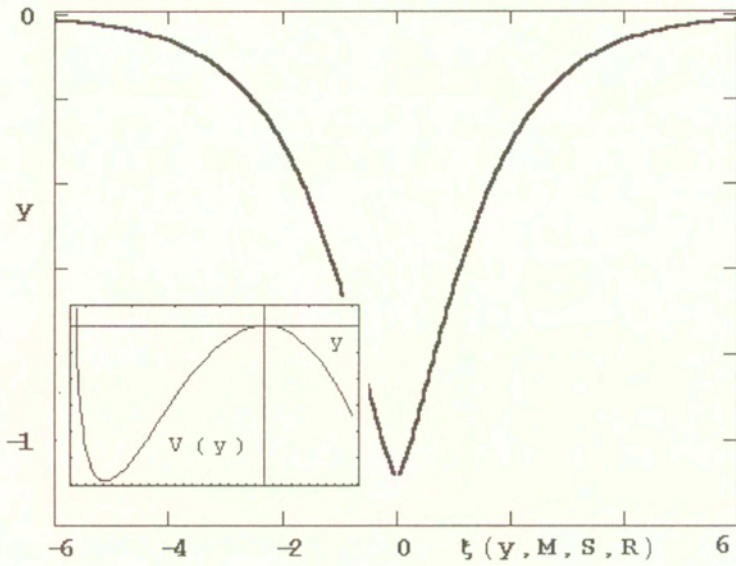


FIG. 5. Sagdeev potentials  $V(y)$ -insert and the respective soliton  $y(\xi)$ . Three-component plasma;  $M=1.5$ ,  $S=0.6$  and  $R=0.01$  (DIAW).

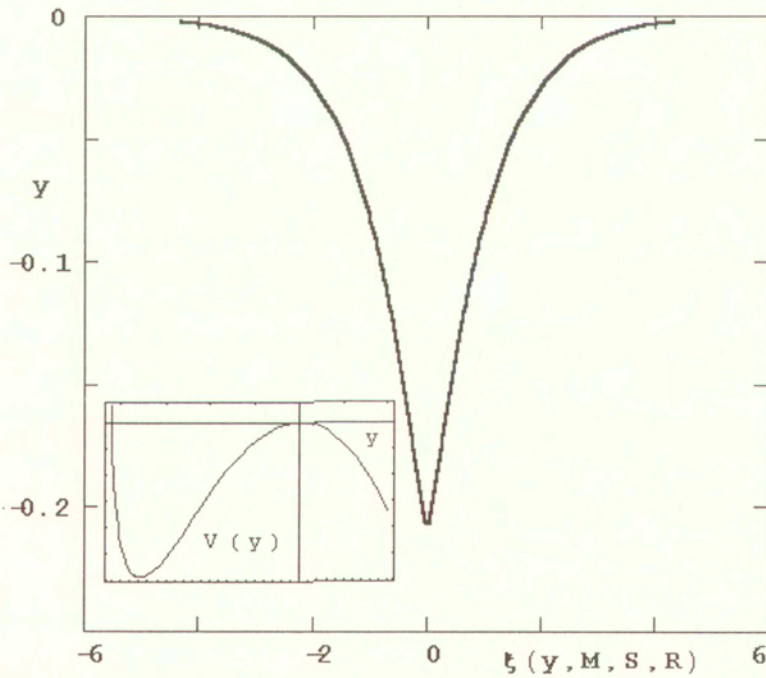


FIG. 6. Sagdeev potentials  $V(y)$ -insert and the respective soliton  $y(\xi)$ . Three-component plasma;  $M=0.65$ ,  $S=0.2$  and  $R=0.9$  (DIAW).

## 5. Conclusions

The initial-value-boundary problem was solved for “far field”, asymptotic solutions, solitons in the case of the fully nonlinear dusty plasma. Landau damping/wave-particle interactions have been excluded by choosing artificial equilibrium distributions. Velocity distributions can be evaluated and the calculation of all moments is possible, e.g. energy flow as well as energy of traveling solitary waves. The dispersion relations here obtained are the same as those in the fluid description of dusty plasmas.

Due to the presence of negatively charged dust grains:

- i) Only negative potential solitons (rarefactive solitons) can exist.
- ii) Linear waves and solitons can exist in dust-ion-acoustic-wave plasmas (DIAW  $R \ll 1$ , non-isothermal ions and electrons) as well as in dust-acoustic-wave plasmas (DAW  $R \simeq 1$ , isothermal ions and electrons).
- iii) The existence of DAW solitons in the case of small amount of dust grains in plasmas ( $S = S_d = 0.2$ ) is secured for the soliton speeds less than the dust-ion-acoustic speed  $c_s$ , which was defined in Sec. 4. The presence of the electron component ( $S < 1$ ) lowers the soliton amplitude as  $R$  is fixed and reduces the range of  $M$ , in which solitons can exist.

For small solitons ( $|y| \ll 1$  and  $S = 1$ ) there is a full resemblance between fluid, see [11], and kinetic solitons revealed in this paper. But in the case of fully nonlinear two-component plasmas,  $S = 1$ , the soliton shape, amplitudes and the soliton existence range of  $M$  are different in these two descriptions. The respective results for fluid description in case of three-component dusty plasmas,  $S < 1$ , are not known to the authors. We note that for DIAW and DAW, we have  $\alpha_i \ll U \ll \alpha_e$  and  $U \ll a_i \ll a_e$ , respectively, and hence the solitons considered here are subjected to insignificant electron and ion Landau damping. It justifies the Dirac delta accepted here and the Heaviside functions as the suitable equilibrium velocity distributions.

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## References

1. U. DE ANGELIS, *The physics of dusty plasmas*, Physica Scripta, **45**, 465–472, 1992.
2. C. K. GEORTZ, *Dusty plasmas in the solar system*, Reviews of Geophysics, **27**, 2, 271–292, May, 1989.
3. X. WANG and A. BHATTACHARJEE, *On a kinetic theory for strongly coupled dusty plasmas*, Phys. Plasmas, **3**, 4, 1189–1191, 1996.

4. A. J. TURSKEI and B. ATAMANIUK, *Far field solutions of Vlasov-Maxwell equations and wave-particle interactions*, J. Techn. Phys., **30**, 2, 147, 1989.
5. R. C. DAVIDSON, *Methods in nonlinear plasma theory*, Academic Press, N. York, 1972.
6. E. INFELD and G. ROWLANDS, *Nonlinear waves, solitons and chaos*, Cambridge Univ. Press, Cambridge 1992.
7. H. L. BERK and K. V. ROBERTS, *Numerical study of Vlasov's equation for special class of distribution functions*, Phys. Fluids, **10**, 1595–1597, 1967.
8. P. K. SHUKLA and V. P. SILIN, *Dust ion-acoustic waves*, Physica Scripta, **45**, 508, 1992.
9. R. L. MERLINO, A. BARKAN, C. THOMPSON and N. D'ANGELO, *Laboratory studies of waves and instabilities in dusty plasmas*, Phys. Plasmas, **5**, 5, 1607–1614, 1996.
10. R. Z. SAGDEEV and M. N. ROZENBLUTH, *Foundations of plasma physics* [in Russian], Vol.1, 2, Suppl., Moskwa, Energo-Atomizdat 1984.
11. A. MAMUN, R. CRAINS and P. SHUKLA, *Solitary potentials in dusty plasmas*, Phys. Plasmas, **3**, 2, 702, 1996.

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## Thermosolutal instability of Walters' rotating fluid (Model B') in porous medium

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THE THERMOSOLUTAL INSTABILITY of Walters' (Model B') fluid in porous medium is considered in the presence of uniform vertical rotation. For the case of stationary convection, the stable solute gradient and rotation have stabilizing effects on the system, whereas the medium permeability has a destabilizing (or stabilizing) effect on the system under certain conditions. The dispersion relation is also analysed numerically. It has also been shown that as rotation parameter increases, the stabilizing range of medium also increases. The kinematic viscoelasticity has no effect on the stationary convection. The stable solute gradient, rotation, porosity and kinematic viscoelasticity introduce oscillatory modes in the system, which did not occur in their absence. The sufficient conditions for the non-existence of overstability are also obtained.

**Key words:** Thermosolutal instability, Walters' (Model B') fluid, Rotation, Porous medium.

### 1. Introduction

A DETAILED ACCOUNT of the theoretical and experimental results of the onset of thermal instability (Bénard convection) in a fluid layer under varying assumptions of hydrodynamics and hydromagnetics has been given in the celebrated monograph by CHANDRASEKHAR [1]. The problem of thermohaline convection in a layer of fluid heated from below and subjected to a stable salinity gradient has been considered by VERONIS [2]. The physics is quite similar to the stellar case in that helium acts like salt in raising the density and in diffusing more slowly than heat. The conditions under which convective motions are important in stellar atmospheres are usually far removed from consideration of a single component fluid and rigid boundaries, and therefore it is desirable to consider a fluid acted on by a solute gradient and free boundaries. The problem of the onset of thermal instability in the presence of a solute gradient is of great importance be-

cause of its applications to atmospheric physics and astrophysics, especially in the case of the ionosphere and the outer layer of the atmosphere. The thermosolutal convection problems also arise in oceanography, limnology and engineering.

With the growing importance of non-Newtonian fluids in modern technology and industries, the investigations on such fluids are desirable. The WALTERS' [3] fluid (Model B') is one such fluid. In another study, SHARMA and KUMAR [4] have studied the steady flow and heat transfer of Walters' fluids (Model B') through a porous pipe of uniform circular cross-section with small suction. SHARMA and KUMAR [5], recently studied the stability of the plane interface separating two viscoelastic Walters' (Model B') fluids of uniform densities and found that for stable configuration, the system is stable or unstable under certain conditions.

In recent years, the investigation of flow of fluids through porous media has become an important topic due to the recovery of crude oil from the pores of reservoir rocks. A great number of applications in geophysics may be found in a recent book by PHILIPS [6]. When the fluid permeates through a porous material, the gross effect is represented by the Darcy law. As a result of this macroscopic law, the usual viscous term in the equation of Walters' fluid (Model B') motion is replaced by the resistance term  $\left[ -\frac{1}{k_1} \left( \mu - \mu' \frac{\partial}{\partial t} \right) \mathbf{q} \right]$ , where  $\mu$  and  $\mu'$  are the viscosity and viscoelasticity of the Walters' fluid,  $k_1$  is the medium permeability and  $\mathbf{q}$  is the Darcian (filter) velocity of the fluid. The problem of thermosolutal convection in fluids in porous medium is of great importance in geophysics, soil sciences, ground water hydrology and astrophysics. Generally, it is accepted that comets consist of a dust "snowball" made of a mixture of frozen gases which, in the process of their journey, changes from solid to gas and vice-versa. The physical properties of comets, meteorites and interplanetary dust strongly suggest the importance of porosity in astrophysical context (MCDONNELL [7]). In recent study, SHARMA *et al.* [8] studied the instability of streaming Walters' viscoelastic fluid B' in a porous medium. In many astrophysical situations, the effect of rotation on thermosolutal convection in a porous medium is also important. Relative to a large volume of published studies on this phenomenon in pure fluids, the thermosolutal convection in porous medium has received only attention, although it has interesting engineering applications: the migration of moisture through the air contained in fibrous insulation, grain storage installations, food processing and the underground spreading of chemical pollutants. Thermosolutal convection in porous medium is also of interest in geophysical systems, electrochemistry and metallurgy. A comprehensive review of the literature concerning thermosolutal convection in a fluid-saturated porous medium may be found in the book by NIELD and BEJAN [9].

Keeping in mind the importance of non-Newtonian fluids in geophysics, soil physics, ground water hydrology, modern technology and various applications

mentioned above, the thermosolutal instability of a Walters' (Model B') fluid in porous medium in the presence of uniform vertical rotation, has been considered in the present paper.

## 2. Formulation of the problem and perturbation equations

Here we consider an infinite, horizontal, incompressible Walters' (Model B') layer of thickness  $d$ , heated and soluted from below so that the temperatures, densities and solute concentrations at the bottom surface  $z = 0$  are  $T_0, \rho_0$  and  $C_0$ , and at the upper surface  $z = d$  are  $T_d, \rho_d$  and  $C_d$ , respectively, and that a uniform temperature gradient  $\beta (= |dT/dz|)$  and a uniform solute gradient  $\beta' (= |dC/dz|)$  are maintained. The gravity field  $\mathbf{g}(0, 0, -g)$  and a uniform vertical rotation  $\mathbf{\Omega}(0, 0, \Omega)$  act on the system. This fluid layer is assumed to be flowing through an isotropic and homogeneous porous medium of porosity  $\varepsilon$  and medium permeability  $k_1$ .

Let  $p, \rho, T, C, \alpha, \alpha', g$  and  $\mathbf{q}(u, v, w)$  denote, respectively, the fluid pressure, density, temperature, solute concentration, thermal coefficient of expansion, an analogous solvent coefficient of expansion, gravitational acceleration and fluid velocity. The equations expressing the conservation of momentum, mass, temperature, solute concentration and equation of state of Walters' (Model B') fluid are

$$(2.1) \quad \frac{1}{\varepsilon} \left[ \frac{\partial \mathbf{q}}{\partial t} + \frac{1}{\varepsilon} (\mathbf{q} \cdot \nabla) \mathbf{q} \right] = - \left( \frac{1}{\rho_0} \right) \nabla p + \mathbf{g} \left( 1 + \frac{\delta \rho}{\rho_0} \right) - \frac{1}{k_1} \left( v - v' \frac{\partial}{\partial t} \right) \mathbf{q} + \frac{2}{\varepsilon} (\mathbf{q} \times \mathbf{\Omega}),$$

$$(2.2) \quad \nabla \cdot \mathbf{q} = 0,$$

$$(2.3) \quad E \frac{\partial T}{\partial t} + (\mathbf{q} \cdot \nabla) T = \kappa \nabla^2 T,$$

$$(2.4) \quad E' \frac{\partial C}{\partial t} + (\mathbf{q} \cdot \nabla) C = \kappa' \nabla^2 C,$$

$$(2.5) \quad \rho = \rho_0 [1 - \alpha(T - T_0) + \alpha'(C - C_0)],$$

where the suffix zero refers to values at the reference level  $z = 0$  and in writing Eq. (2.1) use has been made of Boussinesq approximation. The kinematic viscosity  $\nu$ , the kinematic viscoelasticity  $\nu'$ , the thermal diffusivity  $\kappa$  and the solute diffusivity  $\kappa'$  are all assumed to be constants. Here  $E = \varepsilon + (1 - \varepsilon) \left( \frac{\rho_s c_s}{\rho_0 c_i} \right)$  is a constant and  $E'$  is a analogous to  $E$  but corresponding to solute rather than

heat.  $\rho_s, c_s$  and  $\rho_0, c_i$  stand for density and heat capacity of solid (porous matrix) material and fluid, respectively. The steady state solution is

$$(2.6) \quad \begin{aligned} \mathbf{q} &= (0, 0, 0), & T &= -\beta z + T_0, \\ C &= -\beta' z + C_0, & \rho &= \rho_0(1 + \alpha\beta z - \alpha'\beta' z). \end{aligned}$$

Here we use the linearized stability theory and the normal mode method. Consider a small perturbation on the steady state solution and let  $\delta p, \delta\rho, \theta, \gamma$  and  $\mathbf{q}(u, v, w)$  denote, respectively, the perturbation in pressure  $p$ , density  $\rho$ , temperature  $T$ , solute concentration  $C$  and velocity  $\mathbf{q}(0, 0, 0)$ . The change in density  $\delta\rho$ , caused mainly by the perturbations  $\theta$  and  $\gamma$  in temperature and concentration, is given by

$$(2.7) \quad \delta\rho = -\rho_0(\alpha\theta - \alpha'\gamma).$$

Then the linearized perturbation equations become

$$(2.8) \quad \frac{1}{\varepsilon} \frac{\partial \mathbf{q}}{\partial t} = -\frac{1}{\rho_0} (\nabla \delta p) - \mathbf{g}(\alpha\theta - \alpha'\gamma) - \frac{1}{k_1} \left( v - v' \frac{\partial}{\partial t} \right) \mathbf{q} + \frac{2}{\varepsilon} (\mathbf{q} \times \boldsymbol{\Omega}),$$

$$(2.9) \quad \nabla \cdot \mathbf{q} = 0,$$

$$(2.10) \quad E \frac{\partial \theta}{\partial t} = \beta w + \kappa \nabla^2 \theta,$$

$$(2.11) \quad E' \frac{\partial \gamma}{\partial t} = \beta' w + \kappa' \nabla^2 \gamma.$$

### 3. The dispersion relation

Analysing the disturbances into normal modes, we assume that the perturbation quantities are of the form

$$(3.1) \quad [w, \theta, \gamma, \zeta] = [W(z), \Theta(z), \Gamma(z), Z(z)] \exp(ik_x x + ik_y y + nt).$$

where  $k_x, k_y$  are the wave numbers along the  $x$ - and  $y$ -directions, respectively,  $k = \sqrt{(k_x^2 + k_y^2)}$  is the resultant wave number and  $n$  is the growth rate which is, in general, a complex constant.  $\zeta = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$  stands for the  $z$ -component of vorticity.

Expressing the coordinates  $x, y, z$  in the new unit of length  $d$  and letting  $a = kd, \sigma = \frac{nd^2}{v}, p_1 = \frac{v}{\kappa}, q = \frac{v}{\kappa'}, F = \frac{v}{d^2}, P_l = \frac{k_1}{d^2}$ , and  $D = \frac{d}{dz}$ , Eqs. (2.8)–(2.11), with the help of expression (3.1), in non-dimensional form become

$$(3.2) \quad \left[ \frac{\sigma}{\varepsilon} + \frac{1}{P_l}(1 - \sigma F) \right] (D^2 - a^2)W + \frac{ga^2d^2}{v}(\alpha\Theta - \alpha'\Gamma) - \frac{2\Omega d^3}{\varepsilon v}DZ = 0,$$

$$(3.3) \quad \left[ \frac{\sigma}{\varepsilon} + \frac{1}{P_l}(1 - \sigma F) \right] Z = \left( \frac{2\Omega d}{\varepsilon v} \right) DW,$$

$$(3.4) \quad (D^2 - a^2 - Ep_1\sigma)\Theta = - \left( \frac{\beta d^2}{\kappa} \right) W,$$

$$(3.5) \quad (D^2 - a^2 - E'q\sigma)\Gamma = - \left( \frac{\beta' d^2}{\kappa'} \right) W.$$

Consider the case where both boundaries are free as well as perfect conductors of both heat and solute concentrations. The case of two free boundaries is a little artificial but it enables us to find analytical solutions and to make some qualitative conclusions. The appropriate boundary conditions, with respect to which Eqs. (3.2)–(3.5) must be solved, are (CHANDRASEKHAR [1])

$$(3.6) \quad W = D^2W = 0, \quad \Theta = 0, \quad \Gamma = 0, \quad DZ = 0, \quad \text{at } z = 0 \text{ and } 1.$$

The case of two free boundaries, though a little artificial, is the most appropriate for stellar atmospheres (SPIEGEL [10]). Using the above boundary conditions, it can be shown that all the even order derivatives of  $W$  must vanish for  $z = 0$  and  $1$  and hence, the proper solution of  $W$  characterizing the lowest mode is

$$(3.7) \quad W = W_0 \sin \pi z,$$

where  $W_0$  is a constant.

Eliminating  $\Theta$ ,  $\Gamma$  and  $Z$  between Eqs. (3.2)–(3.5) and substituting the proper solution  $W = W_0 \sin \pi z$ , in the resultant equation, we obtain the dispersion relation

$$(3.8) \quad R_1 = \left( \frac{1+x}{x} \right) \left[ \frac{i\sigma_1}{\varepsilon} + \frac{1}{P} (1 - i\sigma_1 F) \right] (1+x + iEp_1\sigma_1) \\ + T_{A_1} \frac{(1+x + iEp_1\sigma_1)}{x \left( \frac{i\sigma_1}{\varepsilon} + \frac{1}{P} [1 - i\sigma_1 F] \right)} + S_1 \frac{(1+x + iEp_1\sigma_1)}{(1+x + iE'q\sigma_1)},$$

where

$$R_1 = \frac{g\alpha\beta d^4}{v\kappa\pi^4}, \quad S_1 = \frac{g\alpha'\beta'd^4}{v\kappa'\pi^4}, \quad T_{A_1} = \frac{4\Omega^2 d^4}{v^2\pi^4} = \left( \frac{2\Omega d^2}{v\pi^2} \right)^2, \\ x = \frac{a^2}{\pi^2}, \quad i\sigma_1 = \frac{\sigma}{\pi^2}$$



and

$$P = \pi^2 P_l.$$

Equation (3.8) is the required dispersion relation including the effects of rotation, medium permeability, kinematic viscoelasticity and stable solute gradient on the thermosolutal instability of Walters' (Model B') rotating fluid in a porous medium.

#### 4. The stationary convection

When the instability sets in as stationary convection, the marginal state will be characterized by  $\sigma = 0$ . Putting  $\sigma = 0$ , the dispersion relation (3.8) reduces to

$$(4.1) \quad R_1 = \frac{(1+x)^2}{xP} + PT_{A_1} \frac{(1+x)}{x} + S_1,$$

which expresses the modified Rayleigh number  $R_1$  as a function of the dimensionless wave number  $x$  and the parameters  $S_1, T_{A_1}$  and  $P$ . The parameter  $F$  accounting for the kinematic viscoelasticity effect vanishes for the stationary convection.

To investigate the effects of stable solute gradient, rotation and medium permeability, we examine the behaviour of  $\frac{dR_1}{dS_1}$ ,  $\frac{dR_1}{dT_{A_1}}$  and  $\frac{dR_1}{dP}$  analytically. Equation (4.1) yields

$$(4.2) \quad \frac{dR_1}{dS_1} = +1,$$

which implies that the stable solute gradient has a stabilizing effect on thermosolutal instability of Walters' (Model B') rotating fluid in a porous medium. The reverse solute gradient has a destabilizing effect on the system since then  $\frac{dR_1}{dS_1}$  becomes negative. Equation (4.1) also yields

$$(4.3) \quad \frac{dR_1}{dT_{A_1}} = \left( \frac{1+x}{x} \right) P.$$

The rotation, therefore, has always a stabilizing effect on the thermosolutal instability of Walters' (Model B') rotating fluid in a porous medium.

The dispersion relation (4.1) is analysed numerically. In Fig. 1,  $R_1$  is plotted against  $x$  for  $P = 10, T_{A_1} = 5; S_1 = 10$  (for curve 1),  $S_1 = 20$  (for curve 2) and  $S_1 = 30$  (for curve 3). The stabilizing role of the stable solute gradient is clear from the increase of the Rayleigh number with increasing stable solute gradient

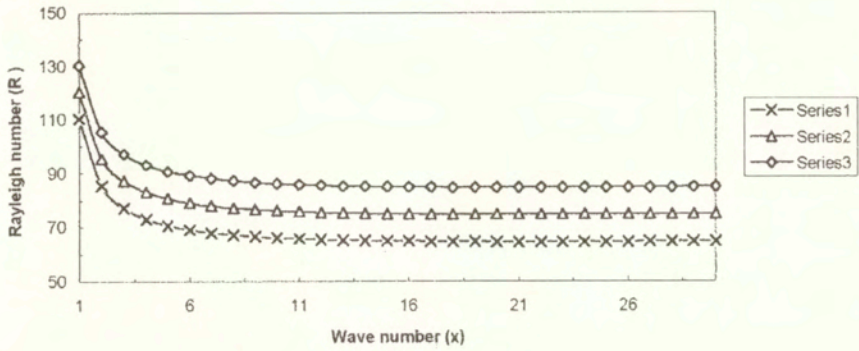


FIG. 1. The variation of Rayleigh number ( $R_1$ ) with wavenumber ( $x$ ) for  $P = 10, T_{A_1} = 5$ ;  $S_1 = 10$  (for curve 1),  $S_1 = 20$  (for curve 2), and  $S_1 = 30$  (for curve 3).

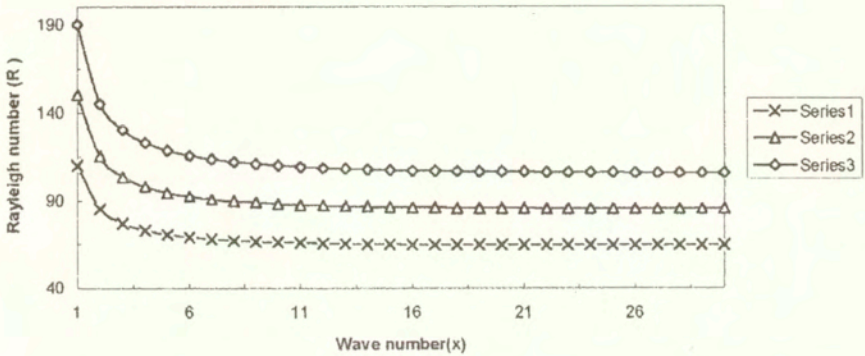


FIG. 2. The variation of Rayleigh number ( $R_1$ ) with wavenumber ( $x$ ) for  $P = 10, S_1 = 10$ ;  $T_{A_1} = 5$  (for curve 1),  $T_{A_1} = 7$  (for curve 2), and  $T_{A_1} = 9$  (for curve 3).

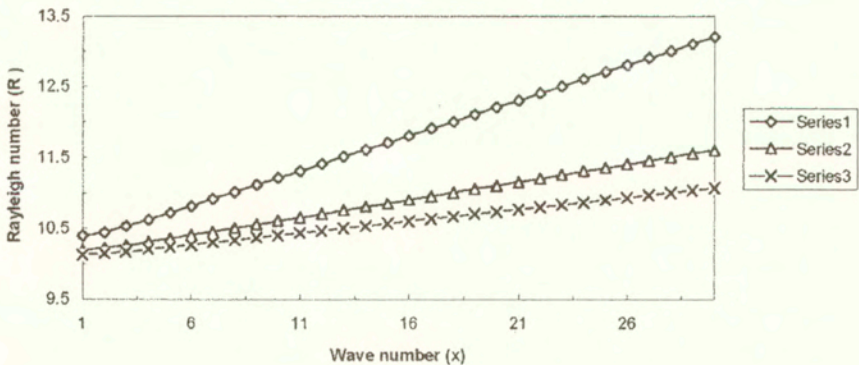


FIG. 3. The variation of Rayleigh number ( $R_1$ ) with wavenumber ( $x$ ) for  $S_1 = 10, T_{A_1} = 0$ ;  $P = 10$  (for curve 1),  $P = 20$  (for curve 2), and  $P = 30$  (for curve 3).

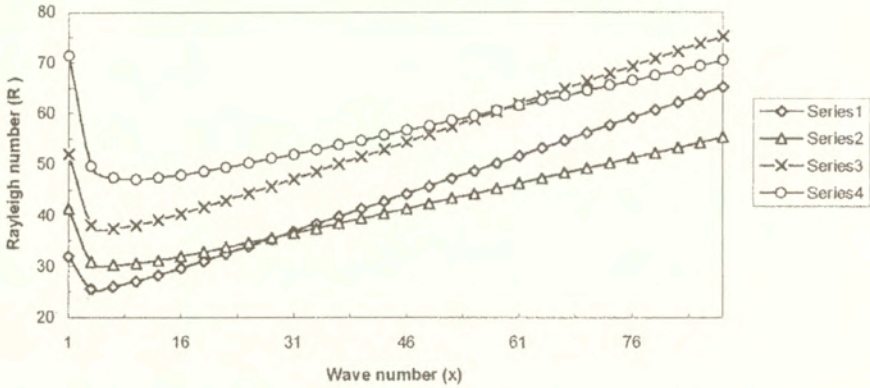


FIG. 4. The variation of Rayleigh number ( $R_1$ ) with wavenumber ( $x$ ) for  $S_1 = 10$ ;  $P = 2, T_{A_1} = 5$  (for curve 1),  $P = 3, T_{A_1} = 5$  (for curve 2),  $P = 2, T_{A_1} = 10$  (for curve 3) and  $P = 3, T_{A_1} = 10$  (for curve 4).

parameter  $S_1$  value. Figure 2 gives  $R_1$  plotted against  $x$  for  $P = 10, S_1 = 10$ ;  $T_{A_1} = 5$  (for curve 1),  $T_{A_1} = 7$  (for curve 2) and  $T_{A_1} = 9$  (for curve 3). Here we also find the stabilizing role of the rotation as the Rayleigh number increases with the increase in rotation parameter  $T_{A_1}$  value. It is evident from (4.1) that

$$(4.4) \quad \frac{dR_1}{dP} = -\left(\frac{1+x}{x}\right) \left[ \frac{1+x}{P^2} - T_{A_1} \right].$$

In the absence of rotation ( $T_{A_1} \rightarrow 0$ ),  $\frac{dR_1}{dP}$  is given by

$$(4.5) \quad \frac{dR_1}{dP} = -\frac{(1+x)^2}{xP^2},$$

which is always negative. The medium permeability, therefore, has a destabilizing effect on thermosolutal instability of Walters' (Model B') fluid in the absence of rotation. In the presence of rotation, the medium permeability has a destabilizing (or stabilizing) effect on the system if

$$(4.6) \quad T_{A_1} < (\text{or } >) \frac{1+x}{P^2}.$$

It has also been shown graphically that for

i)  $S_1 = 10, T_{A_1} = 0$  (i.e. in the absence of rotation);  $P = 10$  (for curve 1),  $P = 20$  (for curve 2) and  $P = 30$  (for curve 3); the medium permeability has always a destabilizing effect (Fig. 3).

ii)  $S_1 = 10, T_{A_1} = 5$ ;  $P = 2$ , (for curve 1),  $P = 3$ , (for curve 2); the medium permeability has a stabilizing influence for  $x < 29$ , and for  $x > 29$  it has a destabilizing effect (Fig. 4).

iii)  $S_1 = 10, T_{AI} = 10; P = 2$ , (for curve 3) and  $P = 3$ , (for curve 4); the medium permeability has a stabilizing influence for  $x < 59$  and for  $x > 59$  it has a destabilizing effect (Fig. 4).

In addition, it has also been shown that as the rotation parameter increases, the stabilizing range of medium permeability also increases (Fig. 4).

## 5. Stability of the system and oscillatory modes

Here we examine the possibility of oscillatory modes, if any, in stability problem due to the presence of kinematic viscoelasticity, stable solute gradient and rotation. Multiplying (3.2) by  $W^*$ , the complex conjugate of  $W$ , and using (3.3)–(3.5) together with the boundary conditions (3.6), we obtain

$$(5.1) \quad \left[ \frac{\sigma}{\varepsilon} + \frac{1}{P_l}(1 - \sigma F) \right] I_1 + \left( \frac{g\alpha' \kappa' a^2}{v\beta'} \right) [I_4 + E'q\sigma^* I_5] \\ + d^2 \left[ \frac{\sigma^*}{\varepsilon} + \frac{1}{P_l}(1 - \sigma^* F) \right] I_6 - \left( \frac{g\alpha\kappa a^2}{v\beta} \right) [I_2 + Ep_1\sigma^* I_3] = 0,$$

where

$$(5.2) \quad I_1 = \int_0^1 (|DW|^2 + a^2 |W|^2) dz, \quad I_2 = \int_0^1 (|D\Theta|^2 + a^2 |\Theta|^2) dz, \\ I_3 = \int_0^1 (|\Theta|^2) dz, \quad I_4 = \int_0^1 (|D\Gamma|^2 + a^2 |\Gamma|^2) dz, \\ I_5 = \int_0^1 (|\Gamma|^2) dz, \quad I_6 = \int_0^1 (|Z|^2) dz.$$

The integrals  $I_1, \dots, I_6$  are all positive definite. Putting  $\sigma = \sigma_r + i\sigma_i$  and equating the real and imaginary parts of equation (5.1), we obtain

$$(5.3) \quad \left[ \left( \frac{1}{\varepsilon} - \frac{F}{P_l} \right) I_1 + \frac{g\alpha' \kappa' a^2}{v\beta'} E'q I_5 + d^2 \left( \frac{1}{\varepsilon} - \frac{F}{P_l} \right) I_6 - \frac{g\alpha\kappa a^2}{v\beta} Ep_1 I_3 \right] \sigma_r \\ = - \left[ \frac{I_1}{P_l} + \frac{g\alpha' \kappa' a^2}{v\beta'} I_4 + \frac{d^2}{P_l} I_6 - \frac{g\alpha\kappa a^2}{v\beta} I_2 \right],$$

$$(5.4) \quad \left[ \left( \frac{1}{\varepsilon} - \frac{F}{P_l} \right) I_1 - \frac{g\alpha'\kappa'a^2}{v\beta'} E'qI_5 - d^2 \left( \frac{1}{\varepsilon} - \frac{F}{P_l} \right) I_6 + \frac{g\alpha\kappa a^2}{v\beta} Ep_1 I_3 \right] \sigma_i = 0.$$

It is evident from (5.3) that  $\sigma_r$  is positive or negative. The system is, therefore, stable or unstable. It is clear from (5.4) that  $\sigma_i$  may be zero or non-zero, meaning that the modes may be non-oscillatory or oscillatory. The oscillatory modes are introduced due to the presence of kinematic viscoelasticity, stable solute gradient and rotation, which were non-existent in their absence.

## 6. The case of overstability

Here we discuss the possibility of whether instability may occur as overstability. Since we wish to determine the Rayleigh number for the onset of instability via a state of pure oscillations, it suffices to find conditions for which (3.8) will admit the solutions with  $\sigma_1$  real.

If we equate real and imaginary parts of (3.8) and eliminate  $R_1$  between them, we obtain

$$(6.1) \quad A_2 c_1^2 + A_1 c_1 + A_0 = 0,$$

where we have put  $c_1 = \sigma_1^2$ ,  $b = 1 + x$  and

$$(6.2) \quad A_2 = b \left( 1 - \frac{\varepsilon F}{P} \right)^2 E'^2 q^2 \left[ b \left( 1 - \frac{\varepsilon F}{P} \right) + \frac{\varepsilon Ep_1}{p} \right],$$

$$(6.3) \quad A_1 = \left\{ \left[ \left( 1 - \frac{\varepsilon F}{P} \right) \left( 1 - \frac{2\varepsilon F}{P} \right) \right] b^4 + \left[ \frac{\varepsilon}{P} Ep_1 \left( 1 - \frac{2\varepsilon F}{P} + \frac{\varepsilon^2 F^2}{P^2} \right) \right] b^3 + \left[ \frac{\varepsilon^2}{P^2} E'^2 q^2 \left( 1 - \frac{\varepsilon F}{P} \right) \right] b^2 + \left[ \varepsilon^2 E'^2 q^2 \left( \frac{\varepsilon \overline{Ep_1}}{p^3} - T_{A_1} + \frac{\varepsilon F}{P} T_{A_1} \right) + \varepsilon(b-1)S_1 \left( 1 - \frac{\varepsilon F}{P} \right) \left( Ep_1 - E'q + \frac{\varepsilon F}{P} E'q \right) \right] b + \left[ \frac{\varepsilon^3}{P} T_{A_1} Ep_1 E'^2 q^2 \right] \right\},$$

$$(6.4) \quad A_0 = \varepsilon^2 b \left\{ \left[ \frac{1}{P^2} \left( 1 - \frac{\varepsilon F}{P} \right) \right] b^3 + \left[ \left( \frac{\varepsilon E p_1}{p^3} - T_{A_1} + \frac{\varepsilon F}{P} T_{A_1} \right) \right] b^2 \right. \\ \left. + \left[ \frac{\varepsilon}{P} T_{A_1} E p_1 \right] b + \left[ \frac{\varepsilon}{P^2} (b-1) S_1 (E p_1 - E' q) \right] b \right\}.$$

Since  $\sigma_1$  is real for overstability, both the values of  $c_1 (= \sigma_1^2)$  are positive. Equation (6.1) is quadratic in  $c_1$  and does not involve any of its roots to be positive if

$$(6.5) \quad E p_1 > E' q, \quad E p_1 > \frac{P^3 T_{A_1}}{\varepsilon} \quad \text{and} \quad \frac{F}{P} < \frac{1}{\varepsilon},$$

what implies

$$(6.6) \quad E' \kappa < E \kappa', \quad \kappa < \frac{\varepsilon v^3 d^2 E}{(2\Omega\pi)^2 k_1^3} \quad \text{and} \quad v < \frac{k_1}{\varepsilon}.$$

Thus  $E' \kappa < E \kappa'$ ,  $\kappa < \frac{\varepsilon v^3 d^2 E}{(2\Omega\pi)^2 k_1^3}$  and  $v < \frac{k_1}{\varepsilon}$  are the sufficient conditions for the nonexistence of overstability, the violation of which does not necessarily imply the occurrence of overstability.

## References

1. S. CHANDRASEKHAR, *Hydrodynamic and hydromagnetic stability*, Dover Publication, New York 1981.
2. G. VERONIS, *J. Marine Res.*, **23**, 1, 1965.
3. K. WALTERS, *Quart. Jour. Mech. Appl. Math.*, **15**, 76, 1962.
4. P. R. SHARMA and H. KUMAR, *Proc. Nat. Acad. Sci. India*, **65(A)**, I 75, 1995.
5. R. C. SHARMA and P. KUMAR, *Czech. J. Phys.*, **47**, 197, 1997.
6. O. M. PHILIPS, *Flow and reaction in permeable rocks*, Cambridge University Press, Cambridge 1991.
7. J. A. M. MCDONNELL, *Cosmic dust*, John Wiley and Sons, Toronto 1978, p. 330.
8. R. C. SHARMA, SUNIL and S. CHAND, *Czech J. Phys.*, **48**, 1, 1998.
9. D. A. NIELD and A. BEJAN, *Convection in porous medium*, Springer, 1992.
10. E. A. SPIEGEL, *Astrophys. J.*, **141** 1068, 1965.

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## Localisation of deformation as a local quasi-static/dynamic transition<sup>(1)</sup>

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THE PROBLEM OF THE MODELLING of the strain localisation in elasto-visco-nonlinear materials and structures submitted to so-called “quasistatic” loadings is here considered. Unlike the usual approaches, which suppose that the localisation band remains in (quasi)static equilibrium, it is here assumed that **localisation is essentially a dynamic phenomenon**, even if the external loadings are “quasistatic”. This means that the localisation criterion proposed is also a “local loss of (quasi)staticity” criterion. As soon as the criterion is verified, the dynamic problem is treated (at least locally) instead of the (quasi)static one.

### 1. Introduction

LOCALISATION OF DEFORMATION is an instability process, accompanying inelastic deformation, widely observed under quasi-static as well as dynamic loading conditions. This mechanism is characterised by the transition from a diffuse mode of deformation to a localised mode associated with the formation of narrow zones in which strains quickly and highly concentrate. Besides, once such bands appear, they persist and under favourable circumstances become immediate precursor to failure. This phenomenon is followed either by the emergence of a macroscopic crack leading to fracture (brittle materials like rocks and concretes) or by a softening regime ending also by fracture events (ductile materials like steels).

Properly modelling the initiation and development of such a material instability could constitute one of the missing links between continuum mechanics framework and fracture mechanics framework.

For a non-viscous material, modelled as rate-independent<sup>(2)</sup>, considered to

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<sup>(2)</sup>Referred to in this paper as elasto-nonlinear materials or ENL.

deform quasi-statically, the usual mathematical method employed to predict the onset of strain localisation is the bifurcation analysis. This approach, within a theoretical framework due to HADAMARD [11], is based on the requirement of traction continuity and a jump of the velocity gradient across a singularity surface limiting the band. These conditions lead to the well-known condition for the singularity of the associated acoustic tensor resulting from a double contraction of the dissipative branch of the tangent operator with the normal to the band (RICE [20]). The vanishing of the determinant of the acoustic tensor at the onset of localisation is connected with the loss of ellipticity of the local rate equilibrium equations and with the occurrence of stationary acceleration waves in the solid.

As a consequence of the loss of uniqueness of the mechanical response, a fundamental difficulty in numerical simulations appears. For grid based methods such as finite elements or finite differences, the width of the band of localisation depends on the size of the elements meshing the zone where the instability is detected. This pathological dependence induces the use of regularisation techniques based either on the kinematics of localisation phenomenon at the elementary level (finite element regularisation method (ORTIZ *et al.* [17])) or by incorporating an internal length scale or a higher order continuum structure in constitutive relations (PIJAUDIER-CABOT and BAZĄNT [19], ZBIB and AIFANTIS [21]).

For a viscous material, modelled as rate-dependent<sup>(3)</sup>, the application of the bifurcation analysis provides a criterion never fulfilled. The tangent operator coincides with the elastic stiffness tensor which remains positive definite. The uniqueness of the solution of the local rate (or incremental) constitutive equations is guaranteed and the initial boundary-value problem remains well posed.

Yet, experimental tests establish the existence of localisation patterns for viscous materials. Moreover, when numerical simulations are performed, even if bifurcation is precluded, by localisation instability is observed; mesh sensitivity is either reduced for slightly viscous materials or suppressed with higher viscosity (FOREST and CAILLETAUD [13]). This apparent paradox may be understood by the fact that finite element method constraints require the use of a pseudo-tangent operator, instead of the real one, allowing the bifurcation of the numerical (incremental) problem in a localised mode. Besides, it is just numerical interpretation that does not provide any answer to defining a localisation criterion for viscous materials.

To remove this difficulty, changes in the mode of deformation may be detected by employing a linear perturbation stability analysis. At any stage of the postulated deformation process, an infinitesimal exponential disturbance is superimposed onto the regular solution. The homogeneous solution is said to be unstable if the analysis reveals the growth of an admissible perturbation. This method has been employed first in one-dimensional problems (CLIFTON [7] and

<sup>(3)</sup>Referred to in this paper as elasto-visco-nonlinear materials or EVNL.



BAI [2]), extended to three-dimensional problems neglecting elasticity (ANAND *et al.* [1]), generalised to three dimensional problems with the effect (among others) of elasticity (DOBOVŠEK and MORAN [9], CANO [4]).

This kind of analysis, as compared to a full non linear study, because of linearisation, predicts only the necessary conditions for the onset of an instability and fails to forecast the evolution of localisation during an extended period of time. The rate of growth value appears in a characteristic stability equation and localisation is detected when this value is sufficiently large compared with the variation of the homogeneous solution (MOLINARI [16]). As noticed by CANO [4], a question remains for qualifying this rate of growth: the highest value admissible seems to be an upper bound to localisation.

In this paper, the aim is to establish an alternative criterion for EVNL materials and structures submitted to quasi-static loadings, also based on a perturbation stability analysis, but grounded on the hypothesis that even for so-called quasi-static loadings localisation is an intrinsically local dynamic phenomenon.

A large class of EVNL materials is first presented in Sec. 2. The initial-boundary value problem associated is then considered in Sec. 3. Next in Sec. 4, we propose to quantify the notion of quasi-staticity: as soon as the inertia terms of the dynamic problem exceed a critical value, the problem to be considered is no longer the quasi-static problem but, at least locally, the dynamic one. This value is then coupled to a critical kinetic power reached at the incipience of localisation. To let the viscosity effects appear, a perturbation stability analysis of the acceleration boundary-value problem is carried out in Sec. 5, which provides a characteristic stability equation function of the rate of growth of the perturbation. At last in Sec. 6, by considering the instability of the acceleration problem corresponding to the reach of the critical value of inertia terms, i.e. by choosing the lowest rate of growth value violating the quasistaticity condition, a loss of quasistaticity/localisation criterion is established.

## 2. Constitutive equations

Attention is focused hereafter on a large class of constitutive equations, established under the small strain framework, within the first gradient theory and under isothermal conditions. We admit the reversible behaviour of the rate-dependent materials considered in this paper (instantaneous elasticity) to be determined by a potential free energy  $w(\epsilon, \alpha)$ , function of the linearised strain  $\epsilon$ , at most quadratic to preserve linear elasticity, and a given number of internal variables  $\alpha_p$ . These internal variables may be scalars, vectors or tensors; for simplicity, they will be denoted as  $\alpha$ .

Thereafter, the stress tensor  $\sigma$  (connected with  $\epsilon$ ) and the thermodynamic forces  $\mathbf{A}$  connected with the internal variables  $\alpha$ , are given by the state laws:

$$(2.1) \quad \boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\epsilon}}(\boldsymbol{\epsilon}, \boldsymbol{\alpha}), \quad \mathbf{A} = -\frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\epsilon}, \boldsymbol{\alpha}),$$

As far as the material irreversible behaviour is concerned, we define a convex reversibility domain limited by the criterion  $f = 0$  (in the space of forces) where  $f$  (the yield function) is a function of  $\mathbf{A}$ , eventually parameterised by  $\boldsymbol{\alpha}$ , i.e.  $f = f(\mathbf{A}; \boldsymbol{\alpha})$ ; inside this domain no irreversibility is possible.

We also assume the existence of a pseudo-potential  $g(\mathbf{A}; \boldsymbol{\alpha})$  from which the evolution laws, assuming  $\dot{\boldsymbol{\alpha}}$ -normality, follow:

$$(2.2) \quad \dot{\boldsymbol{\alpha}} = \Lambda \frac{\partial g}{\partial \mathbf{A}},$$

where  $\Lambda$  is called pseudo-visco-nonlinear multiplier. The elasto-visco-nonlinear class of models considered here is an extension of the elasto-viscoplastic materials first proposed by PERZYNA [18]. The multiplier is given by:

$$(2.3) \quad \Lambda = \frac{1}{\eta} \langle \Phi(f) \rangle^N,$$

where  $\langle \rangle$  are the Macauley brackets ( $\langle x \rangle = \text{Max}(x, 0)$ ),  $\eta$  is a relaxation time. Common choices for the function  $\Phi$  are:

$$(2.4) \quad \begin{array}{ll} \Phi(f) = \frac{f}{K} & \Phi(f) = \left(\frac{f}{K}\right)^N \\ \text{linear form} & \text{power law} \end{array},$$

where  $N$  is a dimensionless viscosity exponent (Norton's coefficient) and  $K$  a resistance coefficient depending on the material mechanical state, say  $K = K(\boldsymbol{\epsilon}, \boldsymbol{\alpha})$ . In the sequel, the power law form of (2.4) is assumed.

By differentiating (2.1) with respect to time, one obtains the rate constitutive equations:

$$(2.5) \quad \dot{\boldsymbol{\sigma}} = \mathbf{E}^w : \dot{\boldsymbol{\epsilon}} + \mathbf{B}(\boldsymbol{\epsilon}, \boldsymbol{\alpha}).$$

$\mathbf{E}^w = \frac{\partial^2 w}{\partial \boldsymbol{\epsilon} \partial \boldsymbol{\epsilon}}$  is the elastic stiffness tensor and  $\mathbf{B}$  is a function of non rate terms:

$$(2.6) \quad \mathbf{B}(\boldsymbol{\epsilon}, \boldsymbol{\alpha}) = -\frac{1}{\eta} \langle \frac{f}{K} \rangle^N \boldsymbol{\chi}^w(\boldsymbol{\epsilon}, \boldsymbol{\alpha}) \bullet \frac{\partial g}{\partial \mathbf{A}}(\mathbf{A}(\boldsymbol{\epsilon}, \boldsymbol{\alpha}), \boldsymbol{\alpha}).$$

The tensor  $\boldsymbol{\chi}^w$  is given by:

$$(2.7) \quad \boldsymbol{\chi}^w = -\frac{\partial^2 w}{\partial \boldsymbol{\epsilon} \partial \boldsymbol{\alpha}}.$$

### 3. Static, quasi-static and dynamic considerations

Let us consider a structure taking up an arbitrary opened domain  $\Omega$  in  $\mathbf{R}^3$  which constitutive material belongs to the general class previously described. This structure, during the time interval  $[0, T]$ , where  $T > 0$ , is subjected to body forces  $\mathbf{f}^g(\mathbf{x}, t)$  and its boundary  $\partial\Omega$  subjected to surface tractions  $\mathbf{F}^g(\mathbf{x}, t)$  on the part  $\partial\Omega_1$ , and to given displacements  $\mathbf{u}^g(\mathbf{x}, t)$  on  $\partial\Omega_2$ , so that  $\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$  and  $\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$ .

One has to solve the nonlinear dynamical initial and boundary value problem  $(P_g)$ :

Find  $\mathbf{u}(\mathbf{x}, t)$ ,  $\boldsymbol{\sigma}(\mathbf{x}, t)$ , and  $\boldsymbol{\alpha}(\mathbf{x}, t)$  defined for  $\mathbf{x} \in \Omega$  and  $0 \leq t \leq T$  satisfying:

$$(3.1) \quad (P_g) \quad \left\{ \begin{array}{l} \bullet \text{ motion equations: } \operatorname{div} \boldsymbol{\sigma} + \mathbf{f}^g = \rho \ddot{\mathbf{u}} \quad \text{in } \Omega \times [0, T], \\ \bullet \text{ constitutive equations given in Sec. 2,} \\ \bullet \text{ compatibility conditions:} \\ \quad \boldsymbol{\epsilon}(\mathbf{u}) = \frac{1}{2}(\operatorname{grad} \mathbf{u} + (\operatorname{grad} \mathbf{u})^T) \quad \text{in } \Omega \times [0, T], \\ \bullet \text{ boundary conditions: } \begin{cases} \mathbf{u} = \mathbf{u}^g & \text{on } \partial\Omega_2 \times [0, T] \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{F}^g & \text{on } \partial\Omega_1 \times [0, T] \end{cases}, \\ \bullet \text{ initial conditions: } \begin{cases} \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}^0 & \text{in } \Omega \\ \boldsymbol{\alpha}(\mathbf{x}, 0) = \boldsymbol{\alpha}^0 & \text{in } \Omega \end{cases}, \end{array} \right.$$

where  $\mathbf{n}$  is the outward unit normal to  $\partial\Omega$ .

The presence in  $(3.1)_1$  of the inertia terms, say  $\rho \ddot{\mathbf{u}}$  qualifies  $(P_g)$  to be the dynamic problem.

When the structure  $\Omega$  undergoes **quasi-static loadings**, i.e. when the loadings are slow with respect to the time dimension, it is usually assumed that inertia terms in Eq.(3.1)<sub>1</sub> may be neglected. Then a new problem, say  $(P)$ , is to be treated, in which  $(3.1)_1$  becomes:

$$(3.2) \quad \operatorname{div} \boldsymbol{\sigma} + \mathbf{f}^g = 0, \quad \text{quasi-static equilibrium conditions.}$$

Actually,  $(P)$  is the **static problem** and coincides with the quasi-static problem as an approximation of  $(P_g)$ .

In the same way, for problems of higher orders undergoing quasi-static loadings, equilibrium equations for both the rate problem  $(\dot{P})$  and the acceleration problem  $(\ddot{P})$  are:

$$(3.3) \quad \begin{aligned} \operatorname{div} \dot{\boldsymbol{\sigma}} + \dot{\mathbf{f}}^g &= 0, \\ \operatorname{div} \ddot{\boldsymbol{\sigma}} + \ddot{\mathbf{f}}^g &= 0. \end{aligned}$$

#### 4. A quantitative definition of the quasi-staticity notion linked to an energetic measure at the onset of localisation

##### 4.1. A condition for the loss of quasi-staticity

Following Sec. 3, one must say that no quantitative definition of the quasi-staticity is usually defined, i.e. a fundamental question is addressed:

When does the problem ( $P$ ) cease to be quasi-static?

or equivalently, when should the general problem ( $P_g$ ) be considered instead of ( $P$ )? Let us point out that external loadings are considered to stay quasi-static.

DEFINITION: *The solution  $\mathbf{u}(\mathbf{x}, t)$  of ( $P_g$ ) will be described as quasi-static when the r.h.s. of the balance of linear momentum equation (3.1)<sub>1</sub> is lower than a critical norm, say  $\gamma_{\text{crit}}$ :*

$$(4.1) \quad \rho |\ddot{\mathbf{u}}(\mathbf{x}, t)| < \gamma_{\text{crit}} \quad \forall \mathbf{x} \forall t.$$

*If not, the solution of ( $P_g$ ) is qualified as dynamic.*

By opposition to the usual hypothesis for qualifying an initial-boundary problem as quasi-static (practically the latter is treated as static, i.e.  $\operatorname{div} \boldsymbol{\sigma} + \mathbf{f}^g = 0$ ), no hypothesis is formulated *a priori* for acceleration, qualified *a posteriori*.

As soon as the inequality (4.1) is not satisfied, the general problem should be solved. But, in fact, we may imagine that in a substructure  $\Omega_i$  of  $\Omega$  the solution of the boundary value subproblem violates the condition of quasi-staticity while in the other subdomains composing  $\Omega$  the inequality (4.1) is still satisfied. Then, the problem should be, at least in the substructure  $\Omega_i$ , solved as dynamic.

##### 4.2. How to connect $\gamma_{\text{crit}}$ to the occurrence of localisation?

Localisation is considered as being an intrinsically dynamic local phenomenon: this idea is akin to observations of LEROY [14] in finite-element simulations of a Von Mises viscous solid under plane strain tensile loading: “*shear-band failure mode can be defined as a continuous increase in strain rate in a band of decreasing thickness. This observation also indicates that localization should be interpreted as a dynamic process even in a kinematically controlled experimental set-up*”.

One suggests, at a given displacement rate  $|\dot{\mathbf{u}}|$ , that  $\gamma_{\text{crit}}$  may be linked to a critical kinetic power at localisation ( $\kappa_{\text{crit}}$ ), experimentally accessible. This

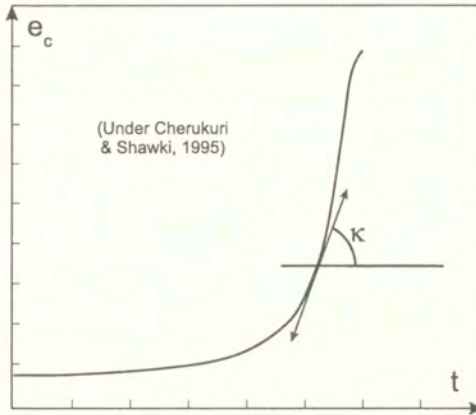


FIG. 1. Evolution of the kinetic energy.

suggestion coincides with the hypothesis of CHERUKURI and SHAWKI [5] for their localisation work under dynamic loadings.

A “pseudo-local” kinetic energy  $e_c$  (“pseudo” because linked to  $\rho_0$ , initial density) and its associated kinetic power  $\dot{e}_c$  are defined first:

$$(4.2) \quad e_c = \frac{1}{2} \rho_0 \dot{\mathbf{u}} \cdot \dot{\mathbf{u}},$$

$$\dot{e}_c = \rho_0 \dot{\mathbf{u}} \cdot \ddot{\mathbf{u}} \leq \rho_0 |\dot{\mathbf{u}}| |\ddot{\mathbf{u}}|.$$

In order to link the parameter  $\gamma_{crit}$  with experimental evidences, let us consider a sample. Whenever no localisation, its response for its gauge length is characteristic of the material behaviour. The local kinetic energy could be estimated by experimental procedures (e.g. by infrared and speckle image processing techniques, see CHRYSOCHOOS *et al.* [6]) because:

$$(4.3) \quad e_c \approx \frac{\rho_0 l_0}{2V_0} \int_S \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} dS,$$

where  $S$  is the gauge length section, where the measures are made. An eventual critical kinetic power  $\kappa_{crit}$  at the localisation onset follows (see Fig. 1):

$$(4.4) \quad \dot{e}_c = \kappa_{crit}.$$

If  $\kappa_{crit}$  is admitted being a material characteristic, independent of the loading path at a given  $|\dot{\mathbf{u}}|$ , linking loss of quasi-staticity (violation of Eq.(4.1)) and localisation (Eq.(4.4)) one may write:

$$(4.5) \quad \gamma_{crit} = \rho (\rho_0 |\dot{\mathbf{u}}|)^{-1} \kappa_{crit} \approx \kappa_{crit} |\dot{\mathbf{u}}|^{-1},$$

this latter approximation being valid in the small strain framework.

## 5. Stability analysis

### 5.1. Description of the linear perturbation method

The essence of the linear perturbation stability analysis is to determine under which conditions, if the homogeneous solution of the boundary value problem is disturbed by a small perturbation, this perturbation is likely to decay or grow while the constitutive and momentum balance equations are still satisfied.

The characteristic stability equation obtained is commonly a function of the rate of growth of the disturbance. A zero root corresponds to a loss of stability of the homogeneous solution. The onset of instability corresponds to a zero value (absolute instability), but such “*an unstable mode can sometimes grow very slowly and therefore be overcome by another mode appearing later with a much higher rate of growth*” (DUDZINSKI and MOLINARI [10]).

In the context of localisation instability process, its utilisation requires the following assumptions:

- in its current configuration ( $t_0$ ), the structure  $\Omega$  is supposed to be homogeneous, homogeneously deformed and evolving slowly.
- the perturbation superimposed is a displacement rate one (or a displacement one).
- the disturbance chosen has a form of an exponential wave that may lead to a localised deformation mode:

$$\dot{\mathbf{u}} = \dot{\mathbf{u}}^0 + \Delta\dot{\mathbf{u}}(\mathbf{x}, t),$$

with  $\Delta\dot{\mathbf{u}}(\mathbf{x}, t) = \delta\dot{\mathbf{u}} \exp(ik\mathbf{x} \cdot \mathbf{n} + \omega(t - t^0))$ ; thus  $\Delta\dot{\boldsymbol{\epsilon}} = ik(\Delta\dot{\mathbf{u}} \otimes \mathbf{n})_s = (\mathbf{g} \otimes \mathbf{n})_s$ , where  $\delta\dot{\mathbf{u}}$  is the initial perturbation amplitude,  $\mathbf{n}$  the propagation direction (unit) that determines the orientation of the localisation surface,  $\omega$  the rate of growth,  $\mathbf{k} = k\mathbf{n}$  the wave vector. The relative orientation of  $\mathbf{n}$  and  $\mathbf{g}$  informs about the type of localisation.

- the perturbation amplitude is sufficiently small to allow the study of the “first-order problem” (linearisation).

- the results of the linear stability analysis are valid only for perturbations whose evolutions are rapid compared to variations of the homogeneous solution. MOLINARI [16] suggests to study the rate of growth of a relative perturbation defined as the disturbance divided by the corresponding homogeneous solution. Implicitly, two time scales are introduced, the former linked to the perturbation (i.e. “small”), the latter macroscopic (i.e. “large”) linked to the regular solution (BATAILLE and KESTIN [3]). These hypotheses allow to consider the coefficients in the linearised perturbed equations to be constant.

Furthermore, it is usually assumed that the perturbation for the other field quantities takes the same exponential form (e.g. [9], [4]), that is to say:  $\dot{\alpha} = \dot{\alpha}^0 + \Delta\dot{\alpha}(\mathbf{x}, t)$  with  $\Delta\dot{\alpha}(\mathbf{x}, t) = \delta\dot{\alpha} \exp(ik\mathbf{x} \cdot \mathbf{n} + \omega(t - t^0))$ . As a consequence, all the disturbed variables present the same rate of growth and stability conditions for the problem ( $\dot{P}$ ) are explored.

## 5.2. Stability of the local acceleration problem

As previously recalled, in the classical linear stability analysis, internal variables are supposed to be perturbed in the same exponential form and with the same rate of growth as the displacement rate (or displacement) perturbation. This assumption is quite disconcerting: since these variables are internal and consequently not measurable by direct observations (LEMAITRE and CHABOCHE [12]), how to justify the way they are perturbed?

In this paper, we do not use the classical linear stability analysis: instead of postulating the way the internal variables are perturbed, we let them evolve freely so that they could take into account the change in displacement rate. Following this assumption, the rate (or incremental) problem ( $\dot{P}$ ), reflecting the instantaneous material response, is considered as stable. Suggesting (as DÉSOYER *et al.* [8]) that the response to a loading of a rate-dependent material is delayed compared to the response obtained for a rate-independent material, one naturally considers the local acceleration problem ( $\ddot{P}$ ).

**5.2.1. Momentum balance acceleration equation.** The acceleration problem ( $\ddot{P}$ ) is written, in the absence of body forces by (3.3)<sub>2</sub>, as:

$$(5.1) \quad \text{div } \ddot{\sigma} = 0.$$

Eq.(5.1) requires the expression of  $\ddot{\sigma}$  to be formulated, which is done by time derivation of Eq.(2.5):

$$(5.2) \quad \ddot{\sigma} = \mathbf{E}^w : \ddot{\epsilon} - V(\epsilon, \alpha) : \dot{\epsilon} + \mathbf{C}(\epsilon, \alpha),$$

where  $\mathbf{V}$  and  $\mathbf{C}$  are non-rate terms:

$$(5.3) \quad \mathbf{C}(\epsilon, \alpha) = \frac{1}{\eta} \left\langle \frac{f}{K} \right\rangle^N \frac{\partial \mathbf{B}}{\partial \alpha} \bullet \frac{\partial g}{\partial \mathbf{A}} \quad \text{and}$$

$$\mathbf{V}(\epsilon, \alpha) = -\frac{1}{\eta} \left\langle \frac{f}{K} \right\rangle^N \frac{\partial \mathbf{E}^w}{\partial \alpha} \bullet \frac{\partial g}{\partial \mathbf{A}} - \frac{\partial \mathbf{B}}{\partial \epsilon}.$$

Using Eq.(2.6), expression of  $\mathbf{V}$  is more precisely given by:

$$(5.4) \quad \eta \mathbf{V}(\boldsymbol{\epsilon}, \boldsymbol{\alpha}) = \begin{cases} \frac{N}{K} < \frac{f}{K} >^{N-1} \left[ \left( \boldsymbol{\chi}^w \bullet \frac{\partial g}{\partial \mathbf{A}} \right) \otimes \left( \frac{\partial f}{\partial \mathbf{A}} \bullet \boldsymbol{\chi}^w - \frac{f}{K} \frac{\partial K}{\partial \boldsymbol{\epsilon}} \right) \right], \\ - < \frac{f}{K} >^N \left[ \frac{\partial \mathbf{E}^w}{\partial \boldsymbol{\alpha}} \bullet \frac{\partial g}{\partial \mathbf{A}} - \boldsymbol{\chi}^w \bullet \frac{\partial^2 g}{\partial \mathbf{A} \partial \mathbf{A}} \bullet \boldsymbol{\chi}^w - \left( \frac{\partial \boldsymbol{\chi}^w}{\partial \boldsymbol{\epsilon}} \right)^T \bullet \frac{\partial g}{\partial \mathbf{A}} \right], \end{cases}$$

where  $\bullet$  denotes the inner product on tensors of required orders.

**5.2.2. Perturbation stability analysis.** The problem is considered to be initially quasi-static, with a structure undergoing quasi-static loadings, initially homogeneous, homogeneously deformed. The homogeneous or regular solution is denoted by  $(\mathbf{u}^0, \boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0)$  at time  $t^0$ .

A perturbation stability analysis is then conducted involving a rate displacement perturbation  $\Delta \dot{\mathbf{u}}$  of the solution  $\dot{\mathbf{u}}^0$  of  $(\dot{P})$ :

$$(5.5) \quad \forall t \geq t^0 \quad \begin{cases} \dot{\mathbf{u}} = \dot{\mathbf{u}}^0 + \Delta \dot{\mathbf{u}}, \\ \Delta \dot{\mathbf{u}}(\mathbf{x}, t) = \delta \dot{\mathbf{u}} \exp(ik\mathbf{x} \cdot \mathbf{n} + \omega(t - t^0)). \end{cases}$$

In the perturbed state equation Eq.(5.2) becomes:

$$(5.6) \quad \ddot{\boldsymbol{\sigma}}(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0, \dot{\boldsymbol{\epsilon}}^0 + \Delta \dot{\boldsymbol{\epsilon}}, \ddot{\boldsymbol{\epsilon}}^0 + \Delta \ddot{\boldsymbol{\epsilon}}) = \mathbf{E}^w(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0) : (\ddot{\boldsymbol{\epsilon}}^0 + \Delta \ddot{\boldsymbol{\epsilon}}) - \mathbf{V}(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0) : (\dot{\boldsymbol{\epsilon}}^0 + \Delta \dot{\boldsymbol{\epsilon}}) + \mathbf{C}(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0).$$

With the regular solution  $(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0)$  assumed to be homogeneous, Eq.(3.3)<sub>2</sub> in the perturbed state, combining Eq.(5.1) and Eq.(5.6),  $\text{div}(\ddot{\boldsymbol{\sigma}}(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0, \dot{\boldsymbol{\epsilon}}^0 + \Delta \dot{\boldsymbol{\epsilon}}, \ddot{\boldsymbol{\epsilon}}^0 + \Delta \ddot{\boldsymbol{\epsilon}})) = 0$  in  $\Omega$  becomes:

$$(5.7) \quad \mathbf{E}^w(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0) \bullet \left( \nabla \cdot (\nabla_s(\Delta \ddot{\mathbf{u}})) \right) - \mathbf{V}(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0) \bullet \left( \nabla \cdot (\nabla_s(\Delta \dot{\mathbf{u}})) \right) = 0 \quad \text{in } \Omega,$$

where  $\nabla$  is the gradient operator. Substituting Eq.(5.5) into (5.7) one obtains:

$$(5.8) \quad \left\{ \mathbf{n} \cdot \left[ \mathbf{E}^w - \frac{1}{\omega} \mathbf{V} \right] \cdot \mathbf{n} \right\} \cdot \delta \dot{\mathbf{u}} = 0.$$



A non-trivial solution of (5.8) is obtained as soon as

$$(5.9) \quad \exists(\mathbf{n}, \boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0) \quad \text{and} \quad \exists \omega > 0 \quad / \quad \det\left(\mathbf{n} \cdot \left\{ \mathbf{E}^w - \frac{1}{\omega} \mathbf{V} \right\} \cdot \mathbf{n}\right) = 0.$$

Owing to the fact that  $\mathbf{n}$  and  $\omega$  are solutions of Eq.(5.9) which is time-dependent, it should be noticed that only necessary conditions for an instability onset could be obtained.

### 5.3. Connection with the occurrence of dynamic effects at localisation

If there exists  $\omega < 0$  satisfying Eq.(5.9), the regular solution of ( $\ddot{P}$ ) is stable; if  $\omega > 0$  satisfying Eq.(5.9) exists, the regular solution is unstable, as existence of a growing-in-time perturbed solution is possible.

In Eq.(5.9), it is possible to find  $\omega$  and  $\mathbf{n}$  as solutions; but by conjecturing the localisation to be an intrinsically dynamic phenomenon, one retains only perturbations violating the quantitative criterion for quasi-staticity (4.1), i.e.:

$$(5.10) \quad \begin{aligned} \rho |\Delta \ddot{\mathbf{u}}| &\geq \gamma_{\text{crit}}, \\ |\Delta \dot{\mathbf{u}}| &= \omega |\delta \dot{\mathbf{u}}|. \end{aligned}$$

The first perturbation fulfilling Eq.(5.10) verifies the condition:

$$(5.11) \quad \rho \omega |\delta \dot{\mathbf{u}}| = \gamma_{\text{crit}} \approx \kappa_{\text{crit}} |\dot{\mathbf{u}}^0|^{-1}.$$

Replacing  $\omega$  from Eq.(5.11) in the instability criterion (5.9), one obtains as a criterion for a localised static/dynamic transition:

$$(5.12) \quad \boxed{\begin{aligned} \exists?(\mathbf{n}, \boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0, \delta \dot{\mathbf{u}}) \quad / \\ \det\left(\mathbf{n} \cdot \left[ \mathbf{E}^w(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0) - \frac{\rho |\delta \dot{\mathbf{u}}| |\dot{\mathbf{u}}^0|}{\kappa_{\text{crit}}} \mathbf{V}(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0) \right] \cdot \mathbf{n}\right) = 0 \end{aligned}}$$

## 6. Discussion

It appears that the criterion proposed depends on material characteristics (viscous parameters  $\eta, N, K$ ) and current mechanical state via,  $(\boldsymbol{\epsilon}^0, \boldsymbol{\alpha}^0)$  but on  $\rho, |\delta \dot{\mathbf{u}}|, |\dot{\mathbf{u}}^0|, \kappa_{\text{crit}}$  as well.

- The  $\kappa_{\text{crit}}$ -dependence and the  $\rho$ -dependence reflect a material feature and a loading rate feature (via  $\dot{\mathbf{u}}^0$ ). This rate-dependence would then exclude a material

classification based only on their behaviour at the onset of the localisation: only a classification based on the material and the loading rate would be relevant. This remark follows the conclusions of BATAILLE and KESTIN [3].

• The  $|\delta\dot{\mathbf{u}}|$ -dependence could also be connected to the loading rate conditions and suggests that the material will not localise if a too small perturbation is introduced compared to the loading displacement rate  $\dot{\mathbf{u}}^0$ .

A new approach of modelling the physical phenomenon of localisation of deformation is thus presented. It is viewed as a local transition from a (quasi)-static behaviour to a dynamic one. The boundary-value problem is to be treated, at least locally, as dynamic after the onset of localisation.

Apart from this new definition, a localisation criterion is proposed, function of parameters usually not encountered: the amplitude of the perturbation, the density of the material, the loading rate displacement and a critical "pseudo-kinetic" energy. This approach, insofar as a critical kinetic power could be experimentally measured, also permits to remove the difficulty of determining the rate of growth of the perturbation.

Considering the dynamic boundary-value problem for the rate-dependent material linked to the post-localisation behaviour, some difficulties stemming from the rate-independent models may arise. These are a null width of the localisation band and a loss of objectivity of the Finite Elements response. It is known that for rate-dependent materials in a dynamic context LOREST and PREVOST [15], a band width naturally appears. Also the mesh sensitivity is suppressed [15] whereas in the quasi-static context it may be only reduced as observed by FOREST and CAILLETAUD [13].

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## References

1. L. ANAND, K. H. KIM and T. G. SHAWKI, *Onset of shear localization in viscoplastic solids*, J. Mech. Phys. Solids, **35**, 4, 407–429, 1987.
2. Y. L. BAI, *Thermo-plastic instability in simple shear*, J. Mech. Phys. Solids, **30**, 195–207, 1982.
3. J. BATAILLE and J. KESTIN, *L'interprétation physique de la thermodynamique rationnelle*, J. Méca., **14**, 2, 365–384, 1975.
4. V. CANO, *Instabilités et rupture dans les solides élastoviscoplastiques*, Thèse de Doctorat de l'Université Paris 6, Décembre 1996.
5. H. P. CHERUKURI and T. G. SHAWKI, *An energy-based localization theory: i. basic framework*, Int. J. Plast., **11**, 2, 15–40, 1995.
6. A. CHRYSOCHOOS, H. LOUCHE, J. M. MURACCIOLE, P. NÉMOZ-GAILLARD, J. L. SAUREL and B. WATTRISSE, *Experimental analysis of localization mechanisms in mild*

- steels by infrared and speckle image processing, [In:] *Advanced Optical Methods and Applications in Solids Mechanics*, IUTAM Symposium, A. Lagarde Editor, Poitiers-Futuroscope, France, August 31 - September 4, 1998.
7. R. J. CLIFTON, *Adiabatic shear*, [In:] Report NMAB-356 of the NRC Committee on Material Response to Ultrasonic Loading Rates, 1978.
  8. T. DÉSOYER, J. L. HANUS and V. KERYVIN, *An instability condition of the deformation process in elasto-(visco)-nonlinear materials*, *Mech. Res. Comm.*, **25**, 4, 437-442, 1998.
  9. I. DOBOVŠEK and B. MORAN, *Materials instabilities in rate-dependent solids*, *Eur. J. Mech.*, A/Solids, **15**, 2, 267-294, 1996.
  10. D. DUDZINSKI and A. MOLINARI, *Perturbation analysis of thermoviscoplastic instabilities in biaxial loading*, *Int. J. Solids Structures*, **27**, 5, 601-628, 1991.
  11. J. HADAMARD, [In:] *Leçons sur la propagation des ondes et les équations de l'hydrodynamique*, Hermann, Paris, 1903.
  12. J. LEMAITRE and J. L. CHABOCHE, *Mécanique des matériaux solides*, Editions Dunod, 1985.
  13. S. FOREST and G. CAILLETAUD, *Strain localization in single crystals: Effect of Boundaries and Interfaces*, *Eur. J. Mech.*, A/Solids, **14**, 5, 747-771, 1995.
  14. Y. LEROY, *Linear stability analysis of rate-dependent discrete systems*, *Int. J. Solids Structures*, **27**, 6, 783-808, 1991.
  15. B. LORET and J. H. PREVOST, *Dynamic strain localization in elasto-(visco)-plastic solids, Part 1: General formulation and one-dimensional examples*, *Comp. Meth. Appl. Mech. Engng.*, **83**, 247-273, 1990.
  16. A. MOLINARI, *Instabilité thermoviscoplastique en cisaillement simple*, *J. Mech. Th. Appl.*, **4**, 5, 659-684, 1985.
  17. M. ORTIZ, Y. M. LEROY and A. NEEDLEMAN, *A finite element method for localized failure analysis*, *Comp. Meth. Appl. Mech. Engng.*, **61**, 189-214, 1987.
  18. P. PERZYNA, *Fundamental problems in viscoplasticity*, *Adv. Appl. Mech.*, **9**, 243-377, 1966.
  19. G. PIJAUDIER-CABOT and Z. P. BAŽANT, *Non-local damage theory*, *J. Engng. Mech.*, **113**, 1512-1533, 1987.
  20. J. R. RICE, *The localisation of plastic deformation*, [In:] *Theoretical and Applied Mechanics*, Proc. IUTAM Cong. ([Ed.] W.Koiter), North-Holland, Amsterdam, 207-220, 1976.
  21. H. M. ZBIB and E. C. AIFANTIS, *On the localization and post-localization of plastic deformation (Parts I, II and III)*, *Res. Mech.*, **23**, 261-305, 1988.

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## Observable plastic spin and comparison with other approaches

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THE OBJECT OF THIS PAPER is to formulate a relation for plastic spin, basing on the work of RANIECKI and MRÓZ [17] and the suggestion of HILL [5].

### 1. Introduction

IN DESCRIPTION of strain-induced anisotropy during finite (large) straining of metals and alloys the use of the concept of plastic spin was found to be instrumental.

As we know, the plastic spin represents the mean relative spin of all material fibers measured with respect to some chosen triad which can be thought as being attached to the substructures. The spin being the difference between the plastic spin and the material spin, takes part in the substructure corotational rates. For completing the constitutive equations, one has to specify three additional equations for plastic spin. As the plastic spin is not measurable explicitly, the representation theorems for isotropic functions have been used in conjunction with the concept of tensorial structure variables to provide explicit forms for it ONAT [12, 13], LORET [9], DAFALIAS [2], PAULUN and PECHERSKI [15]. Another possibility was proposed in the work of RANIECKI and MRÓZ [17] for a model of rigid-plastic solids. They indicate that in certain circumstances the plastic spin can be regarded, at least conceptually, as a measurable quantity. Supposing that the measurable texture orientation is specified by a rigidly rotating triad during consecutive steps of plastic deformation, the plastic spin is defined as the difference of material and texture spin. Such an approach closely follows the ideas of MANDEL [10, 11].

Tensors will be denoted by boldface characters. With the summation over repeated indices implied, the following symbolic operations apply :  $\mathbf{A}\mathbf{B} \rightarrow A_{ij}B_j$ ,  $\mathbf{A} \cdot \mathbf{B} \rightarrow A_{ij}B_{ij}$ ,  $\mathbf{A} \otimes \mathbf{B} \rightarrow A_{ij}B_{kl}$  with proper extension to different orders tensor. The prefix *tr* indicates the trace, a superscript *T* the transpose and a superscripted dot the material time derivative or rate. By **1** we denote the identity tensor and by a superscript  $-1$  the inverse.

## 2. Basic relations

### 2.1. Basic kinematic quantities

Following RANIECKI and MRÓZ [17], consider a uniform deformation of the rigid-plastic material element. Assume that the orientation of the texture can be specified at each instant of the process by three unit mutually orthogonal vectors triad. Let  $\mathbf{t}_i^0$  ( $i = 1, 2, 3$ ) be the triad representing the initial texture orientation in the initial stress-free configuration ( $k_0$ ), see Fig. 1. Assuming that at each subsequent instant  $t$  the orientation of texture is specified by the triad  $\mathbf{t}_i(t)$ , there is  $\mathbf{t}_i(t_0) = \mathbf{t}_i^0$  obviously. Let  $\mathbf{Q}(t)$  be the proper orthogonal tensor ( $\mathbf{Q}\mathbf{Q}^T = \mathbf{1}$ ) which transforms initial triad  $\mathbf{t}_i^0$  into instantaneous  $\mathbf{t}_i(t)$ , that is  $\mathbf{t}_i(t) = \mathbf{Q}(t)\mathbf{t}_i^0$ . The *instantaneous texture spin*  $\omega^t$  is defined as:

$$(2.1) \quad \dot{\mathbf{t}}_i(t) = \omega^t(t) \mathbf{t}_i(t),$$

where

$$(2.2) \quad \omega^t(t) = \dot{\mathbf{Q}}\mathbf{Q}^T = \sum_{i=1}^3 \dot{\mathbf{t}}_i(t) \otimes \mathbf{t}_i(t) \equiv \dot{\mathbf{t}}_i \otimes \mathbf{t}_i.$$

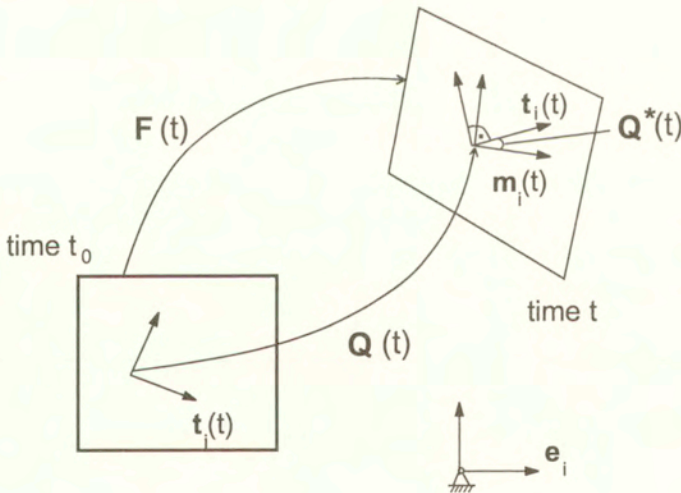


FIG. 1.

Introduce the notion of *texture reference frame*  $\mathbf{m}_i$  selected in the following way: vector  $\mathbf{m}_1$  represents a material fiber lying in a chosen material plane with normal  $\mathbf{m}_2$  and  $\mathbf{m}_3 = \mathbf{m}_1 \wedge \mathbf{m}_2$  (the vector product), see MANDEL [10, 11].

The spin  $\omega^m(m, t)$  of the reference triad  $\mathbf{m}_i$  will be defined as

$$(2.3) \quad \omega^m(m, t) = \dot{\mathbf{m}}_i \otimes \mathbf{m}_i, \quad \dot{\mathbf{m}}_i = \omega^m(m, t) \mathbf{m}_i.$$

Here the symbol  $m$  in brackets emphasize the fact that  $\omega^m(m, t)$  depend on the selection of texture reference frame.

Denote by  $\mathbf{V}$  the spatial velocity gradient  $\mathbf{V} = \dot{\mathbf{F}}\mathbf{F}^{-1}$  where  $\mathbf{F}$  is the deformation gradient. The symmetric and antisymmetric part of  $\mathbf{V}$  are, respectively, the rate of permanent strain  $\mathbf{D}$  and the material spin  $\omega$ . This idea follows the concept of director triad proposed by MANDEL [10, 11] defined on macrolevel. Some experiments of plastic deformation of the metal sheet subjected to the tension test produced the fiber-like textures (see, for example [1]).

To express the spin  $\omega^m$  in terms of  $\mathbf{V}$  and  $\mathbf{m}_i$  we find first the material derivative of the reference triad. The material derivative of vector  $\mathbf{m}_1$  can be found by differentiating the relation  $\mathbf{m}_1 = \frac{d\mathbf{x}}{|d\mathbf{x}|}$  to obtain:

$$(2.4) \quad \dot{\mathbf{m}}_1 = \mathbf{V}\mathbf{m}_1 - (\mathbf{m}_1 \cdot \mathbf{V}\mathbf{m}_1) \mathbf{m}_1.$$

In a similar way one can find the material derivative of vector  $\mathbf{m}_2 = \frac{\text{grad}f}{|\text{grad}f|}$ , where  $f(\mathbf{x}, t) = 0$  is the material surface in actual configuration in the following form:

$$(2.5) \quad \dot{\mathbf{m}}_2 = (\mathbf{m}_2 \cdot \mathbf{V}\mathbf{m}_2) \mathbf{m}_2 - \mathbf{V}^T \mathbf{m}_2.$$

From the relation  $\mathbf{m}_3 = \mathbf{m}_1 \wedge \mathbf{m}_2$  we have

$$(2.6) \quad \dot{\mathbf{m}}_3 = \dot{\mathbf{m}}_1 \wedge \mathbf{m}_2 + \mathbf{m}_1 \wedge \dot{\mathbf{m}}_2.$$

Introducing (2.4), (2.5) and (2.6) into (2.3)<sub>1</sub> it follows that the spin  $\omega^m$  of the triad  $\mathbf{m}_i$  is a very simple function of the strain rate tensor  $\mathbf{D}$  and the chosen triad (see, [7, 18]):

$$(2.7) \quad \begin{aligned} \omega^m(m, t) &= \omega(t) - \hat{\omega}(m, t), \\ 2\hat{\omega}(m, t) &= \hat{\omega}_{ij}(\mathbf{m}_i \otimes \mathbf{m}_j - \mathbf{m}_j \otimes \mathbf{m}_i), \\ \hat{\omega}_{12} &= \mathbf{m}_1 \cdot \mathbf{D}\mathbf{m}_2, \quad \hat{\omega}_{13} = \mathbf{m}_1 \cdot \mathbf{D}\mathbf{m}_3, \quad \hat{\omega}_{32} = \mathbf{m}_2 \cdot \mathbf{D}\mathbf{m}_3. \end{aligned}$$

If the transformation from  $\mathbf{m}_i$  to  $\mathbf{t}_i$  is specified by an orthogonal tensor  $\mathbf{Q}^*$ , then

$$(2.8) \quad \mathbf{t}_i = \mathbf{Q}^*(t) \mathbf{m}_i, \quad \mathbf{Q}^*(t) = \mathbf{t}_i \otimes \mathbf{m}_i.$$

The *relative texture spin*  $\omega^r$  is defined as follows:

$$(2.9) \quad \omega^r(m, t) = \dot{\mathbf{Q}}^* \mathbf{Q}^{*T}.$$

We can write also

$$(2.10) \quad 2\omega^r(m, t) = \dot{Q}_{ik}^*(t)Q_{jk}^*(t) (\mathbf{m}_i \otimes \mathbf{m}_j - \mathbf{m}_j \otimes \mathbf{m}_i),$$

where  $Q_{ij}^r$  is the matrix of direction cosines of angles between the vectors  $\mathbf{t}_i$  and  $\mathbf{m}_j$ :

$$(2.11) \quad Q_{ij}^* = \mathbf{m}_i(t) \cdot \mathbf{t}_j(t) = \mathbf{m}_i \cdot \mathbf{Q}^* \mathbf{m}_j, \quad \mathbf{Q}^* = Q_{ij}^* \mathbf{m}_i \otimes \mathbf{m}_j.$$

Differentiating (2.11)<sub>2</sub> with respect to time and using (2.3)<sub>2</sub>, we obtain

$$\dot{\mathbf{Q}}^* = \dot{Q}_{ij}^* \mathbf{m}_i \otimes \mathbf{m}_j + \omega^m \mathbf{Q}^* - \mathbf{Q}^* \omega^m;$$

then on accounting (2.10) we have

$$(2.12) \quad \dot{\mathbf{Q}}^* \mathbf{Q}^{*\text{T}} = \omega^r + \omega^m - \mathbf{Q}^* \omega^m \mathbf{Q}^{*\text{T}}.$$

On the other hand, differentiation (2.8)<sub>2</sub> with respect to  $t$ , accounting for (2.1) and (2.3)<sub>2</sub>, then multiplying two sides by  $\mathbf{Q}^{*\text{T}}$ , gives

$$(2.13) \quad \dot{\mathbf{Q}}^* \mathbf{Q}^{*\text{T}} = \omega^t - \mathbf{Q}^* \omega^m \mathbf{Q}^{*\text{T}}.$$

From (2.12), (2.13) and (2.7)<sub>2</sub> it follows

$$(2.14) \quad \omega^t = \omega^m + \omega^r = \omega(t) - (\hat{\omega}(m, t) - \omega^r(m, t)).$$

Defining *the plastic texture spin*  $\omega^p(t)$  as the difference of  $\omega(t)$  and  $\omega^t$ , the followings relation between these spins take place [17]

$$(2.15) \quad \omega^p(t) = \omega - \omega^t = \hat{\omega}(m, t) - \omega^r(m, t).$$

The symbol  $m$  in brackets emphasizes the fact that  $\hat{\omega}(m, t)$  depends on the selection of the texture reference frame. Both  $\omega^t$  and  $\omega$  are independent of the selection of the particular texture reference frame. Therefore, from (2.15) it follows that the plastic texture spin  $\omega^p(t)$  is also independent of the choice of  $\mathbf{m}_i$ , and equation (2.15)<sub>2</sub> shows the possibility for measurement of  $\omega^p$  by metallographic methods.

If at generic instant  $t$  the texture reference triad  $\mathbf{m}_i$  is assumed to coincide with  $\mathbf{t}_i$ , then the corresponding tensors are denoted by  $\hat{\omega}$  and  $\omega^r$ , dropping symbol “ $m$ ” in brackets, and are called respectively, *the texture R-spin* and *plastic R-spin*, see Fig. 2. In general, at the subsequent instant  $\mathbf{m}_i(t + \delta t) \neq \mathbf{t}_i(t + \delta t)$ . Setting  $\mathbf{m}_i(t) = \mathbf{t}_i(t)$  in (2.7), (2.9) leads to the expression for *R*-spins:

$$2\hat{\omega} = \hat{\omega}_{ij}(\mathbf{t}_i \otimes \mathbf{t}_j - \mathbf{t}_j \otimes \mathbf{t}_i),$$

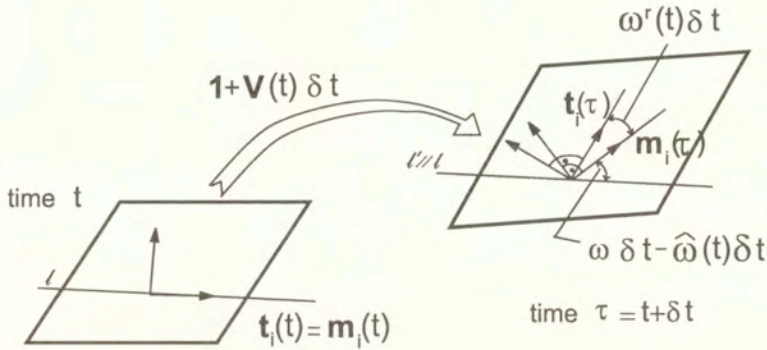


FIG. 2.

$$(2.16) \quad \hat{\omega}_{12} = \mathbf{t}_1 \cdot \mathbf{D} \mathbf{t}_2, \quad \hat{\omega}_{13} = \mathbf{t}_1 \cdot \mathbf{D} \mathbf{t}_3, \quad \hat{\omega}_{32} = \mathbf{t}_2 \cdot \mathbf{D} \mathbf{t}_3,$$

and

$$(2.17) \quad 2\omega^r = \omega_{ij}^r (\mathbf{t}_i \otimes \mathbf{t}_j - \mathbf{t}_j \otimes \mathbf{t}_i).$$

Tensor  $\omega^r \delta t$  represents the angles between vectors  $\mathbf{t}_i(t + \delta t)$  and  $\mathbf{m}_i(t + \delta t)$  while tensor  $(\omega - \hat{\omega}) \delta t$  specifies the angles between  $\mathbf{m}_i(t)$  and  $\mathbf{m}_i(t + \delta t)$ . The relation (2.15) remains valid, so that:

$$(2.18) \quad \omega^p = \omega - \omega^t = \hat{\omega} - \omega^r.$$

The plastic spin is thus divided into two parts. From (2.16), it follows that  $\hat{\omega}$  is a known function of  $\mathbf{t}_i$  and  $\mathbf{D}$ . Both the relative texture spin and plastic reference spin (including  $R$ -spins) are objective tensors. To complete the description, a constitutive equation for  $\omega^r$  should be formulated. This could be verified by metallographic measurements of the texture orientation changes during deformation. Due to the lack of appropriate experimental data, some theoretical assumptions may be proposed to find meaningful constitutive equations. For example, RANIECKI and SAMANTA supposed  $\omega^r = 0$  what means that the variation of texture orientation and the variation of its reference frame is the same during the deformation process [18]. First, we consider the case of simple shear to explain the notions of this section. The more general case of generalized plane strain state was studied in the same paper of RANIECKI and MRÓZ [17].

## 2.2. General structure of evolution rules for rigid-plastic solids

Consider the texture anisotropy assuming that the yield surface is specified by the reduced stress  $\sigma - \alpha$ , where  $\sigma$  is the Cauchy stress and  $\alpha$  is the texture internal stress defining the shift of the yield surface. Let  $\mathcal{A}$  be the set of variable



$$(2.19) \quad \mathcal{A} = (\mathbf{D}, \boldsymbol{\sigma}, \boldsymbol{\alpha}, \mathbf{t}_i, \alpha),$$

where  $\mathbf{t}_i$  is the texture triad and  $\alpha$  is scalar internal variable. Assume that we know the initial orientation  $\mathbf{t}_i^0$  of the texture triad and the initial texture stress  $\boldsymbol{\alpha}(t_0) = \boldsymbol{\alpha}^0$ . A general form of evolution equations for rigid-plastic solids is

$$(2.20) \quad \boldsymbol{\omega}^r = \mathcal{P}(\mathcal{A}), \quad \overset{\circ}{\boldsymbol{\alpha}} = \mathcal{Q}(\mathcal{A}), \quad \dot{\alpha} = \mathcal{K}(\mathcal{A});$$

here  $\overset{\circ}{\boldsymbol{\alpha}}$  is the corotational rate with texture

$$(2.21) \quad \overset{\circ}{\boldsymbol{\alpha}} = \dot{\boldsymbol{\alpha}} + \boldsymbol{\alpha}\boldsymbol{\omega}^t - \boldsymbol{\omega}^t\boldsymbol{\alpha}$$

and  $\mathcal{P}$  is antisymmetric,  $\mathcal{Q}$  is symmetric and  $\mathcal{K}$  is a scalar isotropic functions of all tensor arguments. They are homogeneous functions of degree one of  $\mathbf{D}$  for rate-independent materials. We will use some theoretical assumptions for the form of  $\mathcal{P}$ . For linear kinematic hardening the evolution equation for  $\boldsymbol{\alpha}$  is as follows:

$$(2.22) \quad \overset{\circ}{\boldsymbol{\alpha}} = c\mathbf{D}$$

where  $c = \text{const}$ . For this rule, the equation (2.19)<sub>2</sub> can be integrated to obtain interesting integral form of the equation for the internal variable [17]:

$$(2.23) \quad \boldsymbol{\alpha}(t) = c \left( \int_{t_0}^t \mathbf{t}_i(\tau) \cdot \mathbf{D}(\tau) \mathbf{t}_j(\tau) d\tau \right) \mathbf{t}_i(t) \otimes \mathbf{t}_j(t) + \alpha_{ij}^0 \mathbf{t}_i(t) \otimes \mathbf{t}_j(t);$$

here  $\alpha_{ij}^0$  are the initial texture stress components in the initial texture triad

$$(2.24) \quad \alpha_{ij}^0 = \mathbf{t}_i^0 \cdot \boldsymbol{\alpha}^0 \mathbf{t}_j^0.$$

The first term in (2.23) describes the change of internal stress due to plastic deformation while the second term specifies the rotation of the initial internal stress with the texture.

### 3. Simple shear analysis

#### 3.1. Expressions for the spins of previous section

The motion in simple shear is given by

$$(3.1) \quad x_1 = X_1 + \text{ctg } \chi X_2 = X_1 + \gamma X_2, \quad x_2 = X_2, \quad x_3 = X_3,$$

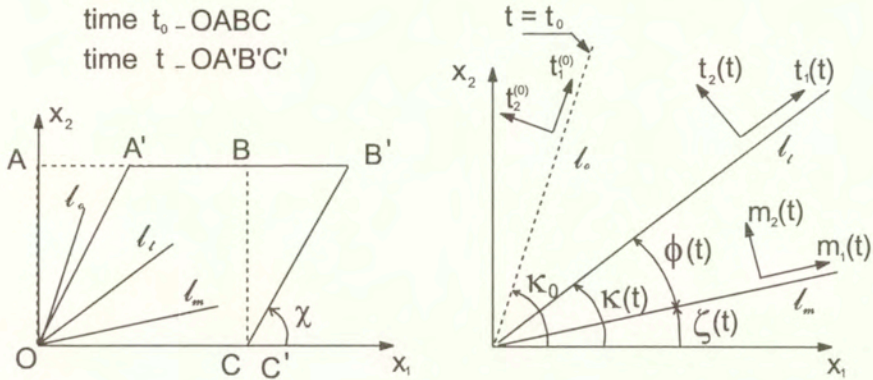


FIG. 3.

where  $x_i$  and  $X_i$ ,  $i = 1, 2, 3$ , are the Cartesian coordinates of the current and initial position of a material point,  $\gamma = \text{ctg } \chi$  is called the engineering shear strain. The deformation gradient  $\mathbf{F}$  in polar decomposition reads  $\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{S}\mathbf{R}$ . After a straightforward computation we obtain the following relations

$$(3.2) \quad \mathbf{S}^2 = \begin{pmatrix} 1 + \gamma^2 & \gamma & 0 \\ \gamma & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The rate of plastic deformation, the material spin and the rate  $\dot{\mathbf{R}}\mathbf{R}^T$  in truncated form (all other components that have an index equal to 3 being identically zero) are

$$(3.3) \quad \mathbf{D} = \frac{\dot{\gamma}}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\omega} = \frac{\dot{\gamma}}{2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

$$\dot{\mathbf{R}}\mathbf{R}^T = \frac{2\dot{\gamma}}{\gamma^2 + 4} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Let the rectangle  $OABC$  be deformed into a parallelogram  $OA'B'C'$  at the instant  $t$ , see Fig. 3. The texture orientation at the initial instant  $t_0$  is specified by the line  $l_0$  (the vector  $\mathbf{t}_1^{(0)}$  is parallel to  $l_0$ ). At the instant  $t$  the texture orientation is presented by the position of the line  $l_t$  (vector  $\mathbf{t}_1(t)$  lies on this direction). The material line coinciding before deformation with the segment  $l_0$  at instant  $t$  occupies the position  $l_m$  (vector  $\mathbf{m}_1(t)$  is parallel to this line). Denote by  $\zeta(t)$  the angle between the axis  $x_1$  and  $l_m$ . Let the angle  $\kappa(t)$  specify the instantaneous orientation of texture  $l_t$  and introduce the rotation  $\phi = \zeta(t) - \kappa(t)$ .

We have at  $t = t_0$ :

$$(3.4) \quad \zeta(t_0) = \kappa(t_0) = \kappa_0, \quad \phi(t_0) = 0.$$

From (2.7) and (3.3) it follows that the orientation of  $l_m$  does not depend on the stretch and shear strain histories:

$$(3.5) \quad \text{ctg } \zeta(t) = \gamma + \text{ctg } \kappa_0$$

and all the spins defined in previous section have now only one independent component with index  $1_2$  which will be dropped:

$$(3.6) \quad \omega(t) = \dot{\gamma}/2 \quad \text{for material spin,}$$

$$(3.7) \quad \omega^t(t) = -\dot{\kappa} \quad \text{for instantaneous texture spin,}$$

$$(3.8) \quad \omega^r(m, t) = \dot{\phi} \quad \text{for relative texture spin,}$$

$$(3.9) \quad \hat{\omega}(m, t) = \frac{\cos 2\zeta}{2} \dot{\gamma} \quad \text{for relative plastic spin,}$$

$$(3.10) \quad \hat{\omega} = \frac{\cos 2\kappa}{2} \dot{\gamma} \quad \text{for plastic } R\text{-spin,}$$

$$(3.11) \quad \omega^r(t) = \dot{\Omega}(t) \quad \text{for texture } R\text{-spin,}$$

$$(3.12) \quad \begin{aligned} \omega^p(t) &= \hat{\omega}(m, t) - \dot{\phi}(t) \quad \text{for total plastic spin.} \\ &= \hat{\omega} - \dot{\Omega}(t) \end{aligned}$$

The equation (2.1) specifying the texture orientation leads to one differential equation for  $\kappa(t)$ . Supposing that the texture R-spin  $\dot{\Omega}$  is known, this equation reads

$$(3.13) \quad \dot{\kappa} + \dot{\Omega} + \dot{\gamma} \sin^2 \kappa = 0.$$

and in the case where the total plastic spin is known:

$$(3.14) \quad \dot{\kappa} = \omega^p(t) - \dot{\gamma}/2.$$

Equations (2.23) give, after some transformation, the expressions for internal stresses

$$\begin{aligned}
 \alpha_{22} - \alpha_{11} &= -c \left[ \cos 2\kappa(\gamma) \int_0^\gamma \sin 2\kappa(g) dg - \sin 2\kappa(\gamma) \int_0^\gamma \cos 2\kappa(g) dg \right] \\
 &\quad + (\alpha_{22}^0 - \alpha_{11}^0) \cos 2(\kappa(\gamma) - \kappa_0) + 2\alpha_{12}^0 \sin 2(\kappa(\gamma) - \kappa_0), \\
 (3.15) \quad \alpha_{22} + \alpha_{11} &= (\alpha_{22}^0 + \alpha_{11}^0), \\
 \alpha_{12} &= \frac{c}{2} \left[ \cos 2\kappa(\gamma) \int_0^\gamma \cos 2\kappa(g) dg + \sin 2\kappa(\gamma) \int_0^\gamma \sin 2\kappa(g) dg \right] \\
 &\quad + (\alpha_{11}^0 - \alpha_{22}^0) \sin 2(\kappa(\gamma) - \kappa_0) + \alpha_{12}^0 \cos 2(\kappa(\gamma) - \kappa_0), \\
 \alpha_{33} &= \alpha_{33}^0.
 \end{aligned}$$

Here the function  $\kappa(\gamma)$  is found from the functions  $\kappa(t)$  and  $\gamma(t)$ ,  $\kappa|_{\gamma=0} = \kappa_0$ . For incompressible materials  $-\alpha_{33}^0 = \alpha_{11}^0 + \alpha_{22}^0$ .

When a Mises-type yield criterion is adopted

$$(3.16) \quad f = \frac{3}{2} (\bar{\sigma} - \alpha) \cdot (\bar{\sigma} - \alpha) - \sigma_0^2 = 0$$

where  $\bar{\sigma}$  is the deviator of  $\sigma$ , one has

$$(3.17) \quad \bar{\sigma}_{11} = \alpha_{11}, \quad \bar{\sigma}_{22} = \alpha_{22}, \quad \bar{\sigma}_{12} = \frac{\sigma_0}{\sqrt{3}} + \alpha_{12},$$

so, for zero initial value of  $\alpha$ , the relations (3.15 - 3.17) lead to the following normalized stresses (with respect to yield):

$$\begin{aligned}
 \sigma'_{11} \equiv \frac{\bar{\sigma}_{11}}{\sigma_0} &= \frac{c}{2\sigma_0} \left[ \cos 2\kappa(\gamma) \int_0^\gamma \sin 2\kappa(g) dg \right. \\
 &\quad \left. - \sin 2\kappa(\gamma) \int_0^\gamma \cos 2\kappa(g) dg \right] = -\sigma'_{22}, \\
 (3.18) \quad \sigma'_{12} \equiv \frac{\bar{\sigma}_{12}}{\sigma_0} &= \frac{1}{\sqrt{3}} + \frac{c}{2\sigma_0} \left[ \cos 2\kappa(\gamma) \int_0^\gamma \cos 2\kappa(g) dg \right. \\
 &\quad \left. + \sin 2\kappa(\gamma) \int_0^\gamma \sin 2\kappa(g) dg \right].
 \end{aligned}$$

### 3.2. Different assumptions for texture orientation

1. When total plastic spin is neglected, from (3.14) one has  $\dot{\kappa} = -\dot{\gamma}/2$  then  $\kappa(\gamma) = \kappa_0 - \gamma/2$ . Introducing this relation to (3.18), the known oscillatory results are obtained:

$$(3.19) \quad \sigma'_{11} = \frac{c}{2\sigma_0} (1 - \cos \gamma), \quad \sigma'_{12} = \frac{1}{\sqrt{3}} + \frac{c}{2\sigma_0} \sin \gamma.$$

2. With the assumption of RANIECKI and SAMANTA  $\omega^r = 0$  [18], from (2.18) one has  $\omega - \omega^t = \hat{\omega}$ , and the last relation leads to the differential equation

$$(3.20) \quad \dot{\kappa} + \dot{\gamma} \sin^2 \kappa = 0,$$

which gives  $\gamma = \cotg \kappa - \cotg \kappa_0$ . After a long but straightforward calculations, one obtains from (3.18):

$$(3.21) \quad \begin{aligned} \sigma'_{11} &= \frac{c}{2\sigma_0(\gamma^2 + 1)} [(\gamma^2 - 1)\ln(\gamma^2 + 1) - 2\gamma(\gamma - 2\arctg \gamma)], \\ \sigma'_{12} &= \frac{1}{\sqrt{3}} + \frac{c}{2\sigma_0(\gamma^2 + 1)} [(\gamma^2 - 1)(\gamma - 2\arctg \gamma) + 2\gamma \ln(\gamma^2 + 1)]. \end{aligned}$$

3. In paper [2] DAFALIAS considered the corotational rates with spin  $\dot{\mathbf{R}}\mathbf{R}^T$ . This rate was also studied by DIENES [3] for hypoelasticity. This case leads to

$$\dot{\kappa} = -\frac{2\dot{\gamma}}{\gamma^2 + 4} \quad \text{or} \quad \kappa = -\arctg \frac{\gamma}{2} + \kappa_0$$

and from (3.18) we obtain

$$(3.22) \quad \begin{aligned} \sigma'_{11} &= \frac{c}{2\sigma_0} \left[ 4 \cos\left(2\arctg \frac{\gamma}{2}\right) \ln\left(\cos \arctg \frac{\gamma}{2}\right) \right. \\ &\quad \left. + \sin\left(2\arctg \frac{\gamma}{2}\right) \left(4\arctg \frac{\gamma}{2} - \gamma\right) \right], \\ \sigma'_{12} &= \frac{1}{\sqrt{3}} + \frac{c}{2\sigma_0} \left[ \cos\left(2\arctg \frac{\gamma}{2}\right) \left(4\arctg \frac{\gamma}{2} - \gamma\right) \right. \\ &\quad \left. - 4 \sin\left(2\arctg \frac{\gamma}{2}\right) \ln\left(\cos \arctg \frac{\gamma}{2}\right) \right], \end{aligned}$$

which can be shown to be the same as in [2].

4. The simple shear process was considered by PAULUN and PEŁCHERSKI [14, 16] by introducing an influence function which produces a retardation of the material spin. In this case, the instantaneous texture spin (3.7) is in the form

$$(3.23) \quad \dot{\kappa} = -\frac{\dot{\gamma}}{2(1+\gamma^2)};$$

then we find  $\kappa = \kappa_0 - 1/2 \operatorname{arctg} \gamma$  and equations (3.18) give the followings relations for stresses as in the papers mentioned above:

$$(3.24) \quad \begin{aligned} \sigma'_{11} &= \frac{c}{2\sigma_0\sqrt{\gamma^2+1}} \left[ 1 - \sqrt{\gamma^2+1} + \gamma \ln \left( \sqrt{\gamma^2+1} + \gamma \right) \right], \\ \sigma'_{12} &= \frac{1}{\sqrt{3}} + \frac{c}{2\sigma_0\sqrt{\gamma^2+1}} \left[ \ln \left( \sqrt{\gamma^2+1} + \gamma \right) + \gamma \left( \sqrt{\gamma^2+1} - 1 \right) \right]. \end{aligned}$$

5. The assumption that every material remains isotropic becomes less good as the deformation continues. Individual crystal grains are elongated in the direction of the greatest tensile strain and the texture of the specimen becomes fibrous (see HILL [5]). Assume that the texture triad coincides with that of the principal axes of the left stretch tensor  $\mathbf{S}$  during the deformation process [19]. In this case, from (3.2) we can find the principal axes of  $\mathbf{S}$  and the instant texture triad is defined as follows:

$$(3.25) \quad \begin{aligned} \mathbf{t}_1 &= \left( \frac{\gamma^2 + \sqrt{\gamma^2(\gamma^2+4)}}{\sqrt{4\gamma^2 + [\gamma^2 + \sqrt{\gamma^2(\gamma^2+4)}]^2}}; \frac{2\gamma}{\sqrt{4\gamma^2 + [\gamma^2 + \sqrt{\gamma^2(\gamma^2+4)}]^2}} \right), \\ \mathbf{t}_2 &= \left( \frac{\gamma^2 - \sqrt{\gamma^2(\gamma^2+4)}}{\sqrt{4\gamma^2 + [\gamma^2 - \sqrt{\gamma^2(\gamma^2+4)}]^2}}; \frac{2\gamma}{\sqrt{4\gamma^2 + [\gamma^2 + \sqrt{\gamma^2(\gamma^2+4)}]^2}} \right), \end{aligned}$$

and the instant orientation of the texture triad is

$$\kappa = \operatorname{arctg} \left( \frac{2}{\gamma + \sqrt{\gamma^2+4}} \right).$$

Now the stresses are

$$(3.26) \quad \begin{aligned} \sigma'_{11} &= \frac{c}{\sigma_0\sqrt{\gamma^2+4}} \left[ \gamma \ln \left( \frac{\gamma + \sqrt{\gamma^2+4}}{2} \right) - \sqrt{\gamma^2+4} + 2 \right], \\ \sigma'_{12} &= \frac{1}{\sqrt{3}} + \frac{c}{2\sigma_0\sqrt{\gamma^2+4}} \left[ \gamma \left( \sqrt{\gamma^2+4} - 2 \right) + 4 \ln \left( \frac{\gamma + \sqrt{\gamma^2+4}}{2} \right) \right]. \end{aligned}$$

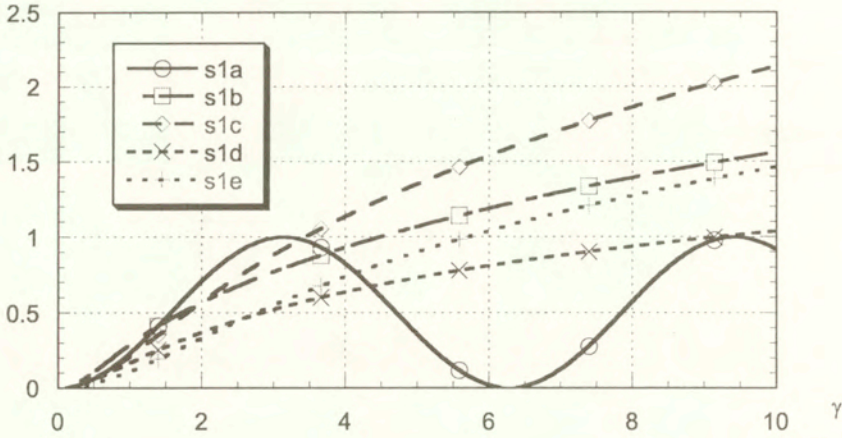


FIG. 4. Normalized stress  $\sigma_{11}/\sigma_0$  vs. strain; s1a – Jaumann; s1b – Raniecki and Samanta; s1c – Dafalias; s1d – Paulun and Pęcherski; s1e – this paper.

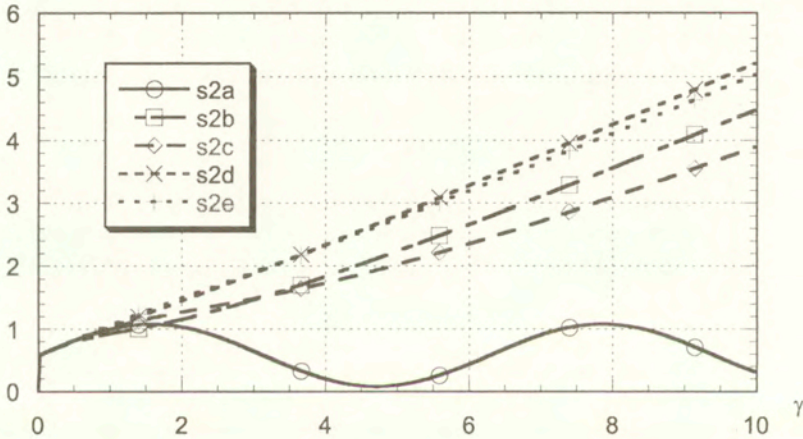


FIG. 5. Normalized stress  $\sigma_{12}/\sigma_0$  vs. strain; s2a – Jaumann; s2b – Raniecki and Samanta; s2c – Dafalias; s2d – Paulun and Pęcherski; s2e – this paper.

We take the material constants for an aluminum alloy from the paper of LEE *et al.* [8]: initial yield stress  $\sigma_0 = 207\text{MPa}$  and modulus of linear hardening  $c = 206.6\text{MPa}$ , to plot the normal  $\sigma'_{11}$  and shear stress  $\sigma'_{12}$  vs. strain  $\gamma$  for all the case considered in this section. They are shown in Fig. 4 and Fig. 5 where curve (a) for Jaumann rate, curve (b) for Raniecki and Samanta's assumption, curve (c) for the case of Dafalias, curve (d) for the case of Paulun and Pęcherski, and curve (e) for the assumption of this paper.

#### 4. The expression for the proposed spin in absolute representation

Decompose the deformation gradient  $\mathbf{F}$  in the polar form

<http://rcin.org.pl>

$$(4.1) \quad \mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{S}\mathbf{R},$$

where  $\mathbf{U}$ ,  $\mathbf{S}$  are, respectively, the right and the left stretch tensors and  $\mathbf{R}$  is proper orthogonal. Let  $\mathbf{N}_i$  and  $\lambda_i$ , ( $i = 1, 2, 3$ ) be respectively, the principal directions and eigenvalues of the stretch tensor  $\mathbf{U}$  (which are also those of  $\mathbf{S}$ )

$$(4.2) \quad \dot{\mathbf{U}} = \lambda_i \mathbf{N}_i \otimes \mathbf{N}_i.$$

Denote by  $\mathbf{n}_i$  the principal directions of  $\mathbf{S}$ ,  $\mathbf{n}_i = \mathbf{R}\mathbf{N}_i$ , then

$$(4.3) \quad \mathbf{S} = \lambda_i \mathbf{n}_i \otimes \mathbf{n}_i.$$

By differentiating this spectral decomposition with respect to time we obtain

$$(4.4) \quad \mathbf{S}\dot{\boldsymbol{\Omega}}^S - \boldsymbol{\Omega}^S\mathbf{S} = \dot{\lambda}_i \mathbf{n}_i \otimes \mathbf{n}_i - \dot{\mathbf{S}}.$$

Supposing  $\mathbf{S}$  known function of  $t$  we can find  $\boldsymbol{\Omega}^S$  from the previous relation. The equation of this form was studied by GUO and others in the paper [4]. Denote by I, II and III the principal invariants of  $\mathbf{S}$ :

$$(4.5) \quad \begin{aligned} \text{I} &= \lambda_1 + \lambda_2 + \lambda_3, \\ \text{II} &= \lambda_2\lambda_3 + \lambda_3\lambda_1 + \lambda_1\lambda_2, \\ \text{III} &= \lambda_1\lambda_2\lambda_3. \end{aligned}$$

In case of distinct eigenvalues, the solution of (4.4) is

$$(4.6) \quad \begin{aligned} \boldsymbol{\Omega}^S &= \Delta^{-2}[(6\text{I} \cdot \text{III} - 5\text{I}^2 \cdot \text{II} + \text{I}^4 + 4\text{II}^2)(\dot{\mathbf{S}}\mathbf{S} - \mathbf{S}\dot{\mathbf{S}}) \\ &\quad + (4\text{I} \cdot \text{II} - \text{I}^3 - 9\text{III})(\dot{\mathbf{S}}\mathbf{S}^2 - \mathbf{S}^2\dot{\mathbf{S}}) + (\text{I}^2 - 3\text{II})(\mathbf{S}\dot{\mathbf{S}}\mathbf{S}^2 - \mathbf{S}^2\dot{\mathbf{S}}\mathbf{S})] \end{aligned}$$

here

$$(4.7) \quad \begin{aligned} \Delta^2 &= (\lambda_2 - \lambda_3)^2(\lambda_3 - \lambda_1)^2(\lambda_1 - \lambda_2)^2 \\ &= 18\text{I} \cdot \text{II} \cdot \text{III} + \text{I}^2 \cdot \text{II}^2 - 4\text{I}^3 \cdot \text{III} - 4\text{II}^3 - 27\text{III}^2. \end{aligned}$$

Note that from (4.1)  $\mathbf{S} = \mathbf{R}\mathbf{U}\mathbf{R}^T$  we can express  $\dot{\mathbf{S}}$  in terms of the velocity gradient using the following relations derived by HOGER [6] (valid in case of distinct eigenvalues)



$$(4.8) \quad \dot{\mathbf{U}} = \frac{1}{\mathbf{I} \cdot \mathbf{II} - \mathbf{III}} \mathbf{R}^T [\mathbf{S}^2 \mathbf{D} \mathbf{S}^2 - \mathbf{I}(\mathbf{S}^2 \mathbf{D} \mathbf{S} + \mathbf{S} \mathbf{D} \mathbf{S}^2) \\ + (\mathbf{I}^2 + \mathbf{II}) \mathbf{S} \mathbf{D} \mathbf{S} - \mathbf{III}(\mathbf{S} \mathbf{D} + \mathbf{D} \mathbf{S}) + (\mathbf{I} \cdot \mathbf{III}) \mathbf{D}] \mathbf{R}$$

and

$$(4.9) \quad \dot{\mathbf{R}} \mathbf{R}^T = \boldsymbol{\omega} + \frac{1}{\mathbf{I} \cdot \mathbf{II} - \mathbf{III}} [\mathbf{I}^2 (\mathbf{D} \mathbf{S} - \mathbf{S} \mathbf{D}) \\ + \mathbf{I}(\mathbf{S}^2 \mathbf{D} - \mathbf{D} \mathbf{S}^2) + (\mathbf{S} \mathbf{D} \mathbf{S}^2 - \mathbf{S}^2 \mathbf{D} \mathbf{S})].$$

In the particular case, where  $\mathbf{D} \mathbf{S} = \mathbf{S} \mathbf{D}$  (HÖGER [6] have proved that this is the necessary and sufficient condition for the corotational Jaumann derivative of  $\ln \mathbf{S}$  to be equal to the stretching tensor  $\mathbf{D}$ ), the relation (4.6) takes the form

$$(4.10) \quad \boldsymbol{\Omega}^S = \Delta^{-2} \left\{ (6\mathbf{I} \cdot \mathbf{III} - 5\mathbf{I}^2 \cdot \mathbf{II} + \mathbf{I}^4 + 4\mathbf{II}^2) [(\boldsymbol{\omega} \mathbf{S} - \mathbf{S} \boldsymbol{\omega}) \mathbf{S} - \mathbf{S}(\boldsymbol{\omega} \mathbf{S} - \mathbf{S} \boldsymbol{\omega})] \right. \\ \left. + (4\mathbf{I} \cdot \mathbf{II} - \mathbf{I}^3 - 9\mathbf{III}) [(\boldsymbol{\omega} \mathbf{S} - \mathbf{S} \boldsymbol{\omega}) \mathbf{S}^2 - \mathbf{S}^2(\boldsymbol{\omega} \mathbf{S} - \mathbf{S} \boldsymbol{\omega})] \right. \\ \left. + (\mathbf{I}^2 - 3\mathbf{II}) [\mathbf{S}(\boldsymbol{\omega} \mathbf{S} - \mathbf{S} \boldsymbol{\omega}) \mathbf{S}^2 - \mathbf{S}^2(\boldsymbol{\omega} \mathbf{S} - \mathbf{S} \boldsymbol{\omega}) \mathbf{S}] \right\},$$

and the relation for plastic spin (2.18) now reads

$$(4.11) \quad \boldsymbol{\omega}^p = \boldsymbol{\omega} - \boldsymbol{\Omega}^S.$$

## 5. Conclusions

In the paper we use the suggestion of HILL to propose the orientation of instant texture triad for accomplishing the description of rigid-plastic material in finite deformation. The paper shows the relation between the two approaches for defining the plastic spin. The considerations presented in the work of Raniecki and Mróz permit to understand the physical meaning and, in principle, shows the possible way to find experimentally the evolution law for plastic spin.

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## References

1. J. M. CARLSON and J. E. BIRD, *Development of sample-scale shear bands during necking of ferrite-austenite sheet*, Acta Mech., **35**, 1675–1701, 1987.
2. Y. F. DAFALIAS, *Corotational rates for kinematic hardening at large plastic deformation*, J. Appl. Mech., **50**, 561–565, 1983.
3. J. K. DIENES, *On the analysis of rotation and stress rate in deforming bodies*, Acta. Mech., **32**, 217–232, 1979.
4. LIANG HAORYUN, GUO ZHONG-HENG, TH. LEHMANN and CHI-SING MAN, *Twirl tensors and the tensors equations  $\mathbf{ax} - \mathbf{xa} = \mathbf{c}$* , J. Elasticity, **27**, 227–245, 1992.
5. R. HILL, *The mathematical theory of plasticity*, Oxford University Press, 1967.
6. ANNE HOGER, *The material time derivative of logarithmic strain*, Int. J. Solids Struct., **22** 9, 1019–1032, 1986.
7. M. KLEIBER AND B. RANIECKI, *Elastic-plastic materials at finite strain*, [In:] A. SAWCZUK, [Ed.], Plasticity Today, 3–46. Elsevier Applied Sci. Pub. Ltd., 1985.
8. E. H. LEE, R. L. MALLETT and R. L. WERTHEIMER, *Stress analysis for anisotropic hardening in finite deformation plasticity*, J. Appl. Mech., **50**, 554–560, 1983.
9. B. LORET, *On the effects of plastic rotation in the finite deformation of anisotropic elasto-plastic materials*, Mech. Materials, **2**, 287–304, 1983.
10. J. MANDEL, *Plasticité et viscoplasticité*, Springer, Udine 1971.
11. J. MANDEL, *Director vectors and constitutive equations for plastic and viscoplastic media*, [In:] A. SAWCZUK, [Ed.], Problems of Plasticity, 135–143. Nordhoff Int. Pub., 1974.
12. E. T. ONAT, *Representation of inelastic behavior in the presence of anisotropy and of finite deformation*, [In:] B. WILSHIRE and D. R. J. OWEN, [Eds.] Recent Advance in Creep and Fracture of Engineering Materials and Structures, 231–254. Pineridge Press, Swansea, U. K. 1982.
13. E. T. ONAT, *Shear flow of kinematically hardening rigid-plastic materials*, [In:] G. J. DVORAK and R. T. SHIELD, [Eds.] Mechanics of material behaviour, 311–324, Elsevier, 1984.
14. J. E. PAULUN and R. PEÇHERSKI, *Study of corotational rates for kinematic hardening in finite deformation plasticity*, Arch. Mech., **37**, 661–677, 1985.
15. J. E. PAULUN and R. PEÇHERSKI, *On the application of the plastic spin concept for the description of anisotropic hardening in finite deformation plasticity*, Int. J. of Plasticity, **3**, 303–314, 1987.
16. J. E. PAULUN and R. PEÇHERSKI, *On the relation for plastic spin*, Arch. Applied Mechanics, **62**, 376–385, 1992.
17. B. RANIECKI and Z. MRÓZ, *On the strain-induced anisotropy and texture in rigid-plastic solids*, [In:] M. KLEIBER and A. KÖNIG [Eds.] Inelastic Solids and Structure, A. Sawczuk Memorial Volume, 13–32, Pineridge Press, 1989.
18. B. RANIECKI and S. K. SAMANTA, *The thermodynamic model of rigid-plastic solids with kinematic hardening*, Arch. Mech., **40**, 1988.
19. NGUYEN HUU VIEM, *An example of strain-induced anisotropy and texture at finite strain*, [In:] Proc.VIIth French-Polish Symposium, 1990.

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Dusty plasma solitons in Vlasov plasmas
- 181 R. C. SHARMA, SUNIL and SURESH CHAND  
Thermosolutal instability of Walters' rotating fluid (Model B') in porous medium
- 193 J. L. HANUS, V. KERYVIN and T. DÉSOYER  
Localisation of deformation as a local quasi-static/dynamic transition
- 207 NGUYEN HUU VIEM and B. RANIECKI  
Observable plastic spin and comparison with other approaches