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PERSPECTIVE OF INTERFACES FROM STAND POINT OF CONTINUUM PHYSICS

Abstract. The aim of our contribution is to draw attention to the fact, which so far has rarely absorbed theoreticians studying continuous media, that a moving surface may carry not only disturbances, but also physical properties different from those of the surrounding media.

Here, we present a unified view of the theory of non-relativistic thermodynamics incorporating phenomena with singularities. These singularities will present as discontinuous functions or their derivatives, and in the form of the discontinuity in respect to the Lebesgue measure of physical quantities.

A special focus exists on the fracture at interfaces. Current topics include the role of thermal residual or processing induced stresses, the detailed role of plasticity, and geometric effects on interface crack driving forces.

We model a situation of this kind by the movement of a surface separating two well-behaved material media, while attributing to the surface the physical properties of a phase change.

For a proper understanding of interfacial (transport) processes, one needs to be familiar with the basic geometrical description of a surface, we present here.

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1. Introduction

The objective of this contribution is to present perspective of physics of interfaces from stand point of continuum physics. This approach develops the foundations more carefully than the traditional approach where there is a tendency to hurry on to the applications, and moreover, provides a background for later advanced study in modern nonlinear continuum physics. Our ultimate intension was to present the subject matter in a sound manner as clear as possible. We hope that the text provides enough insights for understanding of terminology used scientific state-ofthe art papers and to find the "right and straightforward path" in the scientific world of material surface phenomena.

In what follows a few words of general meaning are worthwhile.

While at one time certain theoretical statements were regarded as "laws" of physics, nowadays many theories prefer to regard each theory as a mathematical model of some aspect of nature. But, any mathematical theory of physics must idealized nature. Then, every theory is only "approximate" in respect to nature

itself. Particularly, it stands for continuous distribution of matter which is the principle assumption of continuum physics.

In physical theory, mathematical rigor is of the essence. Than, a theory is tested by experiment. In this sense, a given theory is "good", if a range of application is greater than another's, it is "better" of the two. This holds as well for a continuum physics approach.

Having these in mind, we organize the text as follows.

The text consists of six sections:

Section 1 - Introduction

In Section 2 - "Interface in problems of continuum physics", is designed to cover the essential features of interfaces problems in continuum physics.

For those who have not been exposed to necessary mathematics we have included a Section 3 "Basic notion of geometry and kinematics of surface", since, for proper understanding of the subject matter requires knowledge of tensor calculus.

In Section 4 - "Material displacement derivative", we concentrated on notion of displacement derivative, the quantity which is of most importance in problems of interfaces.

In Section 5 - "The theory of singular surfaces", the basic techniques for study of propagation of interfaces is derived.

In Section 6 - "Balances laws of bulk material and interface", we start with the formulation of a general equation of balance and proceed by listing special cases that are of particular interest in continuum mechanics and surface of discontinuity.

Finally, in writing this part of the monograph, it has been our hope to make available to the physical and material scientist and engineer some of the more sophisticated mathematical techniques.

2. Interface in Problems of Continuum Physics

Continuum physics is concerned with the description of physical phenomena as observed at the macroscopic level, with no reference to the underlying microstructure of the matter constituting the medium in which the phenomena occur. The medium itself is regarded as a continuous distribution of matter and is referred to as a continuous medium (or simply continuum). Physical quantities (such as mass or velocity) are distributed through the medium, and in mathematical terms are treated as fields. These fields are subject to a number of physical laws which express general principles common to all forms of matter.

The balance laws are formulated as integral equations governing fields defined on regions of space occupied by a material body in motion. A disturbance in the continuity of a phenomenon or physical field is termed a singularity. The aim of our contribution is to present a unified view of the theory of non-relativistic thermodynamics incorporating phenomena with singularities. These singularities will present as discontinuous functions or their derivatives, and in the form of the discontinuity in respect to the Lebesgue measure of physical quantities. The examples of the first type of singularity are shock and acceleration waves. The second type is usually associated with surface concentrations of physical quantities. Discontinuities in fields may be caused by discontinuities in material properties or by some discontinuous behavior of the source which gives rise to the fields. In most problems discontinuities in the source function propagate through the medium, and if the source function is prescribed at the boundary, that is on some initial surface, the carrier of the discontinuity is a moving surface in the medium, which in chemical physics are called interfaces.

Our aim is to draw attention to the fact, which so far has rarely absorbed theoreticians studying continuous media, that a moving surface may carry not only disturbances, but also physical properties different from those of the surrounding media. As an example we consider the direct interaction of two different phases of a material. The phases are usually defined so that we can imagine an interfacial region between the phases. We can model a situation of this kind by the movement of a surface separating two well-behaved material media, while attributing to the surface the physical properties of a phase change. Thus, the term interphase mass transfer simply means the transfer of a component between two or more phases in contact with each other. The component being transferred can undergo reactions in one or both of the phases, or it can be conservative (i.e., nonreactive). Other examples may be provided by phenomena such as the motion of surface dislocations, or the propagation of cracks. In fluid mechanics the surface tension of drops provides an example.

Since the pioneering paper by Gibbs [1], phase transformation phenomena in three-dimensional (3D) continua have been also described by introducing into the body a movable singular surface separating two different material phases in thermodynamic equilibrium state. The phase transformation phenomenon manifests itself best in thin layers of matter: films, membranes, plates, and shells. For example, thin films made of shape-memory alloys like NiTi, NiMnGa, NiTiCu, or NiAl can considerably alter their shapes under appropriate stress and/or temperature changes. Full analysis of the phenomenon in such thin-walled structures is often infeasible if one wants to apply the 3D continuum model. The mechanical description of behavior of such structures can conveniently be based on various 2D models consisting of a base surface endowed with various fields modelling an additional microstructure. Then the notion of a movable surface curve separating 2D regions with different material phases in an appropriate and convenient tool for modelling the phase interface in thin-walled shell structures.

A special focus exists on the fracture at interfaces. Current topics include the role of thermal residual or processing induced stresses, the detailed role of plasticity, and geometric effects on interface crack driving forces. Of particular note in a few of the papers is the focus on multi-scale modelling, a critical link for complete material behavior descriptions. The research described is fundamental by nature, but has engineering relevance in the following areas: thin films, multilayers and assemblies in the semiconductor industry, thermal barrier coatings, and structural engineering composites. It is clear that many research opportunities exist in this field, and it is expected that new contributions will provide direction for this future work (Eshelby [2], Maugin [3], Gurtin [4]).

Great effort has been devoted in recent years to determining the bending rigidity K. Conceptually, two different approaches can be distinguished. In the mechanical approach, the response of the membrane to an applied force is measured, from which the bending rigidity is deduced. The extreme softness of these systems is exploited by the second type of method where the bending rigidity is derived from the thermally excited membrane fluctuations. One example of the mechanical approach (Evans [5], Evans and Needham [6]) is provided by studies of tether formation from giant vesicles which are aspirated with a micro-pipette (Bo and Waugh [7]). Bending elasticity or, in its mathematical formulation, curvature energy not only generates a large variety of shapes, it also leads to different fluctuation or excitation spectra of these shapes and different dynamics than is shown by simple liquid interfaces. These phenomena require different mathematical tools for their description, such as conformal transformations in three dimensions.

A prime motivation to investigate membranes arises from biology in our 3D world (see Seifert [8]). The lipid bilayer is the most elementary and indispensable structural component of biological membranes, which form the boundary of all cells and cell organelles (Alberts et al. [9]). In biological membranes, the bilayer consists of many different lipids and other amphiphiles. Biomembranes are 'decorated' with embedded membrane proteins, which ensure the essential functional properties of a biomembrane such as ion pumping, conversion from light energy to chemical energy, and specific recognition. Often a polymeric network is anchored to the membrane endowing it with further structural stability. This stability is particularly spectacular in red blood cells which can squeeze through tiny capillaries and still recover their rest shape countless times in a life cycle.

Many properties of polymeric systems are not controlled directly by the bulk of the materials but its surface and by internal interfaces. This has been recognized very early and the study of polymers at interfaces has become a major area of Polymer Science.

The study of polymer solutions at interfaces has most often been motivated by the effects of polymers on the stability of colloidal suspensions.

Interfacial effects are also very important in polymer melts. The variation of the surface tension of a polymer melt with molecular weight is associated to subtle interactions between the end points and the interface and only starts to be understood.

Some of the major issues for applications such as adhesion or friction are related to the mechanical properties of interfaces.

The interfacial rheology of polymers at a solid interface dominates the friction properties and strongly depends on the degree of slip of polymers on a surface.

In addition to the possible existence of interfacial-tension gradients at surfactantadsorbed fluid interfaces, other interfacial rheological stresses of a viscous nature may arise, such as those relating to interfacial shear and dilatational viscosities (see Edwards et al. [10], Wasan and Mohan [11]).

Understanding the physical properties of the bilayer through the study of vesicles should provide valuable insight into the physical mechanisms that also govern the more complex biomembranes for which, from this perspective, the artificial vesicle is a model system. Striking phenomenological similarities between the budding and exocytosis where small vesicles bud off the cell membrane encourage a thorough analysis of these artificial membranes. Referring to the biological motivation, a distinction has been emphasized between classical 'biophysics' and a field which acquired the somewhat fancy notion of "biologically inspired physics" (Peliti [12]). While the former field is concerned with the detailed modelling of real biological processes often at the cost of many parameters in a theoretical description the latter approach takes the biological material as inspiration for asking questions biologists often may not even find (yet).

It is also well known that certain chemical components of liquid and gaseous phases will accumulate at interfaces. For example, surfactants in detergents accumulate at the interface of soils and water, thereby allowing dirt to be removed from soiled clothing. Some organic molecules with hydrophobic characteristics can accumulate at the air-water interface to such an extend that very few solvent molecules are present at the interface. These surface films have been studied extensively by physical chemists, and in some cases, the mechanics of the film has yielded information on molecular dimensions. Nitrogen gas is also known to accumulate at solid-gas interfaces, and this property allows us to use nitrogen to determine the surface area of very fine or porous surfaces or adsorbents. Likewise, some molecules or ions may be depleted (negatively adsorbed) at interfaces. In either case, something about the interface is either like or disliked by the molecules in question. Accumulation of molecules at the interface at these three examples suggests that this configuration somehow minimizes the Gibbs function for these systems.

When we are dealing with the propagation of interfaces, we are facing with two basic issues:

- The problem of interface morphology (planar or curved interface, cellular structure; unstationary shape, chaotic, turbulent) as a function of the control parameters.
- The problem of propagation velocity, or growth velocity as a function dendritic of the same control parameters.

From mathematical point of view, interface motion is equivalent to the solution of a free boundary problem. The question is to determine a solution for a scalar field (pressure, temperature, concentration of an impurity) or a vector field (such as a fluid velocity field) satisfying a partial derivatives equation (diffusion equation, Euler or Navier-Stokes equation) with boundary conditions applied on the interface. Saffman-Taylor interface dynamics and dendritic growth appear to be prototypes for the understanding of the dynamics of curved fronts.

3. Basic Notion of Geometry and Kinematics of Surface

For a proper understanding of interfacial (transport) processes, one needs to be familiar with the basic geometrical description of a surface, as shown in the following section. For a terminology or notation, the reader may wish to consult any of the standard textbooks of tensor analysis and differential geometry (see for instance Aris [13], do Carmo [14], Millman and Parker [15], Kreyszig [16] and the bibliography in them).

Here we discuss those elements of geometry and kinematics of surface S_t which are important for our further presentation. Since we confine to the real physical problems we consider E_3 – three dimensional Euclidean space – as a space of physical events. Thus a (material) surface S_t is a subspace of E_3 , i.e., $S_t \in E_3$.

The analytical expression for surface S_t , for each t in an open real interval I, is given by

$$(3.1) \qquad \qquad \mathcal{S}_t: \quad f(\mathbf{x},t) = 0,$$

where by \mathbf{x} and t we denote a point in E_3 and time, respectively. It is assumed that function f is of class $r \ge 1$ in (\mathbf{x}, t) .

Taking into account that S_t is two-dimensional manifold, position of any of its point can be defined in relation to allowable coordinate system u^{α} ($\alpha = 1, 2$) of S_t . In that case, the point $\mathbf{x}(x^k)$, (k = 1, 2, 3), as the point of the surface S_t , is defined by relation $\mathbf{x} = \mathbf{x}(\mathbf{u}, t)$, i.e.,

(3.2)
$$x^k = x^k(u^{\alpha}, t), \quad \operatorname{rank}\left(\frac{\partial x^i}{\partial u^{\alpha}}\right) = 2,$$

for every $\mathbf{x} \in S_t$ (or every $\mathbf{u}(u^{\alpha}) \in D$, where D is a domain of R^2). The second expression in (3.2) represents the condition under which the surface S_t is a regular one.

The coordinates u^{α} are called *Gaussian parameters* of surface S, and they are intrinsic to the surface. This way of presentation is called *parameterization of surface*. Relations (3.2) represent one of many possible parameterizations of surface S_t , unlike its representation (3.1), which is unique.

Taking into consideration (3.2), the position vector \mathbf{p} , with respect to a frame in E_3 , of the point $\mathbf{x} \in S_t$ is given by the expression

(3.3)
$$\mathbf{p}(\mathbf{x}) = \mathbf{p}[x^i(u^{\alpha}, t)], \quad \text{or} \quad \mathbf{p}(\mathbf{u}) = \mathbf{p}(u^{\alpha}, t).$$

In order to be able to apply differential calculus to problems we are going to investigate, we must require the existence of a certain number of partial derivatives of \mathbf{p} (or \mathbf{x}) with respect to u^{α} and t. Further, we note that $\mathbf{p}(u^{\alpha}, t)$ is of class $r \ge 1$.

3.1. The Geometry of Surfaces. When considering the geometry of surface the value of parameter t is fixed. We denote by

(3.4)
$$\mathbf{g}_i \stackrel{\text{def}}{=} \frac{\partial \mathbf{p}}{\partial x^i},$$

the spatial covariant base vectors or natural basis of the curvilinear system x^k . Also, by \mathbf{g}^i we denote contravariant base vectors (dual basis or reciprocal basis of natural basis \mathbf{g}_i).

By definition

(3.5)
$$\mathbf{g}_i \cdot \mathbf{g}^j = \delta_i^j.$$

Here and further δ -systems are generally referred to as the Kronecker deltas.

The metric tensor of Euclidean space E_3 is the identity tensor **I**. Its componental representation is: g_{ij} , g^{ij} or δ_i^j , depending on basis, i.e.,

(3.6)
$$g_{kl} = \mathbf{g}_k \cdot \mathbf{g}_l, \quad g^{kl} = \mathbf{g}^k \cdot \mathbf{g}^l$$

It is easy to show, taking into account (3.5) and (3.6), that $\mathbf{g}^k = g^{kl} \mathbf{g}_l$ and $\mathbf{g}_k = g_{kl} \mathbf{g}^l$. Then (see Cohen and Wang [17])

$$\mathbf{g}_{i,j} = \frac{\partial \mathbf{g}_i}{\partial x^j} - \Gamma^k_{ij} \mathbf{g}_k = 0,$$

where $\Gamma_{ij}^k = \frac{\partial \mathbf{g}_i}{\partial x^j} \cdot \mathbf{g}^k$ is Cristoffel's symbol of the second kind. In the same way, from (3.3) and (3.4) follows

(3.7)
$$\mathbf{a}_{\alpha} \equiv \frac{\partial \mathbf{p}}{\partial u^{\alpha}} = x^{i}_{,\alpha} \mathbf{g}_{i}$$

 \mathbf{a}_{α} are called *covariant base vectors* (or *natural basis*) of curvilinear system u^{α} on surface S and $x^{i}_{,\alpha} = \partial x^{i} / \partial u^{\alpha}$.

From (3.7) and (3.5) it follows that

(3.8)
$$x^i_{,\alpha} = \mathbf{g}^i \cdot \mathbf{a}_{\alpha}$$

Reciprocal base vectors \mathbf{a}^{α} of the base vectors \mathbf{a}_{α} are defined, as in (3.5), by

(3.9)
$$\mathbf{a}_{\alpha} \cdot \mathbf{a}^{\beta} = \delta_{\alpha}^{\beta}.$$

We write $a_{\alpha\beta}$, $a^{\alpha\beta}$, δ^{β}_{α} for the components of *metric tensor* **I** of the surface S. Thus, in particular,

(3.10)
$$a_{\alpha\beta} \equiv \mathbf{a}_{\alpha} \cdot \mathbf{a}_{\beta} = g_{ij} x^{i}_{,\alpha} x^{j}_{,\beta}.$$

Further, it is easy to show, using (3.9), that

(3.11)
$$\mathbf{a}_{\alpha} \equiv a_{\alpha\beta} \mathbf{a}^{\beta}, \quad \mathbf{a}^{\alpha} \equiv a^{\alpha\beta} \mathbf{a}_{\beta}, \quad \text{where} \quad a^{\alpha\beta} = \mathbf{a}^{\alpha} \cdot \mathbf{a}^{\beta}.$$

Also, $a_{\alpha\gamma}a^{\gamma\beta} = \delta^{\beta}_{\alpha}$, which directly follows from (3.11) and (3.9).

The unit normal vector \mathbf{n} to the surface is given by

(3.12)
$$\mathbf{n} = \frac{\operatorname{grad} f}{|\operatorname{grad} f|}, \quad \mathbf{n} \cdot \mathbf{n} = 1.$$

Relative to basis \mathbf{g}_i and \mathbf{g}^i , components of the vector \mathbf{n} are, respectively

(3.13)
$$n^{i} = \mathbf{n} \cdot \mathbf{g}^{i} = \frac{g^{ij} f_{,j}}{|\operatorname{grad} f|}, \quad n_{i} = \mathbf{n} \cdot \mathbf{g}_{i} = \frac{f_{,i}}{|\operatorname{grad} f|}.$$

We note that the direction of **n** is such that the *space orientation* of $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{n})$ is positive. This set of vectors makes a vector basis of E_3 on S.

The orthogonality of ${\bf n}$ on ${\cal S}$ implies the relations

(3.14)
$$\mathbf{a}_{\alpha} \cdot \mathbf{n} = 0, \text{ or } \mathbf{a}^{\alpha} \cdot \mathbf{n} = 0,$$

or equivalently, $n_j x_{,\alpha}^j = g_{ij} n^i x_{,\alpha}^j = 0$, because of (3.7) and (3.13).

¹Here and further we adopt the Einstein summation convention: if an index appears twice in the same term, once as a subscript and once as a superscript, the sign Σ will be omitted.

In many cases we shall make use of the decomposition of basic vectors \mathbf{g}^{i} with respect to the bases $(\mathbf{a}^{1}, \mathbf{a}^{2}, \mathbf{n})$. Then, in view of (3.8), (3.12–3.14)

(3.15)
$$\mathbf{g}^i = n^i \mathbf{n} + x^i_{,\alpha} \mathbf{a}^{\alpha}$$

Also, from $\mathbf{n} \cdot \mathbf{n} = 1$ we obtain $\frac{\partial \mathbf{n}}{\partial u^{\alpha}} \cdot \mathbf{n} = 0$, so that

(3.16)
$$\mathbf{n}_{,\alpha} \equiv \frac{\partial \mathbf{n}}{\partial u^{\alpha}} = -b^{\beta}_{\alpha} \mathbf{a}_{\beta}.$$

The symmetric tensor

$$b_{\alpha\beta} = \mathbf{n} \cdot \frac{\partial \mathbf{a}_{\alpha}}{\partial u^{\beta}} = -\mathbf{a}_{\alpha} \cdot \frac{\partial \mathbf{n}}{\partial u^{\beta}}, \quad b_{\alpha}^{\beta} = a^{\beta\gamma} b_{\alpha\gamma}$$

is known as the fundamental quantity of the second order of surface S. Then

(3.17)
$$\frac{\partial \mathbf{a}_{\alpha}}{\partial u^{\beta}} = b_{\alpha\beta}\mathbf{n} + \Gamma^{\gamma}_{\alpha\beta}\mathbf{a}_{\gamma},$$

where $\Gamma^{\gamma}_{\alpha\beta} = \mathbf{a}^{\gamma} \cdot \frac{\partial \mathbf{a}_{\alpha}}{\partial u^{\beta}}$ is Cristoffel's symbol of the second kind defined on \mathcal{S}_t . In view of (3.17), we write

(3.18)
$$\mathbf{a}_{\alpha,\beta} = \frac{\partial \mathbf{a}_{\alpha}}{\partial u^{\beta}} - \Gamma^{\gamma}_{\alpha\beta} \mathbf{a}_{\gamma} = b_{\alpha\beta} \mathbf{n}$$

Furthermore, making use of $x^i_{;\alpha\beta\gamma} - x^i_{;\alpha\gamma\beta} = x^i_{;\delta}R^{\delta}_{,\alpha\beta\gamma}$ (see McConell [18]), we have

(3.19)
$$\mathbf{a}_{\alpha,\beta\gamma} - \mathbf{a}_{\alpha,\gamma\beta} = \mathbf{a}_{\delta} R^{\delta}_{.\alpha\beta\gamma},$$

where $R^{\delta}_{.\alpha\beta\gamma}$ is the Riemann-Christoffel tensor of a surface. On the other hand, by means of (3.18) and (3.16), it follows that

(3.20)
$$\mathbf{a}_{\alpha,\beta\gamma} - \mathbf{a}_{\alpha,\gamma\beta} = (b_{\alpha\beta,\gamma} - b_{\alpha\gamma,\beta}) \mathbf{n} + (b_{\alpha\gamma}b_{\beta}^{\delta} - b_{\alpha\beta}b_{\gamma}^{\delta}) \mathbf{a}_{\delta}.$$

Then, from (3.19) and (3.20) we have

$$\begin{array}{ll} b_{\alpha\beta,\gamma} = b_{\alpha\gamma,\beta} & \mbox{Mainardi-Codazzi equations,} \\ R^{\delta}_{.\alpha\beta\gamma} = b_{\alpha\gamma}b^{\delta}_{\beta} - b_{\alpha\beta}b^{\delta}_{\gamma} & \mbox{Gauss equations.} \end{array}$$

Furthermore by

(3.21)
$$K_M = \frac{1}{2} b^{\alpha}_{\alpha}, \quad K_G = \det \left(b^{\alpha}_{\beta} \right),$$

we denote the mean curvature and Gaussian curvature of \mathcal{S} , respectively.

Further, we need to know the rate of change (with respect to time) of some geometrical and physical quantities defined on S_t

3.2. Kinematics of Surface. Let us continually observe a point \mathbf{x} , defined by (3.3), as it moves. Now, if we differentiate the equation f = 0 with respect to time, then

(3.22)
$$\frac{\partial f}{\partial t} + \operatorname{grad} f \cdot \frac{\partial \mathbf{p}}{\partial t} = 0,$$

where $\partial \mathbf{p}/\partial t$ is called the *velocity of a point* \mathbf{x} (or equivalently, the point \mathbf{u}) of surface S.

The velocity of point \mathbf{x} is given by

(3.23)
$$\frac{\partial \mathbf{p}}{\partial t} = u\mathbf{n} + v^{\alpha}\mathbf{a}_{\alpha}, \quad \text{or} \quad \frac{\partial x^{i}}{\partial t} = un^{i} + v^{\alpha}x^{i}_{,\alpha}$$

where v_{α} is tangential velocity of the point **x**.

The normal velocity of the surface, u, or the *speed of displacement*, is given by

$$u_n \stackrel{\text{def}}{=} \frac{\partial \mathbf{p}}{\partial t} \cdot \mathbf{n},$$

or, by means of (3.22) and (3.12),

(3.24)
$$u_n = -\frac{\partial f/\partial t}{|\operatorname{grad} f|}.$$

Since the term on the right side of (3.24) is determined by the spatial equation (3.1) alone, it is independent of the choice of the parametrization (3.2) or (3.3). Clearly, the velocity $\partial \mathbf{p}/\partial t$ depends on a particular choice of the surface coordinates.

3.2.1. Orthogonal Parametrization. When the parametrization u^{α} of the surface S is such that velocities of the surface points are always orthogonal on it, i.e., when $v^{\alpha} = 0$, then (3.23)

(3.25)
$$\frac{\partial \mathbf{p}}{\partial t}\Big|_{\mathbf{u}} = \underbrace{u\mathbf{n}}_{n} \quad \text{or} \quad \frac{\partial x^{i}}{\partial t}\Big|_{u^{\alpha}} = \underbrace{un^{i}}_{n}.$$

Such parametrization of the surface S is called *orthogonal* (see Fig. 1).

With respect to such parametrization, for observer who is outside the surface, position of the surface points is fixed, because there is no tangential component of the velocity to the surface. Therefore, such coordinates $u^{\alpha} \equiv \zeta^{\alpha}$ have advantage over other allowable coordinate systems of the surface because, with respect to them, expressions are considerably simplified.

We point out that the simplest forms of parametrization of surface S are not always its orthogonal parametrization. Also, in general, orthogonal parametrization has local character.

4. Material displacement derivative

4.1. Componental Formulation and Consideration. Here, we concentrate on notion of a *displacement derivative*, the quantity which is of most importance in dynamical problems of (material) interfaces.

We emphasize that we will here deal, in general, with double tensor fields, which are defined with respect to E_3 and surface S(t) embedded in E_3 . Thus, we will

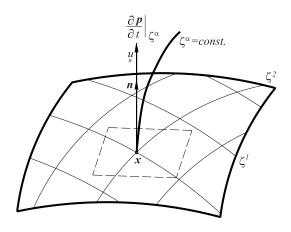


Figure 1

deal with the quantities which obey the transformation law for a tensor under the following groups of transformations $\bar{x}^i = \bar{x}^i(x^j)$, $\bar{u}^\alpha = \bar{u}^\alpha(u^\beta, t)$. In other words, we are interested in the rate of change with respect to time of these quantities when their tensor character is preserved.

Following Thomas [19] we have introduced the notion of displacement derivative (or δ -time derivative) for an arbitrary time-dependent field f in \mathbb{D} confined to the surface S(t), defined as the time derivative of f along the normal trajectory. In order to improve this definition Truesdell and Toupin, [20] suggested a generalization of Thomas's derivative to two-point tensor fields. Their derivative reduces to Thomas's derivative in the case of one-point fields.

However, as pointed out by Bowen and Wang [21], (see also Kosiński [22]) the generalization of the displacement derivation given by Truesdell and Toupin has to be modified: the value of the Truesdell–Toupin derivative of a given geometrical object depends on the basis in which that object is represented, that is whether it is the spatial basis in E_3 or the basis of surface vectors. In order to rectify this error Bowen and Wang introduced what they called the *total displacement derivative* of a function, this being the partial time derivative of the function defined on a surface given in *convected parametrization*². Since, in a convected parametrization ζ^{α} , (Bowen and Wang [21]), the geometrical locus of the surface point $\zeta^{\alpha} = \text{const}$. is the normal trajectory of the surface, the displacement derivative is $\delta \tilde{f}/\delta t$, where $\tilde{f}(\zeta^{\alpha}, t) = f(\mathbf{x}(\zeta^{\alpha}, t), t)$. Thus, it is defined as the time derivative of \tilde{f} if the moving surface S(t) is given in the convected parametrization $\mathbf{x} = \mathbf{x}(\zeta^{\alpha}, t), t$). Jarić and Milanović-Lazarević [23] have extended the definition of the displacement derivative to any (not necessarily convected) surface coordinate system. Cohen and Wang [17] call it *transverse displacement derivative*.

 $^{^{2}}$ Concept of convected coordinates, in both mathematics and continuum mechanics has wider meaning (see Truesell and Toupin [20], Aris [13]).

We shall apply this notion to the time derivative of tensor quantities along the trajectory of a material points of the surface S(t), that is, when $U^{\Delta} = \text{const.}$ We call the time derivative of this kind *material displacement derivative* in order to emphasize its physical meaning. Because of its importance we give its derivation in detail. As before, S(t) is given with respect to the orthogonal parametrization u^{α} .

Let $\Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}(\mathbf{x}, \mathbf{u}, t)$ be a double tensor field on S(t), under the group of transformations $\mathbf{\bar{x}} = \mathbf{\bar{x}}(\mathbf{x})$, $\mathbf{\bar{u}} = \mathbf{\bar{u}}(\mathbf{u}, t)$. Then

$$\bar{\Psi}^{i\ldots j\alpha\ldots\beta}_{k\ldots l\kappa\ldots\lambda} = \Psi^{p\ldots q\pi\ldots\theta}_{r\ldots s\varrho\ldots\sigma} \frac{\partial \bar{x}^{i}}{\partial x^{p}} \ldots \frac{\partial \bar{x}^{j}}{\partial x^{q}} \frac{\partial \bar{u}^{\alpha}}{\partial u^{\pi}} \ldots \frac{\partial \bar{u}^{\beta}}{\partial u^{\theta}} \frac{\partial x^{r}}{\partial \bar{x}^{k}} \ldots \frac{\partial x^{s}}{\partial \bar{x}^{l}} \frac{\partial u^{\varrho}}{\partial \bar{u}^{\kappa}} \ldots \frac{\partial u^{\sigma}}{\partial \bar{u}^{\lambda}}$$

Since, $\mathbf{x} = \mathbf{x}(\mathbf{u}, t)$ and $\mathbf{u} = \mathbf{u}(\mathbf{U}, t)$, where U is material parametrization, then

$$\bar{\mathbf{u}} = \bar{\mathbf{u}}(\mathbf{u}(\mathbf{U},t),t) = \bar{\mathbf{u}}(\mathbf{U},t),$$
$$\bar{\mathbf{x}} = \bar{\mathbf{x}}[\mathbf{x}(\mathbf{u},t)] = \bar{\mathbf{x}}\{\mathbf{x}[\mathbf{u}(\mathbf{U},t),t]\} = \bar{\mathbf{x}}(\mathbf{U},t).$$

Thus, when $U^{\Delta} = \text{const}$

$$(4.1) \quad \frac{d\bar{\Psi}^{i\ldots,j\alpha\ldots,\beta}_{k\ldots,l\kappa\ldots\lambda}}{dt} = \frac{d\Psi^{p\ldots,q\pi\ldots,\theta}_{r\ldots s\varrho\ldots\sigma}}{dt} \frac{\partial\bar{x}^{i}}{\partial x^{p}} \cdots \frac{\partial u^{\sigma}}{\partial\bar{u}^{\lambda}} + \Psi^{p\ldots,q\pi\ldots,\theta}_{r\ldots s\varrho\ldots\sigma} \frac{d}{dt} \left(\frac{\partial\bar{x}^{i}}{\partial x^{p}}\right) \cdots \frac{\partial u^{\sigma}}{\partial\bar{u}^{\lambda}} + \dots + \Psi^{p\ldots,q\pi\ldots,\theta}_{r\ldots s\varrho\ldots\sigma} \frac{\partial\bar{x}^{i}}{\partial x^{p}} \cdots \frac{d}{dt} \left(\frac{\partial u^{\sigma}}{\partial\bar{u}^{\lambda}}\right)$$

Now, we have to calculate the terms which are derivatives of second order, like

$$\frac{d}{dt}\left(\frac{\partial \bar{x}^i}{\partial x^p}\right),\ldots,\frac{d}{dt}\left(\frac{\partial u^{\sigma}}{\partial \bar{u}^{\lambda}}\right).$$

We start with

$$\frac{d\bar{x}^i}{dt} = \frac{\partial \bar{x}^i}{\partial x^a} \frac{\partial x^a}{\partial t}, \quad \frac{d}{dt} \left(\frac{\partial \bar{x}^i}{\partial x^p}\right) = \frac{\partial^2 \bar{x}^i}{\partial x^p \partial x^a} \frac{dx^a}{dt}.$$

But,

$$\frac{\partial^2 \bar{x}^i}{\partial x^p \partial x^a} = \Gamma^b_{pa} \frac{\partial \bar{x}^i}{\partial x^b} + \bar{\Gamma}^i_{cd} \frac{\partial \bar{x}^c}{\partial x^p} \frac{\partial \bar{x}^d}{\partial x^a},$$

so that

(4.2)
$$\frac{d}{dt} \left(\frac{\partial \bar{x}^i}{\partial x^p} \right) = \Gamma^b_{pa} \frac{dx^a}{dt} \frac{\partial \bar{x}^i}{\partial x^b} - \bar{\Gamma}^i_{cd} \frac{d\bar{x}^d}{dt} \frac{\partial \bar{x}^c}{\partial x^p}.$$

On the other hand,

(4.3)
$$\frac{d}{dt}\frac{\partial \bar{u}^{\alpha}}{\partial u^{\pi}} = \frac{\partial}{\partial t}\left(\frac{\partial \bar{u}^{\alpha}}{\partial u^{\pi}}\right) + \frac{\partial^2 \bar{u}^{\alpha}}{\partial u^{\pi} \partial u^{\nu}}\frac{du^{\nu}}{dt}.$$

Also,

$$\frac{d\bar{u}^{\alpha}}{dt} = \frac{\partial\bar{u}^{\alpha}}{\partial t} + \frac{\partial\bar{u}^{\alpha}}{\partial u^{\nu}}\frac{du^{\nu}}{dt},$$

from which we get

(4.4)
$$\frac{\partial}{\partial u^{\pi}} \frac{d\bar{u}^{\alpha}}{dt} = \frac{\partial}{\partial u^{\pi}} \frac{\partial\bar{u}^{\alpha}}{\partial t} + \frac{\partial^{2}\bar{u}^{\alpha}}{\partial u^{\pi}\partial u^{\nu}} \frac{du^{\nu}}{dt} + \frac{\partial\bar{u}^{\alpha}}{\partial u^{\pi}} \frac{\partial}{\partial u^{\nu}} \frac{du^{\pi}}{dt}.$$

From (4.3) and (4.4) we have

(4.5)
$$\frac{d}{dt}\frac{\partial \bar{u}^{\alpha}}{\partial u^{\pi}} = \frac{\partial}{\partial u^{\pi}}\frac{d\bar{u}^{\alpha}}{dt} - \frac{\partial \bar{u}^{\alpha}}{\partial u^{\pi}}\frac{\partial}{\partial u^{\nu}}\frac{du^{\pi}}{dt}.$$

The term $\frac{d}{dt}\frac{\partial u^{\alpha}}{\partial \bar{u}^{\pi}}$ follows directly from (4.5) when we strictly interchange the role of u^{α} and \bar{u}^{α} . Then, substituting (4.2) and (4.3) into (4.1), after long calculation and rearranging the terms, we get

$$\frac{\delta_m \bar{\Psi}_{k\dots l\kappa\dots\lambda}^{i\dots j\alpha\dots\beta}}{\delta t} = \frac{\delta_m \Psi_{r\dots s\varrho\dots \sigma}^{p\dots q\pi\dots \theta}}{\delta t} \frac{\partial \bar{x}^i}{\partial x^p} \cdots \frac{\partial x^s}{\partial \bar{x}^l} \frac{\partial u^{\varrho}}{\partial \bar{u}^{\kappa}} \cdots \frac{\partial u^{\sigma}}{\partial \bar{u}^{\lambda}}.$$

where by $\delta_m/\delta t$ we denote material displacement derivative, i.e.,

(4.6)
$$\frac{\delta_m \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}}{\delta t} \stackrel{\text{def}}{=} \frac{d\Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}}{dt} \Big|_{\mathbf{U}} + \pounds \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta} \\ = \frac{\partial \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}}{\partial t} \Big|_{\mathbf{x},\mathbf{u}} + \Psi_{k...l\kappa...\lambda,m}^{i...j\alpha...\beta} \frac{dx^m}{dt} + \pounds \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}$$

But, in view of (3.25),

(4.7)
$$\frac{\delta_m \mathbf{x}}{\delta t} = \frac{\partial \mathbf{x}}{\partial t} \Big|_{\mathbf{u}} + \dot{u}^{\alpha} \mathbf{a}_{\alpha} \quad \text{or} \quad \frac{dx^i}{dt} = \frac{\partial x^i}{\partial t} \Big|_{\mathbf{u}} + \dot{u}^{\alpha} x^i_{,\alpha} = u_n n^i + \dot{u}^{\alpha} x^i_{,\alpha},$$

so that

(4.8)
$$\frac{\delta_m \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}}{\delta t} \stackrel{\text{def}}{=} \frac{\partial \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}}{\partial t} \Big|_{\mathbf{x},\mathbf{u}} + \Psi_{k...l\kappa...\lambda,mn}^{i...j\alpha...\beta} un^m + \Psi_{k...l\kappa...\lambda,mn}^{i...j\alpha...\beta} x_{\gamma}^m \dot{u}^{\gamma} + \pounds \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta},$$

where

$$\begin{split} \pounds \Psi_{\mathbf{\dot{u}}}^{i...j\alpha...\beta} \stackrel{\text{def}}{=} \dot{u}^{\nu} \frac{\partial \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}}{\partial u^{\nu}} + \Psi_{k...l\nu...\lambda}^{i...j\alpha...\beta} \frac{\partial \dot{u}^{\nu}}{\partial u^{\kappa}} + \dots + \Psi_{k...l\kappa...\nu}^{i...j\alpha...\beta} \frac{\partial \dot{u}^{\nu}}{\partial u^{\lambda}} \\ &- \Psi_{k...l\kappa...\lambda}^{i...j\nu...\beta} \frac{\partial \dot{u}^{\alpha}}{\partial u^{\nu}} - \dots - \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\nu} \frac{\partial \dot{u}^{\beta}}{\partial u^{\nu}} \\ &= \dot{u}^{\nu} \Psi_{k...l\kappa...\lambda,\nu}^{i...j\alpha...\beta} + \Psi_{k...l\nu...\lambda}^{i...j\alpha...\beta} \dot{u}_{,\kappa}^{\nu} + \dots + \Psi_{k...l\kappa...\nu}^{i...j\alpha...\beta} \dot{u}_{,\lambda}^{\nu} \\ &- \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta} \dot{u}_{,\nu}^{\alpha} - \dots - \Psi_{k...l\kappa...\lambda}^{i...j\alpha...\nu} \dot{u}_{,\nu}^{\beta} \end{split}$$

is the *Lie derivative* of the field $\Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}$ with respect to the velocity field $\dot{\mathbf{u}} = \dot{u}^{\alpha} \mathbf{a}_{\alpha}$. We point out that, according to this definition,

$$\dot{u}^{\alpha} \stackrel{\text{def}}{=} \frac{\delta_m u^{\alpha}}{\delta t} \Big|_{U^{\Delta} = \text{const}} = \frac{du^{\alpha}}{dt}.$$

It is easy to show that the material displacement derivative has the following properties:

- (i) the material displacement derivative of a sum of tensor fields equals the sum of the material displacement derivative of the summands;
- (ii) the rule of Leibniz holds for tensor product of tensor quantities and for product of tensor fields.

Remark. The expression (4.8) for material displacement derivative differs both by form and by content from displacement derivative defined by Truesdell and Toupin [20, Eq. (179.5)]

(4.9)
$$\frac{\delta_d \Psi_{k\dots l \kappa \dots \lambda}^{i\dots j \alpha \dots \beta}}{\delta t} \stackrel{\text{def}}{=} \frac{\partial \Psi_{k\dots l \kappa \dots \lambda}^{i\dots j \alpha \dots \beta}}{\partial t} \Big|_{\mathbf{x}, \mathbf{u}} + \Psi_{k\dots l \kappa \dots \lambda, m_n}^{i\dots j \alpha \dots \beta} m^m + \pounds \Psi_{k\dots l \kappa \dots \lambda}^{i\dots j \alpha \dots \beta}.$$

This is obvious if (4.8) is written in the following form

$$\frac{\delta_m \Psi_{k\dots l \kappa \dots \lambda}^{i\dots j \alpha \dots \beta}}{\delta t} = \frac{\delta_d \Psi_{k\dots l \kappa \dots \lambda}^{i\dots j \alpha \dots \beta}}{\delta t} + \Psi_{k\dots l \kappa \dots \lambda, m}^{i\dots j \alpha \dots \beta} x_{\gamma}^m \dot{u}^{\gamma}.$$

Thus $\delta_m/\delta t$ and $\delta_d/\delta t$ are the same only when $u^{\alpha} = \delta^{\alpha}_{\Delta} U^{\Delta}$.

4.2. Material Displacement Derivative of Basic Surface Quantities.

a. Surface base vectors. Material displacement derivative can be applied to all systems, independently of their nature, which satisfy the law of transformation of tensor quantities. Particularly, for the base vectors \mathbf{g}_i it is easy to show that

(4.10)
$$\frac{\delta_m \mathbf{g}_k}{\delta t} = \mathbf{0}.$$

However, it is not the case when the material displacement derivative of surface base vectors \mathbf{a}_{α} are in question. Then \mathbf{a}_{α} dependents explicitly on time so that, in view of (4.6),

$$\frac{\delta_m \mathbf{a}_\alpha}{\delta t} = \frac{\partial \mathbf{a}_\alpha}{\partial t} + \mathbf{a}_{\alpha,k} \frac{dx^k}{dt} + \pounds_{\dot{\mathbf{u}}} \mathbf{a}_\alpha.$$

But, according to (3.25) and (3.16),

$$\frac{\partial \mathbf{a}_{\alpha}}{\partial t} = \frac{\partial}{\partial t} \frac{\partial \mathbf{p}}{\partial u^{\alpha}} = \frac{\partial}{\partial u^{\alpha}} \frac{\partial \mathbf{p}}{\partial t} = \frac{\partial}{\partial u^{\alpha}} (u\mathbf{n}) = u_{n,\alpha}\mathbf{n} - u_{n}b_{\alpha}^{\beta}\mathbf{a}_{\beta},$$

 $\mathbf{a}_{\alpha,k} = 0$ and $\underset{\dot{\mathbf{u}}}{\pounds} \mathbf{a}_{\alpha} = \dot{u}^{\beta} \mathbf{a}_{\beta,\alpha} + \mathbf{a}_{\beta} \dot{u}_{,\alpha}^{\beta} = \dot{u}^{\beta} b_{\alpha\beta} \mathbf{n} + \mathbf{a}_{\beta} \dot{u}_{,\alpha}^{\beta}$, so that

(4.11)
$$\frac{\delta_m \mathbf{a}_{\alpha}}{\delta t} = \left(u_{n,\alpha} + b_{\alpha\beta} \dot{u}^{\beta} \right) \mathbf{n} + \left(\dot{u}_{,\alpha}^{\beta} - u_n^{\beta} b_{\alpha}^{\beta} \right) \mathbf{a}_{\beta}.$$

Than making use of $\mathbf{a}_{\alpha} = x_{:\alpha}^{i} \mathbf{g}_{i}$, (4.10) and (4.11), we get

(4.12)
$$\frac{\delta_m x_{;\alpha}^i}{\delta t} = \left(u_{,\alpha} + b_{\alpha\beta} \dot{u}^\beta\right) n^i + \left(\dot{u}_{,\alpha}^\beta - u_n^\beta b_\alpha^\beta\right) x_{,\beta}^i.$$

b. Unit normal vector to a surface. In the same way, it is easy to show that

$$\frac{\delta_m \mathbf{n}}{\delta t} = \frac{d\mathbf{n}}{dt} = -\left(\underbrace{u}_{n,\alpha} + b_{\alpha\beta} \dot{u}^\beta\right) \mathbf{a}^\alpha.$$

c. Metric tensor (first fundamental tensor) of a surface. Trivially, from (3.6) and (4.10), we have

(4.13)
$$\frac{\delta_m g_{ij}}{\delta t} = 0, \quad \frac{\delta_m g^{ij}}{\delta t} = 0.$$

Than, from (3.10), (4.13) and (4.12), we get

(4.14)
$$\frac{\delta_m a_{\alpha\beta}}{\delta t} = 2 \left[\dot{u}_{(\alpha,\beta)} - u b_{\alpha\beta} \right].$$

d. Determinant of metric tensor of a surface. Let $a = \det(a_{\alpha\beta})$. Then

$$\frac{\delta_m a}{\delta t} = \frac{\partial a}{\partial a_{\alpha\beta}} \frac{\delta_m a_{\alpha\beta}}{\delta t} = a a^{\alpha\beta} \frac{\delta_m a_{\alpha\beta}}{\delta t}.$$

But, $a_{,\alpha} = 0$ so that

(4.15)
$$\frac{\delta_m a}{\delta t} = 2a \left(\dot{u}^{\alpha}_{,\alpha} - u b^{\alpha}_{\alpha} \right)$$

where we made use of (4.14).

For further discussion the following relation is required

$$\frac{\delta_m \sqrt{a}}{\delta t} = \sqrt{a} \left(\dot{u}^{\alpha}_{,\alpha} - u b^{\alpha}_{\alpha} \right),$$

which follows directly from (4.15).

e. Second fundamental tensor of a surface. In order to calculate the material displacement derivative $b_{\alpha\beta}$ we start with (3.18). Then,

(4.16)
$$\frac{\delta_m b_{\alpha\beta}}{\delta t} = \frac{\delta_m \mathbf{a}_{\alpha,\beta}}{\delta t} \cdot \mathbf{n} = \left(\frac{\partial \mathbf{a}_{\alpha,\beta}}{\partial t} + \pounds \mathbf{a}_{\alpha,\beta}\right) \cdot \mathbf{n}$$
$$= \underbrace{u}_{n,\alpha\beta} - \underbrace{u}_{n} b_{\alpha\gamma} b_{\beta}^{\gamma} + b_{\alpha\beta,\gamma} \dot{u}^{\gamma} + b_{\alpha\gamma} \dot{u}_{,\beta}^{\gamma} + b_{\beta\gamma} \dot{u}_{,\alpha}^{\gamma}.$$

f. Contravariant and mixed representation of material derivative. From (4.13) we see that the tensors g_{ij} , g^{ij} and δ^i_j behave as though they were constants in material differentiation with respect to t. However, this is not the case with surface metric tensor $a_{\alpha\beta}$ as can be seen from (4.14), and it is the consequence of its explicit dependence of time. Then the operation of raising and lowering of indices of tensor fields with respect to $a_{\alpha\beta}$ is not, generally, commutative with material time derivative. Particularly, this is true for $a^{\alpha\beta}$. Indeed, it is easy to show that

$$\frac{\delta_m a^{\alpha\beta}}{\delta t} = -a^{\alpha\gamma} a^{\beta\delta} \frac{\delta_m a_{\gamma\delta}}{\delta t} = -2 \left[\dot{u}^{(\alpha,\beta)} - u b^{\alpha\beta} \right],$$

where we have used $(4.14)^3$.

Another quantity of importance for further investigation is b_{α}^{β} . Then, from the relation $b_{\alpha}^{\beta} = b_{\alpha\gamma} a^{\gamma\beta}$, after some calculation, we get

(4.17)
$$\frac{\delta_m b^{\gamma}_{\alpha}}{\delta t} = u_{n,\alpha}^{\gamma} + u_n b_{\alpha\beta} b^{\beta\gamma} + b^{\gamma}_{\beta} \dot{u}^{\beta}_{,\alpha} + b^{\gamma}_{\alpha,\beta} \dot{u}^{\beta} - b^{\beta}_{\alpha} \dot{u}^{\gamma}_{,\beta}.$$

³It is important to notice that $\frac{\delta_m \delta^{\alpha}_{\beta}}{\delta t} = 0$, since, by definition $\frac{\delta_m \delta^{\alpha}_{\beta}}{\delta t} = \frac{\partial \delta^{\alpha}_{\beta}}{\partial t} + \pounds \delta^{\alpha}_{\beta} = \pounds \delta^{\alpha}_{\beta} \equiv 0$.

g. Mean curvature of the surface. In the same way, we can derive material derivatives of the other quantities as $b = \det b_{\alpha\beta}$, K_M , K_G , etc. Thus, from (4.17), contraction with respect to indices α and β , leads to

(4.18)
$$2\frac{\delta_m K_M}{\delta t} = u_{n,\alpha}^{\ \alpha} + u_n b_{\alpha}^{\gamma} b_{\gamma}^{\alpha} + 2K_{M,\gamma} \dot{u}^{\gamma}.$$

This relation can be reduced, by using the Cayley-Hamilton's theorem,

$$(4.19) B2 - IBB + I \det B = 0,$$

where $\boldsymbol{B} = \|b_{\beta}^{\alpha}\|$ and $\boldsymbol{I} = \|\delta_{\beta}^{\alpha}\|$. But, $I_B = \operatorname{tr} \boldsymbol{B} = 2K_M$ and $\det \boldsymbol{B} = K_G$, which follows from (3.21). Also, $\operatorname{tr} \boldsymbol{B}^2 = b_{\alpha}^{\gamma} b_{\gamma}^{\alpha} = 2(2K_M^2 - K_G)$. Then (4.18) can be written in the following form

$$\frac{\delta_m K_M}{\delta t} = K_{M,\alpha} \dot{u}^{\alpha} + \underset{n}{u} \left(2K_M^2 - K_G \right) + \frac{1}{2} \underset{n}{u}_{,\alpha}^{\alpha},$$

or more concisely

$$\frac{\delta_m K_M}{\delta t} = \frac{1}{2} \Delta_s u_n + u_n \left(2K_M^2 - K_G \right) + \dot{\mathbf{u}} \cdot \nabla_s K_M,$$

where surface gradient and surface Laplace operator on S_t are denoted by ∇_s and Δ_s , respectively.

h. Gaussian curvature of a surface. In order to determine $\delta_m K_G/\delta t$ we use the following identities

$$\frac{\delta_m K_M}{\delta t} \equiv \frac{1}{2} \frac{\delta_m (\operatorname{tr} \boldsymbol{B})}{\delta t} = \frac{1}{2} \operatorname{tr} \frac{\delta_m \boldsymbol{B}}{\delta t},$$
$$\frac{\delta_m K_G}{\delta t} \equiv 4 \frac{\delta_m K_M}{\delta t} K_M - \operatorname{tr} \left(\frac{\delta_m \boldsymbol{B}}{\delta t} \boldsymbol{B} \right)$$

where last identity follows from (4.19). From (4.16), after some calculation, we get

$$\operatorname{tr}\left(\frac{\delta_m \boldsymbol{B}}{\delta t}\boldsymbol{B}\right) = u_{n,\alpha\beta}b^{\alpha\beta} + 2uK_M\left(4K_M^2 - 3K_G\right) + b_\beta^\alpha b_{\alpha,\gamma}^\beta \dot{u}^\gamma.$$

Then

$$\frac{\delta_m K_G}{\delta t} = u_{n,\alpha}^{\ \beta} \left(2K_M \delta_\beta^\alpha - b_\beta^\alpha \right) + 2u_n K_M K_G + \left(4K_M K_{M,\gamma} - b_\beta^\alpha b_{\alpha,\gamma}^\beta \right) \dot{u}^\gamma$$

or finally

$$\frac{\delta_m K_G}{\delta t} = u_{n,\alpha}^{\ \beta} \left(2K_M \delta_\beta^\alpha - b_\beta^\alpha \right) + 2u_n K_M K_G + \dot{\mathbf{u}} \cdot \nabla_s K_G$$

4.2.1. The List of Basic Results. For later reference, we record the following formulas:

$$\frac{\delta_m \mathbf{a}_{\alpha}}{\delta t} = \left(u_{n,\alpha} + b_{\alpha\beta} \dot{u}^{\beta} \right) \mathbf{n} + \left(\dot{u}_{,\alpha}^{\beta} - u_n^{\beta} b_{\alpha}^{\beta} \right) \mathbf{a}_{\beta},$$
$$\frac{\delta_m \mathbf{n}}{\delta t} = - \left(u_{n,\alpha} + b_{\alpha\beta} \dot{u}^{\beta} \right) \mathbf{a}^{\alpha},$$
$$\frac{\delta_m a_{\alpha\beta}}{\delta t} = 2 \left[\dot{u}_{(\alpha,\beta)} - u_n^{\beta} b_{\alpha\beta} \right],$$

$$(4.20) \qquad \qquad \frac{\delta_m a^{\alpha\beta}}{\delta t} = 2 \left[u b^{\alpha\beta} - \dot{u}^{(\alpha,\beta)} \right], \\ \left(4.20 \right) \qquad \qquad \frac{\delta_m \sqrt{a}}{\delta t} = \sqrt{a} \left(\dot{u}^{\alpha}_{,\alpha} - u b^{\alpha}_{,\alpha} \right) = \sqrt{a} \left(\nabla_s \cdot \dot{\mathbf{u}} - 2 u K_M \right), \\ \left(\frac{\delta_m b_{\alpha\beta}}{\delta t} = u_{,\alpha\beta} - u b_{\alpha\gamma} b^{\gamma}_{,\beta} + b_{\alpha\gamma} \dot{u}^{\gamma}_{,\beta} + b_{\beta\gamma} \dot{u}^{\gamma}_{,\alpha} + b_{\alpha\beta,\gamma} \dot{u}^{\gamma}, \\ \left(\frac{\delta_m b^{\alpha}_{,\alpha}}{\delta t} = u_{,\alpha}^{,\beta} + u b_{\alpha\gamma} b^{\beta\gamma} + b^{\beta}_{,\gamma} \dot{u}^{\gamma}_{,\alpha} + b^{\beta}_{,\alpha,\gamma} \dot{u}^{\gamma} - b^{\gamma}_{,\alpha} \dot{u}^{\beta}_{,\gamma}, \\ \left(\frac{\delta_m K_M}{\delta t} = \frac{1}{2} \Delta_s u + u_n \left(2 K_M^2 - K_G \right) + \dot{\mathbf{u}} \cdot \nabla_s K_M, \\ \left(\frac{\delta_m K_G}{\delta t} = u_{,\alpha}^{,\beta} \left(2 K_M \delta^{\alpha}_{,\beta} - b^{\alpha}_{,\beta} \right) + 2 u K_M K_G + \dot{\mathbf{u}} \cdot \nabla_s K_G. \end{cases}$$

Remark. It would be appropriate here to emphasize the difference between material surface derivatives $\delta_m/\delta t$ and D_m/D defined by Truesdell and Toupin [20]. Namely, the concept of $\delta_m/\delta t$ is more general than D_m/D and it reduces to D_m/D in the case when the surface is stationary, that is, when u = 0.

When $U^{\Delta} = \delta^{\Delta}_{\alpha} u^{\alpha}$, then $U^{\Delta} = \text{const}$ is orthogonal trajectory of material particles of surface. From mathematical point of view, it means that we are talking about orthogonal parametrization as the referent one. Then

$$\frac{\delta_{m}\mathbf{a}_{\alpha}}{\delta t} = u_{n,\alpha}\mathbf{n} - u_{n}b_{\alpha}^{\beta}\mathbf{a}_{\beta},
\frac{\delta_{m}\mathbf{n}}{\delta t} = -u_{n,\alpha}\mathbf{a}^{\alpha},
\frac{\delta_{m}a_{\alpha\beta}}{\delta t} = -2ub_{\alpha\beta},
\frac{\delta_{m}a^{\alpha\beta}}{\delta t} = 2ub^{\alpha\beta},
\frac{\delta_{m}\sqrt{a}}{\delta t} = -u_{n}\sqrt{a}b_{\alpha}^{\alpha} = -2u\sqrt{a}K_{M},
\frac{\delta_{m}b_{\alpha\beta}}{\delta t} = u_{n,\alpha\beta} - ub_{\alpha\gamma}b_{\beta}^{\gamma},
\frac{\delta_{m}b_{\alpha}^{\beta}}{\delta t} = u_{n,\alpha\beta} + ub_{\alpha\gamma}b^{\beta\gamma},
\frac{\delta_{m}K_{M}}{\delta t} = \frac{1}{2}\Delta_{s}u_{n} + u_{n}\left(2K_{M}^{2} - K_{G}\right),
\frac{\delta_{m}K_{G}}{\delta t} = u_{n,\alpha}^{\beta}\left(2K_{M}\delta_{\beta}^{\alpha} - b_{\beta}^{\alpha}\right) + 2uK_{M}K_{G}.$$

These relations are identical with corresponding expressions of Truesdell and Toupin [20] and then $\frac{\delta_m}{\delta t} \equiv \frac{\delta_d}{\delta t}$ (see also Kosiński [22], Müller [24] and Jarić et al. [25]).

4.2.2. General Consideration. Until now, we have discussed the material displacement derivative of tensor quantities which are defined by their components

with respect to an arbitrary admissible coordinate systems x^i in E_3 and u^{α} in S_t , for example for $\Psi_{k...l\kappa...\lambda}^{i...j\alpha...\beta}(\mathbf{x}, \mathbf{u}, t)$. However, generally we need the expression of material displacement derivative for

$$\Psi = \Psi_{p...q\Lambda...\Sigma}^{k...m\Gamma...\Delta} \mathbf{g}_k \cdots \otimes \mathbf{g}_m \otimes \mathbf{g}^p \otimes \cdots \mathbf{g}^q \otimes \mathbf{a}_{\Gamma} \cdots \otimes \mathbf{a}_\Delta \otimes \mathbf{a}^\Lambda \cdots \otimes \mathbf{a}^\Sigma$$

given in U^{Δ} .

Then, in view of its properties and (4.10), we have

$$\frac{\delta_m}{\delta t} \Psi = \left(\frac{\delta_m}{\delta t} \Psi_{p \cdots q \Lambda \cdots \Sigma}^{k \cdots m \Gamma \cdots \Delta}\right) \mathbf{g}_k \cdots \otimes \mathbf{g}_m \otimes \mathbf{g}^p \otimes \cdots \mathbf{g}^q \otimes \mathbf{a}_{\Gamma} \cdots \otimes \mathbf{a}_{\Delta} \otimes \mathbf{a}^{\Lambda} \cdots \otimes \mathbf{a}^{\Sigma} + \Psi_{p \cdots q \Lambda \cdots \Sigma}^{k \cdots m \Gamma \cdots \Delta} \mathbf{g}_k \cdots \otimes \mathbf{g}_m \otimes \mathbf{g}^p \otimes \cdots \mathbf{g}^q \otimes \frac{\delta_m}{\delta t} \mathbf{a}_{\Gamma} \cdots \otimes \mathbf{a}_{\Delta} \otimes \mathbf{a}^{\Lambda} \cdots \otimes \mathbf{a}^{\Sigma}$$
(1.22)

+
$$\Psi_{p...,q\Lambda...\Sigma}^{k...m\Gamma...\Delta}$$
 $\mathbf{g}_k \cdots \otimes \mathbf{g}_m \otimes \mathbf{g}^p \otimes \cdots \mathbf{g}^q \otimes \mathbf{a}_{\Gamma} \cdots \otimes \mathbf{a}_{\Delta} \otimes \mathbf{a}^{\Lambda} \cdots \otimes \frac{\delta_m}{\delta t} \mathbf{a}^{\Sigma}$,

Particularly, in the case of orthogonal parametrization we obtained

$$\frac{\delta_d}{\delta t} \Psi = \left(\frac{\delta_d}{\delta t} \Psi_{p...,q\Lambda...\Sigma}^{k...m\Gamma...\Delta}\right) \mathbf{g}_k \cdots \otimes \mathbf{g}_m \otimes \mathbf{g}^p \otimes \cdots \mathbf{g}^q \otimes \mathbf{a}_{\Gamma} \cdots \otimes \mathbf{a}_{\Delta} \otimes \mathbf{a}^{\Lambda} \cdots \otimes \mathbf{a}^{\Sigma} + \Psi_{p...,q\Lambda...\Sigma}^{k...m\Gamma...\Delta} \mathbf{g}_k \cdots \otimes \mathbf{g}_m \otimes \mathbf{g}^p \otimes \cdots \mathbf{g}^q \otimes \frac{\delta_d}{\delta t} \mathbf{a}_{\Gamma} \cdots \otimes \mathbf{a}_{\Delta} \otimes \mathbf{a}^{\Lambda} \cdots \otimes \mathbf{a}^{Sigma} :$$

$$+ \Psi_{p...,q\Lambda...\Sigma}^{k...m\Gamma...\Delta} \mathbf{g}_k \cdots \otimes \mathbf{g}_m \otimes \mathbf{g}^p \otimes \cdots \mathbf{g}^q \otimes \mathbf{a}_{\Gamma} \cdots \otimes \mathbf{a}_{\Delta} \otimes \mathbf{a}^{\Lambda} \cdots \otimes \frac{\delta_d}{\delta t} \mathbf{a}^{\Sigma}.$$

Note that in both cases, (4.22) and (4.23), it can be seen that the change of base surface vectors affects material derivatives of the quantity Ψ .

For example, displacement derivative (4.9), defined by Truesdell and Toupin [20], depends on base vectors used to present the object, that is, whether the base is of E_3 (spatial) or surface S.

a. Material displacement derivative of higher order

The material displacement derivative of higher order, i.e., $\delta_m^k \Psi / \delta t^k$, k = 2, 3, ... can be obtained from (4.22). Obviously, their expressions are, generally, very long and complicate. As such they are no of much use. The simplest case appears when we calculate $\delta_m / \delta t$ along $u^{\alpha} = \text{const}$, i.e., when $\dot{u}^{\alpha} = 0$. From mathematical point of view, it means that we are talking about orthogonal parametrization as the referent one. In any case, for their derivation we need the material displacement derivatives of $\delta_m^k \mathbf{a}^{\alpha} / \delta t^k$, $\delta_m^k \mathbf{n} / \delta t^k$, k = 2, 3, ...⁴ Fortunately, in practice, we need material displacement derivatives of second and, eventually, of third order.

Then in addition to (4.21), we need

(4.24)
$$\frac{\delta \mathbf{a}^{\alpha}}{\delta t} = u_{n}^{\alpha} \mathbf{n} + u_{n}^{\beta} b_{\beta}^{\alpha} \mathbf{a}^{\beta},$$

⁴Here, in order to simplify the notation, instead of $\frac{\delta_m^k}{\delta t^k}$ we write $\frac{\delta^k}{\delta t^k}$

as well as

$$\begin{split} \frac{\delta^{2}\mathbf{a}^{\alpha}}{\delta t^{2}} &= \frac{\delta u^{,\alpha}}{\delta t}\mathbf{n} + u^{,\alpha}_{n}\frac{\delta \mathbf{n}}{\delta t} + \frac{\delta(ub_{\beta}^{\alpha})}{\delta t}\mathbf{a}^{\beta} + ub_{\beta}^{\alpha}\frac{\delta \mathbf{a}^{\beta}}{\delta t} = \\ &= \frac{\delta u^{,\alpha}}{\delta t}\mathbf{n} - u^{,\alpha}_{n}u_{n,\beta}\mathbf{a}^{\beta} + \frac{\delta(ub_{\beta}^{\alpha})}{\delta t}\mathbf{a}^{\beta} + ub_{\beta}^{\alpha}\left[u^{,\beta}_{n}\mathbf{n} + ub_{\beta}^{\alpha}\mathbf{a}^{\beta}\right] \\ &= \frac{\delta^{2}\mathbf{a}^{\alpha}}{\delta t^{2}} = \left[\frac{\delta u^{,\alpha}}{\delta t} + ub_{\beta}^{\alpha}u^{,\beta}\right]\mathbf{n} + \left[-u^{,\alpha}_{n}u_{n,\beta} + \frac{\delta(ub_{\beta}^{\alpha})}{\delta t} + u^{2}b_{\gamma}^{\alpha}b_{\beta}^{\gamma}\right]\mathbf{a}^{\beta}. \end{split}$$

Further, from $(4.21)_2$ and (4.24), we obtain

$$\frac{\delta^2 \mathbf{n}}{\delta t^2} = -\frac{\delta u^{,\,\alpha}}{\delta t} \mathbf{a}^{\alpha} - u^{,\,\alpha} \frac{\delta \mathbf{a}^{\alpha}}{\delta t} = u^{,\,\alpha} u_{n,\,\alpha} \mathbf{n} + \begin{bmatrix} \frac{\delta u^{,\,\alpha}}{n} - u_{n,\,\beta} b^{\beta}_{\alpha} \end{bmatrix} \mathbf{a}^{\alpha}.$$

Under the above assumption from (4.7) we obtain

(4.25)
$$\frac{\delta \mathbf{x}}{\delta t} = u\mathbf{n}.$$

Then, in view of $(4.21)_2$,

(4.26)
$$\frac{\delta^2 \mathbf{x}}{\delta t^2} = \frac{\delta u}{\delta t} \mathbf{n} + u_n \frac{\delta \mathbf{n}}{\delta t} = \frac{\delta u}{\delta t} \mathbf{n} - u_{nn,\alpha} \mathbf{a}^{\alpha}.$$

4.2.3. Decomposition of a General Tensor Field. Generally, the decomposition of tensor field defined on surface $\sigma(t)$ gives better insight on the geometrical structures as well as physical nature of the field. For instance, from (3.23) and (3.24) we see that the normal and tangential components of velocity of geometrical point **x** of $\sigma(t)$ are of different nature. Thus, u is independent of the parametrization contrary to v^{α} which depends of parametrization $\sigma(t)$.

In what follows we shall see the other advantages of such presentation of tensor fields. Because of that, we proceed keeping the argument on the highest level of generality, in order to present the theory which can be applied to different field quantities of importance in material sciences, instead of giving the final formulas.

Particularly, applying this procedure to the problem of surface of singularity, we call this approach a direct one contrary to the iterative approach given by Truesdell and Toupin [20], since, this decomposition consists in representing a tensor field, defined on the singular surface, with respect to the naturale bases, which consists of the tangent vectors \mathbf{a}_{α} , $\alpha = 1, 2$, and unite normal vector of the surface.

Let $\mathbf{T}(\mathbf{x}, t) = T_{i_1...i_k} \mathbf{g}^{i_1} \otimes \cdots \otimes \mathbf{g}^{i_k}$ be a tensor field in E_3 . In general case **T** has 3^k independent components. At the points of $\sigma(t)$ tensor **T**, according to (3.15), is given by

(4.27)
$$\mathbf{T}(\mathbf{u},t) = \mathbf{T}(\mathbf{x}(\mathbf{u},t),t) = T_{i_1\dots i_k} \left(n^{i_1}\mathbf{n} + x^{i_1}_{,\alpha_1}\mathbf{a}^{\alpha_1} \right) \otimes \dots \otimes \left(n^{i_k}\mathbf{n} + x^{i_k}_{,\alpha_k}\mathbf{a}^{\alpha_k} \right).$$

In order to simplify further calculation we make use of the following quantities:

(4.28)
$$\mathbf{A}^{i} = n^{i}\mathbf{n}, \quad \mathbf{B}^{i} = x^{i}_{,\alpha}\mathbf{a}^{\alpha}.$$

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(4.29)
$$\mathbf{T} = T_{i_1\dots i_k} \left(\mathbf{A}^{i_1} + \mathbf{B}^{i_1} \right) \otimes \dots \otimes \left(\mathbf{A}^{i_k} + \mathbf{B}^{i_k} \right).$$

Obviously, $(\mathbf{A}^{i_1} + \mathbf{B}^{i_1}) \otimes \cdots \otimes (\mathbf{A}^{i_k} + \mathbf{B}^{i_k})$ has 2^k addends. The explicit form of (4.29) can be writhen by collecting the addends which contain the same numbers of terms \mathbf{A} , or \mathbf{B} .

First term of representative addend is

(4.30)
$$\mathbf{A}^{i_1} \otimes \cdots \otimes \mathbf{A}^{i_{\lambda}} \otimes \mathbf{B}^{i_{\lambda+1}} \otimes \cdots \otimes \mathbf{B}^{i_k}$$

All other terms of this addend have the same order of indices

$$i_1,\ldots,i_\lambda,i_{\lambda+1},\ldots,i_k.$$

It is convenient in writing them to use a table. For example, for terms of the form $\mathbf{A}^i \otimes \mathbf{A}^j \otimes \mathbf{A}^k \otimes \mathbf{B}^l \otimes \mathbf{B}^m$ the following table is appropriate:

i	j	k	l	m
Α	Α	Α	В	В
A	A	В	Α	В
A	A	В	В	Α
Α	B	A	Α	в
Α	B	A	в	Α
Α	B	в	Α	Α
B	Α	Α	Α	В
B	Α	Α	в	Α
В	Α	в	Α	Α
В	B	A	Α	Α

This reduces to the combination without repetition of k elements of λ -th class. The total numbers of them is $\binom{k}{\lambda}$. Thus, for all possible classes $\lambda = 0, 1, \ldots, k$, we will have $\sum_{\lambda=0}^{k} {k \choose \lambda} = 2^{k}$ elements. From (4.28), (4.29) and (4.30) it follows that the first representative term of

decomposition (4.29) is

$$T_{i_1\dots i_{\lambda}i_{\lambda+1}\dots i_k}n^{i_1}\dots n^{i_{\lambda}}x^{i_{\lambda+1}}_{,\alpha_1}\dots x^{i_k}_{,\alpha_{k-\lambda}}\mathbf{n}\otimes\dots\otimes\mathbf{n}\otimes\mathbf{a}^{\alpha_1}\otimes\dots\otimes\mathbf{a}^{\alpha_{k-\lambda}},$$
$$0\leqslant\lambda\leqslant k$$

Particularly,

$$T_{i_1\dots i_k} n^{i_1} \cdots n^{i_k} \mathbf{n} \otimes \cdots \otimes \mathbf{n}, \quad \text{for} \quad \lambda = k,$$

$$T_{i_1\dots i_k} x_{,\alpha_1}^{i_1} \cdots x_{,\alpha_k}^{i_k} \mathbf{a}^{\alpha_1} \otimes \cdots \otimes \mathbf{a}^{\alpha_k} \quad \text{for} \quad \lambda = 0$$

In the case when **T** is symmetric, the term $T_{i_1...i_{\lambda}i_{\lambda+1}...i_k}n^{i_1}\cdots n^{i_{\lambda}}x^{i_{\lambda+1}}_{,\alpha_1}\cdots x^{i_k}_{,\alpha_{k-\lambda}}$ will be common for all terms which can be derived from

$$\mathbf{n}\otimes\cdots\otimes\mathbf{n}\otimes\mathbf{a}^{\alpha_1}\otimes\cdots\otimes\mathbf{a}^{\alpha_{k-\lambda}},$$

as the elements of the combination without repetition of k elements of λ -th class.

This is the case of k-th gradient of tensor \mathbf{T} , i.e., of the tensor

$$abla^{(k)}\mathbf{T} = \mathbf{T}_{,\,i_1\ldots i_k}\otimes \mathbf{g}^{i_1}\otimes \cdots \otimes \mathbf{g}^{i_k},$$

where ∇ denotes gradient. Obviously, this decomposition is very complicated and the expressions are very large. In writing them we need to express

$$\mathbf{T}_{,i_1\ldots i_\lambda i_{\lambda+1}\ldots i_k} n^{i_1}\cdots n^{i_\lambda} x^{i_{\lambda+1}}_{,\alpha_1}\cdots x^{i_k}_{,\alpha_{k-\lambda}}$$

in final form over all indices α .

We shall illustrate this decomposition for gradients of \mathbf{T} in E_3 up to order 3:

(4.31)
$$\nabla \mathbf{T} = \mathbf{T}_{,i} n^{i} \otimes \mathbf{n} + \mathbf{T}_{,i} x^{i}_{,\alpha} \otimes \mathbf{a}^{\alpha} = \partial_{\mathbf{n}} \mathbf{T} \otimes \mathbf{n} + \mathbf{T}_{,\alpha} \otimes \mathbf{a}^{\alpha},$$

where $\partial_{\mathbf{n}} \mathbf{T}$ denotes the normal derivative of tensor \mathbf{T} . Next,

$$\nabla^{(2)}\mathbf{T} = \mathbf{T}_{,ij}n^{i}n^{j}\otimes\mathbf{n}\otimes\mathbf{n} + \mathbf{T}_{,ij}n^{i}x^{j}_{,\alpha}\otimes(\mathbf{n}\otimes\mathbf{a}^{\alpha} + \mathbf{a}^{\alpha}\otimes\mathbf{n}) + \mathbf{T}_{,ij}x^{i}_{,\alpha}x^{j}_{,\beta}\otimes\mathbf{a}^{\alpha}\otimes\mathbf{a}^{\beta}.$$
But $\mathbf{T}_{,ij}x^{i}_{,\alpha}x^{j}_{,\beta} = \mathbf{T}_{,\alpha\beta} - b_{\alpha\beta}\partial_{\mathbf{n}}\mathbf{T}$ and $\mathbf{T}_{,ij}n^{i}x^{j}_{,\alpha} = (\partial_{\mathbf{n}}\mathbf{T})_{,\alpha} + b^{\beta}_{\alpha}\mathbf{T}_{,\beta}$, or finally
(4.32) $\nabla^{(2)}\mathbf{T} = \partial^{(2)}_{\mathbf{n}}\mathbf{T}\otimes\mathbf{n}\otimes\mathbf{n} + \left[(\partial_{\mathbf{n}}\mathbf{T})_{,\alpha} + b^{\beta}_{\alpha}\mathbf{T}_{,\beta}\right]\otimes(\mathbf{n}\otimes\mathbf{a}^{\alpha} + \mathbf{a}^{\alpha}\otimes\mathbf{n}) + (\mathbf{T}_{,\alpha\beta} - b_{\alpha\beta}\partial_{\mathbf{n}}\mathbf{T})\otimes\mathbf{a}^{\alpha}\otimes\mathbf{a}^{\beta}.$

In the same one can derive the expression of $\delta^{(q)}\mathbf{T}$, $q \ge 3$. So obtained results sa well as the procedure can be compared with the results given by Podio-Guidugli [26].

4.2.4. The Decomposition of Displacement (material) Derivative. Let $\mathbf{T} = \mathbf{T}(\mathbf{x}, t)$, $\mathbf{x} = (x^1, \ldots, x^n)$. Obviously, $\mathbf{T} = \mathbf{x}$ is particular case. Therefore, the expression for displacement (material) derivative of $\mathbf{T}(\mathbf{x}, t)$ can be used for this particular case.

Then on $\sigma(t)$ tensor field **T** is, according to (4.27), a function of u^{α} and t. The displacement derivative of **T** on $\sigma(t)$ is the quantity defined by

$$\frac{\delta \mathbf{T}}{\delta t} = \frac{\partial \mathbf{T}}{\partial t} + \frac{\delta \mathbf{x}}{\delta t} \cdot \nabla \mathbf{T}.$$

(see $(4.6)_2$ and (4.22)). By means of (4.25), this can be written as

$$\frac{\delta \mathbf{T}}{\delta t} = \frac{\partial \mathbf{T}}{\partial t} + \underset{n}{u}\mathbf{n} \cdot \nabla \mathbf{T} = \frac{\partial \mathbf{T}}{\partial t} + \underset{n}{u} \partial_{\mathbf{n}} \mathbf{T},$$

or equivalently,

(4.33)
$$\frac{\partial \mathbf{T}}{\partial t} = -\frac{u}{n}\partial_{\mathbf{n}}\mathbf{T} + \frac{\delta \mathbf{T}}{\delta t}.$$

The same process yields the following expression for the $\delta \nabla \mathbf{T} / \delta t$. Thus,

(4.34)
$$\frac{\delta \nabla \mathbf{T}}{\delta t} = \frac{\partial \nabla \mathbf{T}}{\partial t} + \frac{\delta \mathbf{x}}{\delta t} \cdot \nabla^{(2)} \mathbf{T} = \frac{\partial \nabla \mathbf{T}}{\partial t} + u\mathbf{n} \cdot \nabla^{(2)} \mathbf{T}$$

But, because of (4.32), it follows that

$$\mathbf{n} \cdot \nabla^{(2)} \mathbf{T} = \partial_{\mathbf{n}}^{(2)} \mathbf{T} \otimes \mathbf{n} + \left[\left(\partial_{\mathbf{n}} \mathbf{T} \right)_{,\,\alpha} + b_{\alpha}^{\beta} \mathbf{T}_{,\beta} \right] \otimes \mathbf{a}^{\alpha},$$

so that (4.34) becomes

(4.35)
$$\frac{\delta \nabla \mathbf{T}}{\delta t} = \frac{\partial \nabla \mathbf{T}}{\partial t} + u_n \left\{ \partial_{\mathbf{n}}^{(2)} \mathbf{T} \otimes \mathbf{n} + \left[(\partial_{\mathbf{n}} \mathbf{T})_{,\,\alpha} + b_{\alpha}^{\beta} \mathbf{T}_{,\beta} \right] \otimes \mathbf{a}^{\alpha} \right\}.$$

On the other hand

(4.36)
$$\frac{\delta \nabla \mathbf{T}}{\delta t} = \mathbf{C} \otimes \mathbf{n} + \mathbf{C}_{\alpha} \otimes \mathbf{a}^{\alpha}.$$

But, from (4.36), we obtain

$$\mathbf{C} = \mathbf{n} \cdot \frac{\delta \nabla \mathbf{T}}{\delta t} = \frac{\delta \mathbf{n} \cdot \nabla \mathbf{T}}{\delta t} - \frac{\delta \mathbf{n}}{\delta t} \cdot \nabla \mathbf{T} = \frac{\delta \partial_{\mathbf{n}} \mathbf{T}}{\delta t} + u_n^{\alpha} \mathbf{a}_{\alpha} \cdot \nabla \mathbf{T}$$
$$= \frac{\delta \partial_{\mathbf{n}} \mathbf{T}}{\delta t} + u_n^{\alpha} \mathbf{T}_{\alpha},$$

where we made use of (4.31).

Furthermore, it is easily seen from (4.36) and $(4.21)_1$, that

$$\mathbf{C}_{\alpha} = \mathbf{a}_{\alpha} \cdot \frac{\delta \nabla \mathbf{T}}{\delta t} = \frac{\delta \mathbf{a}_{\alpha} \cdot \nabla \mathbf{T}}{\delta t} - \frac{\delta \mathbf{a}_{\alpha}}{\delta t} \cdot \nabla \mathbf{T}$$
$$= \frac{\delta \mathbf{T}_{,\alpha}}{\delta t} - \left(u_{n,\alpha} \mathbf{n} - u_{n} b_{\alpha}^{\beta} \mathbf{a}_{\beta} \right) \cdot \nabla \mathbf{T} = \frac{\delta \mathbf{T}_{,\alpha}}{\delta t} - u_{n,\alpha} \partial_{\mathbf{n}} \mathbf{T} + u_{n} b_{\alpha}^{\beta} \mathbf{T}_{,\beta}.$$

The substitution of these two last expressions into (4.36) yields

(4.37)
$$\frac{\delta \nabla \mathbf{T}}{\delta t} = \left(\frac{\delta \partial_{\mathbf{n}} \mathbf{T}}{\delta t} + u_{n}^{,\,\alpha} \mathbf{T}_{,\,\alpha}\right) \otimes \mathbf{n} + \left(\frac{\delta \mathbf{T}_{,\,\alpha}}{\delta t} - u_{n,\,\alpha}^{,\,\alpha} \partial_{\mathbf{n}} \mathbf{T} + u_{n}^{b} \partial_{\alpha}^{\beta} \mathbf{T}_{,\,\beta}\right) \otimes \mathbf{a}^{\alpha}.$$

Finally, from (4.35) and (4.37), it therefore follows that

(4.38)
$$\frac{\partial \nabla \mathbf{T}}{\partial t} = \left(\frac{\delta \partial_{\mathbf{n}} \mathbf{T}}{\delta t} + u^{\alpha} \mathbf{T}_{,\alpha} - u \partial_{\mathbf{n}}^{(2)} \mathbf{T}\right) \otimes \mathbf{n} + \left[\frac{\delta \mathbf{T}_{,\alpha}}{\delta t} - (u \partial_{\mathbf{n}} \mathbf{T})_{,\alpha}\right] \otimes \mathbf{a}^{\alpha}.$$

We now wish determine the expression for $\delta^2 \mathbf{T} / \delta t^2$. Proceeding in the same manner as above the following important formula is derived:

$$\frac{\delta^2 \mathbf{T}}{\delta t^2} = \frac{\delta}{\delta t} \left(\frac{\partial \mathbf{T}}{\partial t} + \frac{\delta \mathbf{x}}{\delta t} \cdot \nabla \mathbf{T} \right) = \frac{\delta}{\delta t} \frac{\partial \mathbf{T}}{\partial t} + \frac{\delta^2 \mathbf{x}}{\delta t^2} \cdot \nabla(\mathbf{T}) + \frac{\delta \mathbf{x}}{\delta t} \frac{\delta}{\delta t} \nabla \mathbf{T}$$
$$= \frac{\partial^2 \mathbf{T}}{\partial t^2} + 2 \frac{\delta \mathbf{x}}{\delta t} \cdot \frac{\partial \nabla \mathbf{T}}{\partial t} + \operatorname{tr} \left(\frac{\delta \mathbf{x}}{\delta t} \otimes \frac{\delta \mathbf{x}}{\delta t} \right) \nabla^{(2)} \mathbf{T} + \frac{\delta^2 \mathbf{x}}{\delta t^2} \cdot \nabla \mathbf{T}.$$

By virtue of (4.25) and (4.26), after some manipulation, we obtain

$$\frac{\delta^2 \mathbf{T}}{\delta t^2} = \frac{\partial^2 \mathbf{T}}{\partial t^2} + u_n^2 \partial_{\mathbf{n}}^{(2)} \mathbf{T} + 2u_n \frac{\delta \partial_{\mathbf{n}} \mathbf{T}}{\delta t} + \frac{\delta u}{\delta t} \partial_{\mathbf{n}} \mathbf{T} + u_{nn}^{u,\alpha} \mathbf{T}_{,\alpha},$$

or equivalently,

(4.39)
$$\frac{\partial^2 \mathbf{T}}{\partial t^2} = -\frac{u^2}{n} \partial_{\mathbf{n}}^{(2)} \mathbf{T} - 2u \frac{\delta \partial_{\mathbf{n}} \mathbf{T}}{\delta t} - \frac{\delta u}{\delta t} \partial_{\mathbf{n}} \mathbf{T} - \frac{uu}{nn} \partial_{\mathbf{n}} \mathbf{T}, \alpha - \frac{\delta^2 \mathbf{T}}{\delta t^2}.$$

5. The Theory of Singular Surfaces

Following the classical approach the *phases* are described by a *field* φ . In this theory, an *interface* is not a surface but, rather, a transition layer across which φ varies smoothly. The thickness of such layers is constitutively determined. We can consider a version of the phase-field theory that, due to a special choice of *constitutive equations* and a special scaling, allows us to control the thickness of transition layers. We may then investigate the ramification of shrinking that thickness. The phase-field theory allows for two approaches to deriving sharp-interface equations. We refer to these approaches as "*direct*" and "*indirect*". While these yield the same analytical results, the insights that they afford are very different.

The direct approach, which involves, for instance, the *configurational force balance* of the phase-field theory, yields more insight.

This is the main reason why, in this text, we have adopted this widely accepted device of representing a phase interface by a *singular surface*, rather than as a threedimensional region of some thickness (see Slattery [27] and Edvards et al. [10]). Like everything else we do in continuum mechanics, this should be regarded as a model for reality. Our understanding of the phase interface is by no means complete, but there is good experimental evidence that indicates density may be a continuous function of position through the interfacial regions. Perhaps all of the intensive variables we are concerned with, including velocity, should more accurately be regarded as continuous functions of position in going from one phase to the next.

The phase interface in general is not material. We observe mass moving across a phase interface when an ice cube melts. Here the *speed of displacement* of the phase interface is controlled by the rate of heat transfer to the system. Sometimes the speed of displacement of the phase interface might be specified by the rate of a chemical relation. In general, the speed of displacement is given in the problem statement, or it is one of the unknowns which must be determined.

Generally, from physical point of view, field φ suffer discontinuity at the interface. Than such interface is call a *surface of discontinuity*. More precisely, a disturbance in the continuity of a phenomenon or physical field is termed a *singularity*. The singularity will present as discontinuous functions or their derivatives. The examples of the first type of singularity are *shock* and *acceleration waves* (A surface that is singular with respect to some quantity and that has a nonzero speed of propagation is said to be a propagating singular surface or *wave*).

The second type is usually associated with the surface concentrations of physical quantities. Discontinuity in fields may be caused by some discontinuous behavior of the source which gives rise to the fields. In most problems discontinuities in the source function propagate to through the medium, and if the source function is prescribed at the boundary, that is on some initial surface, the carrier of the discontinuity is a moving surface in the medium. In the rest of the paper we are concern with the problem of surface singularities, i.e., with the derivation of compatibility relations for functions suffering jump discontinuities across a surface.

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Compatibility conditions are representation formulas for the *jumps* of partial derivatives of tensor fields in general in terms of the jumps of the tangential, the normal and the displacement derivatives of the tensor field at its singular surface.

In order to find the formulas of compatibility conditions we proceed from very general point of view.

The study provides a natural generalization and unification of the classical treatments of compatibility conditions for moving surfaces and curves as submanifolds of E_3 . The motivation for such a generalization is twofold.

First, it is desirable to exhibit the compatibility conditions in a single unified set of formulas expressed in terms of standard quantities from *differential geometry* and explicitly displaying the features that are common to all submanifolds regardless of their dimensions.

Secondly, it may be of some benefit to the science of continuum physics to have a general theory which treats the phenomena connected with continua of diverse dimensions on an equal footing.

Here we present the essential ideas of the theory and gather the results which are necessary for the following sections. The interested reader is reefer to the article by Truesdell and Toupin [20, Chapters 172–194], perhaps, to the best single reference in connection with this topic.

Consider the surface $\sigma(t)$ which the common boundary of two regions \Re^+ and $\Re^$ in E_3 . The unit normal **n** of $\sigma(t)$ is directed toward the region \Re^+ . Let $\varphi(\mathbf{x}, \mathbf{u}, t)$ be a scalar-valued, vector-valued or tensor valued function such that $\varphi(\cdot, \cdot, t)$ is continuous within each of the regions \Re^+ and \Re^- , and let $\varphi(\cdot, \cdot, t)$ have definite limits φ^+ and φ^- as **x** approaches a point on the surface $\sigma(t)$ from the paths entirely within the regions \Re^+ and \Re^- , respectively.

Definition 1. The jump of $\varphi(\cdot, \cdot, t)$ across $\sigma(t)$ is defined by

$$[[\varphi]] = \varphi^+ - \varphi^-.$$

Clearly, for each time t, the jump $\llbracket \varphi \rrbracket$ of $\varphi(\cdot, \cdot, t)$ can be a function of the position on $\sigma(t)$. Therefore, it is expressible in surface coordinates and time only.

Definition 2. The surface $\sigma(t)$ is said the singular surface with respect to $\varphi(\cdot, \cdot, t)$ if $[\![\varphi]\!] \neq 0$.

This definition may be extended to include the spatial and temporal derivatives of φ .

Definition 3. If the jump $\llbracket \varphi \rrbracket$ of tensor field φ is normal to $\sigma(t)$, the discontinuity of φ is said to be longitudinal; if tangent to $\sigma(t)$, transversal.

In a metric space, the jump of any tensor may be resolved unequally into longitudinal and transversal components.

The entire differential theory of singular surfaces grows from the application of modified Hadamard's lemma to $\varphi_{;\alpha} = \varphi_{,\alpha} + \varphi_{,k} x^k_{,\alpha}$ so that

(5.2)
$$\llbracket \varphi \rrbracket_{;\alpha} = \llbracket \varphi \rrbracket_{,\alpha} + \llbracket \varphi_{,k} \rrbracket x_{,\alpha}^k,$$

which asserts that the jump of a total tangential derivative is total tangential derivative of the jump.

Particulary, for $\varphi(\mathbf{x}, t)$

(5.3)
$$\llbracket \varphi \rrbracket_{,\alpha} = \llbracket \varphi_{,\alpha} \rrbracket = \llbracket \varphi_{,k} x_{,\alpha}^k \rrbracket = \llbracket \varphi_{,k} \rrbracket x_{,\alpha}^k,$$

i.e., the jump of a tangential derivative is the tangential derivative of the jump.

Since the values of $\varphi(\mathbf{x}, \mathbf{u}, t)$ in \Re^+ and \Re^- are in general entirely unrelated to one another, the limiting values of the normal derivatives of $\varphi(\cdot, \cdot, t)$ on two sides of the singular surface $\sigma(t)$

(5.4)
$$\left[\left[\frac{\partial \varphi}{\partial n} \right] \right]$$
 is unrestricted.

Assuming also that the limiting values φ^+ and φ^- are continuously differentiable functions of t in \Re^+ and \Re^- , respectively, we derive a condition that the discontinuity in $\varphi(\cdot, \cdot, t)$ persists in time rather than appearing and disappearing at some particular instant. In a metric space, however, the existence of a definite speed of displacement u_n for the moving surface enable one to write the kinematical condition of compatibility for a spatial tensor field

(5.5)
$$\left[\!\left[\frac{\delta_d\varphi}{\delta t}\right]\!\right] = \left[\!\left[\frac{\partial\varphi}{\partial t}\right]\!\right] + u_n [\![\varphi_{,k}]\!] n^k,$$

where $\delta_d \varphi / \delta t$ is displacement derivative defined by Truesdell and Toupin [20]. We shall come to this formula latter. The formulas (5.2)–(5.5) are essential in the theory of singular surfaces. Henceforth, we shall make very often use of them.

Note that

(5.6)
$$\left[\left[\frac{\delta_d \varphi}{\delta t} \right] \right] = \left(\frac{\delta_d \varphi}{\delta t} \right)^+ - \left(\frac{\delta_d \varphi}{\delta t} \right)^- = \frac{\delta_d \varphi}{\delta t}^+ - \frac{\delta_d \varphi}{\delta t}^- = \frac{\delta_d}{\delta t} \llbracket \varphi \rrbracket$$

To simplify the calculation we consider the notion of the jump defined by (5.1) as the application of the operator $[\![\,]\!]$ applied to the tensor field φ . Then we state the following properties of $[\![\,]\!]$.

i) [] is linear operator. Indeed, from the definition (5.1), we have

$$\llbracket a\varphi + b\psi \rrbracket = a\llbracket \varphi \rrbracket + b\llbracket \psi \rrbracket.$$

for any $a, b \in R$ and any tensor fields φ , ψ of the same order and type. R is the set of real numbers.

ii) $\llbracket \varphi \psi \rrbracket = \langle \varphi \rangle \llbracket \psi \rrbracket + \langle \psi \rangle \llbracket \varphi \rrbracket$, where $\langle \varphi \rangle$ and $\langle \psi \rangle$ are mean values of φ and ψ , respectively, i.e., $\langle \varphi \rangle = 1/2(\varphi^+ + \varphi^-)$ and $\langle \psi \rangle = 1/2(\psi^+ + \psi^-)$. We already state the Hadamar's lemma by (5.2).

From ii) and (5.1) we conclude that if φ is continuos, i.e., if $\varphi_1 = \varphi_2 = \varphi$ then

$$[5.7) \qquad \qquad \llbracket \varphi \psi \rrbracket = \varphi \llbracket \psi \rrbracket.$$

5.1. Singular Surfaces Associated with a Motion. Thus far we have introduced the basic concepts of the theory of moving singular surfaces. However, there are certain conditions, the geometrical conditions of compatibility and kinematical conditions of compatibility, which must be satisfied across the singular surfaces. The geometrical conditions of compatibility relates the jump in the derivatives of $\varphi^{\dots}(\cdot, t)$ to the jump of the normal derivatives of $\varphi^{\dots}(\cdot, t)$, the tangential derivatives of the jump of $\varphi^{\dots}(\cdot, t)$ and the geometrical properties of the singular surfaces. Usually these conditions are iterated to yield higher order conditions of compatibility relations of the singular surfaces. The derivations of these conditions of compatibility are quite lengthy though rather straightforward. The interested reader should consult the work of Thomas [19] and Truesdell and Toupin [20] in which detailed derivations of these conditions are presented.

Definition 4. The order of a singular surface is (usually defined as) the lower order k + l of the derivative $\frac{\partial^l}{\partial t^l} \varphi_{i1\dots i_k}^{\cdots}$ which suffers a finite jump across the surface.

Therefore, the zeroth order singular surface is such that the tensor field $\varphi^{\cdots}(\cdot, t)$ itself suffers a discontinuity across it.

Here, as in all follows, we assume that in region \Re^+ and \Re^- on each side of the singular surface $\sigma(t)$ the function $\varphi(\mathbf{x}, \mathbf{u}, t)$ and all its derivatives up to the highest order considered exist and are continuously differentiable functions of \mathbf{x} , \mathbf{u} and t, while on $\sigma(t)$ they approach definite limits which are continuously differentiable functions of position.

There is no compelling reason to allow only discontinuities of this special type. Jump discontinuities upon surfaces are not the only ones that occur in physical problems. Boundaries, slip surfaces, dislocations, and tears are excluded as not being defined by sufficiently smooth jump discontinuities in function of the material variables. Singularities at isolated lines or points are common. In the case of jump discontinuities on surfaces, there is no a priori ground to expect that he limit values on each side of the surface be continuously differentiable on the surface, as we have assumed. The reason for considering here only singularities of this kind are first, that for more general singularities other than those analyzed above, scarcely any definite results are known except in very particular cases, and, second, that singular surfaces of the above types are frequently found useful in special theories of materials.

This definition of order of the singular surfaces is independent of the motion of any material medium. We now suppose that a medium consisting of particles \mathbf{X} is in motion through the space of places \mathbf{x} according to $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$, $\mathbf{X} = \mathbf{X}(\mathbf{x}, t)$. We assume that these functions are single-valued and continuous. Modifications appropriate to motion suffering discontinuous will be given later. We consider a surface $\sigma(t)$ given by a representation of the form (3.1), and set

 $F(\mathbf{X},t) \equiv f(\mathbf{x}(\mathbf{X},t),t), \text{ so that } f(\mathbf{x},t) \equiv F(\mathbf{x}(\mathbf{X},t),t),$

identically in **x**, **X** and *t*. Alternative representations of the moving surface are thus $\sigma(t) : f(\mathbf{x}, t) = 0$, $\Sigma(t) : F(\mathbf{X}, t) = 0$. The two representatives are the duals of

one another. The other dual quantities, we are going to use frequently here, are the outward unit normal vectors \mathbf{n} and \mathbf{N} of σ and Σ , respectively; also, Grad $\mathbf{x} \equiv \mathbf{F}$ and grad $\mathbf{X} \equiv \mathbf{F}^{-1}$ denote material and space gradients of motion.

In the special case when $f(\mathbf{x}) = 0$ we say that the surface σ is stationary; when $F(\mathbf{X}) = 0$ the surface Σ is material. In the former case, the surface σ consists always of the same places; in the latter, Σ , of the same particles.

Although $\sigma(t)$ and $\Sigma(t)$ are but different means of representing the same phenomenon, the two surfaces so defined are, in general, entirely different from one another geometrically. The surface $f(\mathbf{x}, t) = 0$ is a surface in the space of places, while the surface $F(\mathbf{X}, t) = 0$ is the locus, in the space of particles, of the *initial* positions of the particles \mathbf{X} that are situate upon the surface $f(\mathbf{x}, t) = 0$ at time t.

The dual of the speed of displacement, u, is the speed of propagation

$$U_N = -\frac{\partial F/\partial t}{|\operatorname{Grad} F|}.$$

Many of the singularities of greatest interest are included in the case when $\varphi = \mathbf{x}(\mathbf{X}, t)$, i.e., are surfaces across which the motion itself, or one of its derivatives, is discontinuous. By the order of a singular surface henceforth we shall mean, unless some other quantity is mentioned explicitly, that we are taking $\varphi = \mathbf{x}$. Than at a singular surface of order 0, the motion $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ suffers a jump discontinuity. This must be interpreted as starting that the particles \mathbf{X} upon the singular surface at time t are simultaneously occupying two places \mathbf{x}^+ and \mathbf{x}^- or jump instantaneously from \mathbf{x}^+ to \mathbf{x}^- . Such discontinuity have been found in field theory of fracture mechanics.

Since fracture of the body is excluded from our consideration, the motion on a surface is assumed to be continuous. Therefore, a singular surface of order zero is assumed not to exist, and on every singular surface the relation $[\![\mathbf{x}]\!] = 0$ is supposed to hold.

On a singular surface of order 1 the deformation gradient and the velocity of the medium may suffer finite discontinuity. Such a propagating singular surface will be called a *shock wave*.

On a singular surface of order 2, the deformation gradients and the velocity of the medium will be continuous, while the second gradients of motion and the acceleration of material particles may suffer jumps. Such a propagating singular surface will be called an *acceleration wave*.

Higher-order singular surfaces are similarly defined.

Clearly, the definition of the order of a singular surface may be expressed alternatively in terms of the covariant derivatives with respect to material variables \mathbf{X} , i.e., $\varphi_{,K_1...K_q}$. No modification in the results is needed to allow us to substitute double tensors of the type $\varphi_{p...q\gamma...\delta}^{k...m\alpha...\beta}$ in the various jump conditions. For example, in the case of a surface which is singular with respect to φ and also a singular surface of order 2 or greater with respect to the motion itself, the principle of duality when applied to (5.5) yields

$$\left[\!\left[\frac{\delta_d \varphi}{\delta t}\right]\!\right] = \left[\!\left[\frac{\partial \varphi}{\partial t}\right]\!\right] + \underset{N}{U}\!\left[\!\left[\varphi_{,K}\right]\!\right]\!N^K,$$

where the displacement derivative $\delta_d/\delta t$ is defined in terms of the motion of the material diagram $F(\mathbf{X}, t) = 0$. This results follows at once because, corresponding to any selected initial state, there is a unique speed of propagation U.

5.2. Conditions of Compatibility. Now, we are ready to write the compatibility conditions making use of the results of Sections 4.5 and 4.6. In this way, we demonstrate the advantage of this procedure over iterative procedure (see Truesdel-Tupin $[20, \S\S176, 181]$). Particularly, we confine ourselves to the expressions: (4.31), (4.32), (4.33), (4.38) and (4.39). Then, making use of (5.3), (5.4), (5.6) and (5.7) we write for

5.2.1. Geometrical Conditions of Compatibility.

$$\begin{split} \llbracket \nabla \mathbf{T} \rrbracket &= \llbracket \partial_{\mathbf{n}} \mathbf{T} \rrbracket \otimes \mathbf{n} + \llbracket \mathbf{T} \rrbracket_{,\,\alpha} \otimes \mathbf{a}^{\alpha}, \\ \llbracket \nabla^{(2)} \mathbf{T} \rrbracket &= \llbracket \partial_{\mathbf{n}}^{(2)} \mathbf{T} \rrbracket \otimes \mathbf{n} \otimes \mathbf{n} \\ &+ \left[\llbracket \partial_{\mathbf{n}} \mathbf{T} \rrbracket_{,\,\alpha} + b_{\alpha}^{\beta} \llbracket \mathbf{T} \rrbracket_{,\beta} \right] \otimes \left(\mathbf{n} \otimes \mathbf{a}^{\alpha} + \mathbf{a}^{\alpha} \otimes \mathbf{n} \right) \\ &+ \left(\llbracket \mathbf{T} \rrbracket_{,\,\alpha\beta} - b_{\alpha\beta} \llbracket \partial_{\mathbf{n}} \mathbf{T} \rrbracket \right) \otimes \mathbf{a}^{\alpha} \otimes \mathbf{a}^{\beta}, \end{split}$$

. .

5.2.2. Kinematical Conditions of Compatibility.

$$\begin{split} \left[\!\left[\frac{\partial \mathbf{T}}{\partial t}\right]\!\right] &= -\frac{u}{n} \left[\!\left[\partial_{\mathbf{n}} \mathbf{T}\right]\!\right] + \frac{\delta[\![\mathbf{T}]\!]}{\delta t}, \\ \left[\!\left[\frac{\partial \nabla \mathbf{T}}{\partial t}\right]\!\right] &= \left(\frac{\delta[\![\partial_{\mathbf{n}} \mathbf{T}]\!]}{\delta t} + \frac{u}{n}^{,\alpha} \left[\![\mathbf{T}]\!]_{,\,\alpha} - \frac{u}{n} \left[\!\left[\partial_{\mathbf{n}}^{(2)} \mathbf{T}\right]\!\right]\!\right) \otimes \mathbf{n} + \left[\frac{\delta[\![\mathbf{T}]\!]_{,\,\alpha}}{\delta t} - \left(\!\frac{u}{n} \left[\!\left[\partial_{\mathbf{n}} \mathbf{T}\right]\!\right]\!\right)_{,\,\alpha}\right] \otimes \mathbf{a}^{\alpha}, \\ \left[\!\left[\frac{\partial^{2} \mathbf{T}}{\partial t^{2}}\right]\!\right] &= -\frac{u^{2}}{n} \left[\!\left[\partial_{\mathbf{n}}^{(2)} \mathbf{T}\right]\!\right] - 2u_{n}^{\,\delta} \frac{\left[\!\left[\partial_{\mathbf{n}} \mathbf{T}\right]\!\right]}{\delta t} - \frac{\delta u}{\delta t} \left[\!\left[\partial_{\mathbf{n}} \mathbf{T}\right]\!\right] - \frac{uu^{,\,\alpha}}{\delta t} \left[\!\left[\partial_{\mathbf{n}} \mathbf{T}\right]\!\right] - \frac{uu^{,$$

C T cm T

There are several special cases of importance in continuum physics.

a) If \mathbf{T} is continuous, i.e., if $\llbracket \mathbf{T} \rrbracket = 0$, then

b) If in addition to **T**, ∇ **T** is continuous, i.e., if $[[\mathbf{T}]] = [\partial_{\mathbf{n}}\mathbf{T}] = 0$, then ∂ **T** $/\partial t$ is also continuous. But,

$$\llbracket \nabla^{(2)} \mathbf{T} \rrbracket = \llbracket \partial_{\mathbf{n}}^{(2)} \mathbf{T} \rrbracket \otimes \mathbf{n} \otimes \mathbf{n}, \quad \left[\begin{bmatrix} \frac{\partial \nabla \mathbf{T}}{\partial t} \end{bmatrix} = -u_n^{\mathbb{I}} \begin{bmatrix} \partial_{\mathbf{n}}^{(2)} \mathbf{T} \end{bmatrix} \otimes \mathbf{n}, \quad \left[\begin{bmatrix} \frac{\partial^2 \mathbf{T}}{\partial t^2} \end{bmatrix} = -u_n^2 \llbracket \partial_{\mathbf{n}}^{(2)} \mathbf{T} \end{bmatrix}.$$

Let $\mathbf{T} = \mathbf{x}$ and $[[\mathbf{x}]] = 0$. Then, in accordance with the definition of the order of singular surfaces, we have

c) for a singular surface of order 1,

(5.8)
$$\llbracket \operatorname{Grad} \mathbf{x} \rrbracket = \mathbf{a} \otimes \mathbf{N}, \quad \llbracket \dot{\mathbf{x}} \rrbracket = -\frac{U}{N} \mathbf{a},$$

where $\mathbf{a} = \llbracket \operatorname{Grad} \mathbf{x} \cdot \mathbf{N} \rrbracket$. In componental form these read

$$\llbracket x_{;K}^k \rrbracket = a^k N_K, \quad \llbracket \dot{x}^k \rrbracket = -ua^k$$

where $a^{k} = [\![x_{;K}^{k} N^{K}]\!]$.

The vector \mathbf{a} is the singularity vector; while (5.8) shows it to be parallel to the jump of velocity, its magnitude varies with the choice of the initial state and thus does not furnish a measure of the strength of the singularity.

It is convenient to divide singular surfaces of order 1 into two classes:

- 1. Material singularities, which affect only the deformation gradients;
- 2. Waves, including both shock waves and propagating vortex sheets.

For the former, the choice of the initial state is of prime importance. For the latter, it is not, and the nature of the waves is best specified in terms of the jump of velocity itself, $[\![\dot{\mathbf{x}}]\!]$, which may be arbitrary both in direction and in magnitude. Indeed, if we adopt a strictly spatial standpoint, we may say the only geometrical and kinematical requirement is that discontinuities in velocity be propagated, both the amount of the discontinuity and the speed of propagation being arbitrary. Moreover, it follows that a jump in velocity is impossible unless it is accompanied by jumps in the deformation gradients.

d) for a singular surface of order 2

$$\llbracket \operatorname{Grad}^2 \mathbf{x} \rrbracket = \mathbf{b} \otimes \mathbf{N} \otimes \mathbf{N}, \quad \llbracket \operatorname{Grad} \dot{\mathbf{x}} \rrbracket = - \underset{N}{U} \mathbf{b} \otimes \mathbf{N}, \quad \llbracket \ddot{\mathbf{x}} \rrbracket = - \underset{N}{U^2} \mathbf{b},$$

where $\mathbf{b} = [\![\mathbf{N} \cdot (\operatorname{Grad}^2 \mathbf{x})\mathbf{N}]\!]$. In componental form these read

$$\llbracket x_{;KL}^k \rrbracket = b^k N_K N_L, \quad \llbracket \dot{x}_{;K}^k \rrbracket = - \bigcup_N b^k N_K, \quad \llbracket \ddot{x}^k \rrbracket = - \bigcup_N b^k,$$

where $b^k = \begin{bmatrix} x_{;KL}^k N^K N^L \end{bmatrix}$.

These formulae show that a singular surface of order 2 is completely determined by a vector **b** and the speed of propagation U_N . In particular, material discontinuities of second order affect only the derivatives $x_{,KL}^k$, while discontinuities in the acceleration and in the velocity gradient are necessarily propagated, and conversely, every wave of second order carries jumps in the velocity gradient and the acceleration. Waves of second order are therefore called *acceleration waves*.

5.2.3. Dynamical Conditions of Compatibility. When a singular surface involves field variables that are affected by the motion and deformation of the medium, the geometrical and kinematical compatibility conditions should be supplemented by restrictions originating from the local balance equations. These conditions are called the *dynamical conditions of compatibility*. The dynamical conditions of compatibility are due to the local conservation of mass, balance of linear and angular momenta, balance of energy, and the local Clausius–Duhem inequality on $\sigma(t)$.

These conditions are of fundamental importance in the investigation of many theoretical and practical problems, such as a wave propagation, in continuum physics. Their investigation will not be considered here.

6. Balances Laws of Bulk Material and Interface

Since the primary objective of continuum physics is to determine the fields of density, motion and temperature, field equations are needed. It is customary to base such field equations upon the equations of balance of mechanics and thermodynamics. These are the equations of balance of mass, momentum, moment of momentum and energy or, in other terms, the continuity equation, Newton's laws of motion and the first, as well as the second law of thermodynamics for both: bulk material and interface.

In case of electro-magnetism, the Maxwell equations must be taken into consideration. They are the set of four fundamental equations governing electromagnetism (i.e., the behavior of electric and magnetic fields).

Particulary, we consider materials surfaces which are *permeable*, *semi-permeable* as well as *impermeable* material surface.

Rather than considering the individual transport processes separately governing the balance of mass, momentum, species, etc., we focus now on a single, abstract, generic conservation law, known under the name *general balance law*, governing the transport of all extensive physical properties, in continuous three-dimensional media, and then in discontinuous media. Ultimately, the generic balance equations will be applied in later chapters to specific physical circumstances.

6.1. Transport Theorem. A kinematical theorem that proves useful in the derivation of balance laws in continuum physics is the Reynolds theorem (Reynolds [28]), in the literature known as *transport theorem*. We give it in a generalized form in order that it might apply to a material region through which a phase interface is moving.

Once more, instead of a phase interface, we say that the material region is divided by a surface which is discontinuous (singular) with respect to a quantity Ψ .

In the analysis of phenomena involving singular surfaces two cases should be distinguished:

a) σ is a material surface,

b) σ is not a material surface, but a surface passing through the medium.

In case a) the same material particles remain on the surface during its motion, and the analysis concerns a film or layer, while in case b) the analysis is applicable mainly to wave propagation problems and phase transition phenomena. Moreover, in a number of free boundary problems surfaces may be applied in modeling as well as in analysis.

We state here standard forms of transport theorems: for a volume which contains discontinuity surfaces and for a surface in E_3 (Müller [24]).

6.1.1. Transport Theorem for a Volume which Contains Discontinuity Surfaces. We consider the material volume v of the body B which is divided by singular surface σ into two parts v^+ and v^- (Fig. 2).

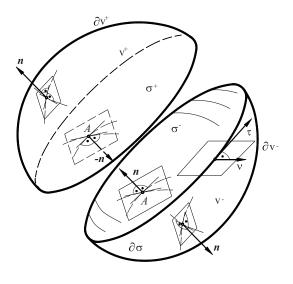


FIGURE 2

The outward unit normal to ∂v , the boundary of v, is denoted by **n**. The velocity of particle of the body is denoted by $\dot{\boldsymbol{\xi}}$

The singular surface, assumed smooth, may be in motion with any speed of displacement u. Is also assumed that $\sigma(t)$ is a persistent singular surface with respect to a quantity Ψ and possibly also with respect to $\dot{\boldsymbol{\xi}}$, the velocity of particle of the body denoted by $\boldsymbol{\xi}^{5}$.

Further the outward normal of σ , pointing to v^+ is denoted also by **n**. The outward normal of $\partial \sigma$, the intersection of σ and $\partial \sigma$, is denoted by ν , which is tangent vector field to σ defined at the points of $\partial \sigma$.

Then, any additive quantities Ψ associated to the body B the following transport theorem holds

$$\frac{D_m}{Dt} \int_{v-\sigma} \Psi \, dv = \int_{v-\sigma} \left(\dot{\Psi} + \Psi \operatorname{div} \dot{\boldsymbol{\xi}} \right) dv + \int_{\sigma} \left[\!\! \left[\Psi \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}} \right) \right] \!\! \right] \cdot \mathbf{n} \, da,$$

where $\llbracket \Psi \rrbracket = \Psi^+ - \Psi^-$ indicates the jump of $\Psi \operatorname{across} \sigma$.

⁵It should be noticed that in the previous considerations we write **x** and $\dot{\mathbf{x}}$ for the placement of the material particle and its velocity independently of the dimension of the body, i.e., whether the body is three-dimensional. This kind of notation will be used later as well except when one-dimensional or two-dimensional continuum is observed. It is the case, for instance, when the material surface is contained in three-dimensional body. In that case **x** and $\dot{\mathbf{x}}$ are quantities which are related to two-dimensional body. With $\boldsymbol{\xi} = \boldsymbol{\xi}(\boldsymbol{\Xi}, t)$ we denote the position of the material particle $\boldsymbol{\xi}$ of three-dimensional material body. Also with $\dot{\boldsymbol{\xi}} = \frac{D_m \boldsymbol{\xi}}{Dt} = \frac{d\boldsymbol{\xi}}{dt}|_{\boldsymbol{\xi}=\text{const}}$, we denote the velocity of that particle (see Truesdell and Toupin [20]).

6.1.2. Transport Theorem for a Surface. Let φ be any additive quantity defined on surface s(t) (see Fig. 3). Then the following transport theorem is valid

$$\frac{\delta_m}{\delta t} \int\limits_{s} \varphi \, da = \int\limits_{s} \left[\frac{\delta_m \varphi}{\delta t} + \varphi \left(\nabla_s \cdot \dot{\mathbf{u}} - 2u K_M \right) \right] \, da,$$

where

$$\frac{\delta_m}{\delta t} da = \left(\nabla_s \cdot \dot{\mathbf{u}} - 2u K_M \right) \, da.$$

Thus follows from $da = \sqrt{a} du^1 du^2$ and $(4.20)_5$.

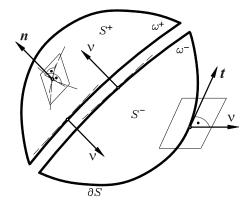


FIGURE 3

For more detailed analysis of the transport theorem for a surface, which contains discontinuity line ω (see Jarić and Golubović [29]).

6.2. Balance Laws for a Single Body. Generally an equation of balance can be written for all additive quantities, irrespective of their physical nature. Therefore this chapter starts with the formulation of a general equation of balance and it proceeds by listing special cases that are of particular interest to continuum mechanics. To start in a fairly general manner, we shall consider a material volume of a body which is separated into two parts v^+ and v^- by a singular surface σ (see Fig. 2).

Let Ψ be an additive quantity associated with the body so that its amount in v may be written as

$$\Psi = \int_{v^+ \cup v^-} \psi_v \, dv + \int_{\sigma} \psi_\sigma \, da,$$

where ψ_v , ψ_σ are the volume and surface densities, of Ψ , respectively.

The existence of the second integral is evidence of the occurrence of surface effects associated with a concentration of the quantity Ψ on a singular surface σ .

The existence of the second integral is evidence of the occurrence of surface effects associated with a concentration of the quantity Ψ on a (singular) surface σ .

In the analysis of phenomena involving singular surfaces two cases should be distinguished: (a) σ is a material surface, (b) σ is not a material surface, but a surface passing through the medium. In case (a) the same material particles remain on the surface during its motion, and the analysis concerns a film or layer, while in case (b) the analysis is applicable mainly to wave propagation problems and phase transition phenomena. Moreover, in a number of free boundary problems surfaces may be applied in modelling as well as in analysis.

Then the balance of the rate of change of Ψ is given by (see Moeckel [30], Kosiński [22], Müler [24])

$$\frac{D_m}{Dt} \int_{v^+ \cup v^-} \psi_v \, dv + \frac{\delta_m}{\delta t} \int_{\sigma} \psi_\sigma \, da = \int_{\partial v - \sigma} \Phi_v \mathbf{n} \, da + \int_{v - \sigma} p_v \, dv + \int_{\partial \sigma} \Phi_\sigma \boldsymbol{\nu} d\ell + \int_{\sigma} p_\sigma \, da,$$

where Φ_v and Φ_σ are flux densities of ψ ; p_v , p_σ are supply (production) densities in the volume and on the singular surface, respectively.

The use of transport theorems (A) and (B), as well as the divergence theorems

$$\int_{v-\sigma} \operatorname{div} \mathbf{w} \, dv + \int_{\sigma} \llbracket \mathbf{w} \rrbracket \cdot \mathbf{n} \, da = \int_{\partial v-\sigma} \mathbf{w} \cdot \mathbf{n} \, da,$$
$$\int_{S-\omega} \operatorname{div}_{S} \mathbf{t} \, da + \int_{\omega} \llbracket \mathbf{t} \rrbracket \cdot \boldsymbol{\nu} \, ds = \int_{\partial S-\omega} \mathbf{t} \cdot \boldsymbol{\nu} \, ds,$$

for all vectors \mathbf{w} in E_3 , and tangential vectors field \mathbf{t} , will provide more explicit expressions for (6.1), i.e.,

(6.2)
$$\int_{v} \left(\frac{D_{m}\psi_{v}}{Dt} + \psi_{v}\nabla\cdot\dot{\boldsymbol{\xi}} - \nabla\cdot\boldsymbol{\Phi}_{v} - p_{v} \right) dv + \int_{\sigma} \left[\frac{\delta_{m}\psi_{\sigma}}{\delta t} + \psi_{\sigma} \left(\nabla_{\sigma}\cdot\dot{\mathbf{u}} - 2uK_{M} \right) - \nabla_{\sigma}\cdot\boldsymbol{\Phi}_{\sigma} - p_{\sigma} \right] da + \int_{\sigma} \left[\psi_{v}(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \boldsymbol{\Phi}_{v}big \right] \cdot \mathbf{n} \, da = 0.$$

The localization of (6.2) now gives the local balance laws

(6.3)
$$\frac{D_m \psi_v}{Dt} + \psi_v \nabla \cdot \dot{\boldsymbol{\xi}} - \nabla \cdot \boldsymbol{\Phi}_v - p_v = \hat{p}_v, \quad \text{in } v - \sigma$$
$$\frac{\delta_m \psi_\sigma}{\delta t} + \psi_\sigma \left(\nabla_\sigma \cdot \dot{\mathbf{u}} - 2u K_M \right) - \nabla_\sigma \cdot \boldsymbol{\Phi}_\sigma - p_\sigma$$
$$+ \left[\left[\psi_v \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}} \right) - \boldsymbol{\Phi}_v \right] \right] \cdot \mathbf{n} = \hat{p}_\sigma, \quad \text{on } \sigma$$

where

(6.5)
$$\int_{v-\sigma} \hat{p}_v \, dv + \int_{\sigma} \hat{p}_{\sigma} \, da = 0.$$

The quantities \hat{p}_v and \hat{p}_{σ} are called *nonlocal volume and surface effects* (or *residuals*), respectively (see Eringen [31]).

Taking into account the influence of the quantities \hat{p}_v and \hat{p}_σ when describing the behaviour of continuum takes us out from the local into nonlocal continuum theory. In the local continuum theory, absence of such quantities is a priori assumed; then $\hat{p}_v = 0$ and $\hat{p}_\sigma = 0$. Restriction (6.5) to nonlocal residuals is generally valid. In most cases it is assumed

(6.6)
$$\int_{v-\sigma} \hat{p}_v \, dv = 0, \quad \int_{\sigma} \hat{p}_\sigma \, da = 0.$$

This assumption is physically justified in case when surface and volume residuals \hat{p}_v and \hat{p}_σ are independent or when their interaction is poor.

The relations (6.3) and (6.4) constitute the generic, volumetric and surface balance equations for continuous three-dimensional media at each point of the continuum with a surface of discontinuity.

It is important to notice that adequate quantities in general balance law are defined over volume, surface and length units, respectively. Since volume, surface and line are geometrical concepts, it is more appropriate, from the physical point of view, to define physical quantities over mass unit whenever it is possible. Having in mind that $dm = \rho dV$ and $dm_{\sigma} = \gamma da$, where ρ and γ are mass density of three-dimensional and two-dimensional body, respectively, we write

$$\begin{split} \psi_v &\to \varrho \psi_v, \quad p_v \to \varrho p_v, \quad \hat{p}_v \to \varrho \hat{p}_v, \\ \psi_\sigma &\to \gamma \psi_\sigma, \quad p_\sigma \to \gamma p_\sigma. \end{split}$$

We call the reader's attention to the fact that so defined new quantities ψ_v and ψ_σ do not change their physical dimensions. Now local balance laws (6.3) and (6.4) become

(6.7)
$$\frac{D_m \varrho \psi_v}{Dt} + \varrho \psi_v \nabla \cdot \dot{\boldsymbol{\xi}} - \nabla \cdot \boldsymbol{\Phi}_v - \varrho p_v = \hat{p}_v,$$

(6.8)
$$\frac{\partial_m \gamma \psi_\sigma}{\delta t} + \gamma \psi_\sigma \left(\nabla_\sigma \cdot \dot{\mathbf{u}} - 2uK_M \right) - \nabla_\sigma \cdot \mathbf{\Phi}_\sigma \\ - \gamma p_\sigma + \left[\varrho \psi_v (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{\Phi}_v \right] \cdot \mathbf{n} = \hat{p}_\sigma.$$

Particularly, for $\psi_v = 1$, $\Phi_v = 0$, $\rho p_v = 0$, $\rho \hat{p}_v = \hat{\rho}$, from (6.7), we obtain (a) Balance of mass

(6.9)
$$\frac{D_m \varrho}{Dt} + \varrho \nabla \cdot \dot{\boldsymbol{\xi}} = \hat{\varrho} \quad \text{or equivalently} \quad \frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \dot{\boldsymbol{\xi}}) = \hat{\varrho}.$$

By substituting (6.9) into (6.7) we get, for bulk material, ⁶ (b) Local balance law of ψ_v

(6.10)
$$\varrho \frac{D_m \psi_v}{Dt} - \nabla \cdot \mathbf{\Phi}_v - \varrho p_v = \varrho \hat{p}_v - \hat{\varrho} \psi_v.$$

⁶The material occupying the region $v - \sigma$ is called bulk material.

Here we confine our investigation mainly to the physical phenomena of nonpolar⁷ nonlinear continuous bodies which are exposed to the thermodynamical (mechanical) effects. Other effects, like chemical, electrical, electromagnetic, ... can be treated in the same way.

Now, the basic fields of thermodynamics in the bulk materials on the interface, other then mass density, are: motion and temperature. Then the field equations are based upon the equations of balance (6.10), with Ψ chosen as: momentum, moment of momentum, energy and entropy. The other quantities are identified in accordance with their physical meaning in continuum mechanics. They are concisely given in the table below (see Moeckel [30], Eringen [31], Müler [24]).

ψ	ψ_v	$\mathbf{\Phi}_v$	p_v	\hat{p}_v
momentum	Ė	Т	f	Î
moment of momentum	$\mathbf{p} imes \dot{oldsymbol{\xi}}$	$\mathbf{p}\times\mathbf{T}$	$\mathbf{p}\times \mathbf{f}$	$\mathbf{p} imes \hat{\mathbf{f}}$
energy	$\frac{1}{2}\dot{\boldsymbol{\xi}}\cdot\dot{\boldsymbol{\xi}}+arepsilon$	$\mathbf{T}^T \dot{\boldsymbol{\xi}} + \mathbf{q}$	$\mathbf{f}\cdot\dot{\boldsymbol{\xi}}+h$	$\hat{\mathbf{f}}\cdot\dot{\boldsymbol{\xi}}+\hat{h}$
entropy	η	s	h/ heta	$\hat{h}/ heta$

Physical meaning of the quantities given in the table are:

 $\mathbf{T} = T^{kl} \mathbf{g}_l \otimes \mathbf{g}_k - \text{stress tensor}^8,$

 $\begin{aligned} \varepsilon &- \text{ internal energy,} \\ \mathbf{q} &= q^k \mathbf{g}_k - \text{heat flux,} \\ \eta &- \text{ entropy density,} \\ \mathbf{s} &= s^k \mathbf{g}_k - \text{ entropy flux,} \\ \mathbf{f} &= f^k \mathbf{g}_k - \text{ body force per unit mass,} \\ h &- \text{ supply of energy per unit mass,} \\ \theta &- \text{ absolute temperature;} \\ h/\theta &- \text{ entropy production.} \end{aligned}$

 h/θ – entropy production. Further, all quantities with "^" are nonlocal residuals of corresponding quantities. For definiteness they are called nonlocal volume and surface effects (or residuals).

By "…" we denote the summation convention over two pair of successive indices. Thus, $\boldsymbol{\epsilon} \cdot \cdot \mathbf{T} = \varepsilon_{ijk} T^{jk} \mathbf{g}^i$, where $\boldsymbol{\epsilon}$ is the Ricci alternation tensor. We also have $\mathbf{p} \times \mathbf{T} = \varepsilon_{ijk} \xi^i T^{lj} \mathbf{g}^k \otimes \mathbf{g}_l$.⁹

 $^{^7\}mathrm{When}$ material bodies are referred to as nonpolar, it means that all torques acting on the material are the results of forces.

⁸This way of representing tensors $\mathbf{T} = T^{kl} \mathbf{g}_l \otimes \mathbf{g}_k$ differs from the representation $\mathbf{T} = T^{kl} \mathbf{g}_k \otimes \mathbf{g}_l$ only when \mathbf{T} is not symmetric. In continuum mechanics this difference comes from the representation of stress vector $\mathbf{t}_{(n)} = \mathbf{t}^k n_k$, where $\mathbf{n} = n^k \mathbf{g}_k$, \mathbf{t}_k -stress vectors acting on coordinate surface. Then, if we write $\mathbf{t}_k = t^{kl} \mathbf{g}_l$ we arrive to the representation $\mathbf{T} = T^{kl} \mathbf{g}_l \otimes \mathbf{g}_k$ (see for instance Eringen [31], Chadwick [32],...). But, if we write $\mathbf{t}_k = t^{lk} \mathbf{g}_l$ we arrive to the representation $\mathbf{T} = T^{kl} \mathbf{g}_k \otimes \mathbf{g}_l$ (see for instance Truesdell and Toupin [20], Gurtin [33], Holzapfel [34],...).

⁹The cross product of a vector and a tensor is a tensor. It is a consequence of the product $\mathbf{g}_i \times (\mathbf{g}_j \otimes \mathbf{g}_k) = (\mathbf{g}_i \times \mathbf{g}_j) \otimes \mathbf{g}_k = \varepsilon_{ijl} \mathbf{g}^l \otimes \mathbf{g}_k$. But, $(\mathbf{g}_i \otimes (\mathbf{g}_j) \times \mathbf{g}_k) = \mathbf{g}_i \otimes (\mathbf{g}_j \times \mathbf{g}_k) = \varepsilon_{jkl} \mathbf{g}_i \otimes \mathbf{g}^l$. Then $\mathbf{a} \times \mathbf{A} = \varepsilon_{ijk} a^i A^{jl} \mathbf{g}^k \otimes \mathbf{g}_l$, $\mathbf{A} \times \mathbf{a} = \varepsilon_{ijk} A^{li} a^j \mathbf{g}_l \otimes \mathbf{g}^k$, where \mathbf{a} and \mathbf{A} are any vector and second order tensor (see Fredrickson [35]). Then $\mathbf{p} \times \mathbf{An} = (\mathbf{p} \times \mathbf{A})\mathbf{n}$. Also $\mathbf{nA} \times \mathbf{a} = -\mathbf{a} \times (\mathbf{nA}) =$

With the notation introduced in the table, the equations of balance of microinertia, momentum, moment of momentum, energy and entropy read: (c) Momentum

(6.11)
$$\nabla \cdot \mathbf{T} + \varrho (\mathbf{f} - \dot{\boldsymbol{\xi}}) = \hat{\varrho} \dot{\boldsymbol{\xi}} - \varrho \hat{\mathbf{f}},$$

(d) Moment of momentum

(6.12)
$$\boldsymbol{\epsilon} \cdot \cdot \mathbf{T} = \varrho \mathbf{p} \times \hat{\mathbf{f}},$$

(e) Energy (I law of thermodynamics)

(6.13)
$$-\varrho\dot{\varepsilon} + \operatorname{tr} \mathbf{T} \left(\nabla \dot{\boldsymbol{\xi}}\right)^T + \nabla \cdot \mathbf{q} + \varrho h = \hat{\varrho} \left(\varepsilon - \frac{1}{2} \dot{\boldsymbol{\xi}} \cdot \dot{\boldsymbol{\xi}}\right) + \varrho \hat{\mathbf{f}} \cdot \dot{\boldsymbol{\xi}} - \varrho \hat{h},$$

(f) Entropy inequality (II law of thermodynamics)

(6.14)
$$\varrho\dot{\eta} - \nabla \cdot \mathbf{s} - \varrho \frac{h}{\theta} \ge \varrho \frac{\hat{h}}{\theta} - \hat{\varrho}\eta.$$

In classical, unlike rational, thermodynamics entropy flux is postulated in the form $\mathbf{s} = \mathbf{q}/\theta$. Then from (6.13) and (6.14) follows that

$$-\varrho(\dot{\varepsilon}-\theta\dot{\eta}) + \operatorname{tr} \mathbf{T} (\nabla \dot{\boldsymbol{\xi}})^T + \mathbf{q} \cdot \nabla(\ln \theta) \ge \hat{\varrho} (\varepsilon - \theta\eta - \frac{1}{2} \dot{\boldsymbol{\xi}} \cdot \dot{\boldsymbol{\xi}}) + \varrho \hat{\mathbf{f}} \cdot \dot{\boldsymbol{\xi}},$$

In solving specific problems it is necessary to express balance laws in the componental form. It is useful to write them in general coordinate system. But, the choice of particular coordinate system dependents on the problem which has to be solved. In general, from mathematical point of view, we have to deal with the system of partial differential equations.

Thus, the balance laws (6.9), (6.11)–(6.14), read: (g) Balance of mass

$$\dot{\varrho} + \varrho \dot{\xi}^k_{,k} = \hat{\varrho}$$

(h) Balance of momentum

$$T^{kl}_{,k} + \varrho \left(f^l - \ddot{\xi}^l \right) = \hat{\varrho} \dot{\xi}^l - \varrho \hat{f}^l,$$

(i) Balance of moment of momentum

$$\varepsilon^{lmn}T_{mn} = \varrho \varepsilon^{lmn} p_m \hat{f}_n,$$

(j) Balance of energy (I law of thermodynamics)

$$-\varrho\dot{\varepsilon} + T^{kl}\dot{\xi}_{l,k} + q^{k}_{,k} + \varrho h = \hat{\varrho}(\varepsilon - \frac{1}{2}\dot{\xi}^{k}\dot{\xi}_{k}) + \varrho\hat{f}^{k}\dot{\xi}_{k} - \varrho\hat{h},$$

(k) Entropy inequality (II law of thermodynamics)

$$-\varrho(\dot{\varepsilon}-\theta\dot{\eta})+T^{kl}\dot{\xi}_{l,k}+q^k(\ln\theta)_{,k}\geqslant\hat{\varrho}\big(\varepsilon-\theta\eta-\frac{1}{2}\dot{\xi}^k\dot{\xi}_k\big)+\varrho\hat{f}^k\dot{\xi}_k.$$

It is important to note that $(6.6)_1$ holds for the set $(\hat{\varrho}, \varrho \hat{f}^l, \varrho \hat{h})$ of the residuals over their domains of definitions, i.e.,

$$\int_{v-\sigma} \left(\hat{\varrho}, \varrho \hat{f}^l, \varrho \hat{h}\right) dv = 0.$$

 $^{-\}mathbf{a} \times \mathbf{A}^T \mathbf{n} = -(\mathbf{a} \times \mathbf{A}^T)\mathbf{n}$. These relations are useful for the calculation of the surface integrals (see Brand [36]).

In many cases it is more convenient to use the material representation of these balance laws:

$$T^{Kl}_{,K} + \varrho_0 (f^l - \ddot{\xi}^l) = \hat{\varrho}_0 \dot{\xi}^l - \varrho_0 \hat{f}^l, - \varrho_0 \dot{\varepsilon} + T^K_{,k} \dot{\xi}^k_{;K} + Q^K_{,K} = \hat{\varrho}_0 (\varepsilon - \frac{1}{2} \dot{\xi}^k \dot{\xi}_k) + \varrho_0 \hat{f}^k \dot{\xi}_k - \varrho_0 (\hat{h} + h)$$

and entropy inequality

$$-\varrho_o(\dot{\varepsilon}-\theta\dot{\eta})+T_k^K\dot{\xi}_{;K}^k+Q^K(\ln\theta)_{,K}\geqslant\hat{\varrho}_o\big(\varepsilon-\theta\eta-\frac{1}{2}\dot{\xi}^k\dot{\xi}_k\big)+\varrho_o\hat{f}^k\dot{\xi}_k$$

 ${\rm where}^{10}$

$$\varrho_o = \varrho J, \quad J = \det\left(\xi_{;K}^k\right), \quad \hat{\varrho}_o = \hat{\varrho}J, \quad T^{Kl} \equiv J X_{;k}^K t^{kl}, \quad Q^K \equiv J X_{;k}^K q^k,$$

6.3. Nonmaterial Interface. Boundary Conditions. In the case when discontinuity surface is not material (for example the surface propagate as a wave), $\gamma = 0$ by definition. Then, all the quantities which are related to the surface are equal zero, except surface nonlocal effect \hat{p}_{σ} (see (b)): ψ_{σ} , Φ_{σ} and p_{σ} . Then (6.8) becomes

(6.15)
$$\left[\!\left[\varrho\psi_v(\dot{\boldsymbol{\xi}}-\dot{\mathbf{x}})-\boldsymbol{\Phi}_v\right]\!\right]\cdot\mathbf{n}=\hat{p}_{\sigma}.$$

Formally, (6.15) states general boundary condition corresponding to the equation by which balance law of the quantity ψ_v is expressed. Specially, (6.15) defines the boundary condition for ρ

$$\left[\varrho(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}})\right] \cdot \mathbf{n} = \hat{\gamma},$$

since then $\psi_v = 1$, $\Phi_v = 0$ and $\hat{p}_{\sigma} = \hat{\gamma}$.

The other explicit form of boundary conditions for the specific physical quantity ψ_v is obtained by using data from table 1:

$$\llbracket \varrho \dot{\boldsymbol{\xi}} \otimes (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{T} \rrbracket \mathbf{n} = \hat{\mathbf{f}}_{\sigma}, \quad 0 = \hat{\boldsymbol{\ell}}_{\sigma} - \mathbf{p} \times \hat{\mathbf{f}}_{\sigma}, \\ \llbracket \varrho (\varepsilon + \frac{1}{2} \dot{\boldsymbol{\xi}} \cdot \dot{\boldsymbol{\xi}}) (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \dot{\boldsymbol{\xi}} \mathbf{T} - \mathbf{q} \rrbracket \mathbf{n} = \hat{\boldsymbol{\varepsilon}}_{\sigma}, \quad \llbracket \varrho \eta (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{s} \rrbracket \cdot \mathbf{n} = \hat{\mathbf{n}}_{\sigma},$$

which present boundary conditions for balance of momentum (6.11), balance of moment of momentum (6.12), balance of energy (6.13) and balance of entropy (6.14).

6.3.1. Material Interface. The singular surface will be also used as a mathematical model for a thin wall or a membrane which separates one part of the body under consideration from another part.

Then the interfacial balance law (6.8) can be used in the way which is completely analogous to the procedure of using balance law (6.7) of three-dimensional body (bulk material). Thus for $\psi_{\sigma} = 1$, $\Phi_{\sigma} = 0$, $p_{\sigma} = 0$, $\hat{p}_{\sigma} = \hat{\gamma}$, as well as $\psi_v = 1$ and $\Phi_v = 0$ we obtain

(a) Balance of mass of interface

(6.16)
$$\frac{\delta_m \gamma}{\delta t} + \gamma \left(\nabla_{\sigma} \cdot \dot{\mathbf{u}} - 2u K_M \right) + \left[\left[\varrho \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}} \right) \right] \right] \cdot \mathbf{n} = \hat{\gamma}$$

From (6.8) and (6.16) we get, in the case of general parametrization of interface

¹⁰Note that ρ_0 is reduced to referent density only in the case when $\hat{\rho} = 0$.

(b) Local balance law of the quantity ψ_{σ}

(6.17)
$$\gamma \frac{\delta_m \psi_\sigma}{\delta t} - \nabla_\sigma \cdot \mathbf{\Phi}_\sigma - \gamma p_\sigma + \left[\!\!\left[\varrho(\psi_v - \psi_\sigma)(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{\Phi}_v\right]\!\!\right] \mathbf{n} = \hat{p}_\sigma - \hat{\gamma}\psi_\sigma,$$
where
$$\delta_m \psi_\sigma = \partial \psi_\sigma + \rho_\phi$$

$$\frac{\partial_m \psi_\sigma}{\delta t} = \frac{\partial \psi_\sigma}{\partial t} + \pounds \psi_\sigma.$$

It is more usual in the literature to use orthogonal parametrization, since then (6.17) can be written in more simplified form.

From mathematical point of view, problems of two-dimensional bodies are more complex because of the geometry of the bodies. In general case, here we are dealing with the Riemann geometry of surface, which is much more complicated than Euclidean geometry. Having this in mind, mathematical models of two-dimensional bodies are primarily simplified by disregarding the effects which can be physically justified, as some nonlocal influences, such as surface mass residual, microinertion influence etc. Then for the general balance law (6.17) we write

(6.18)
$$\gamma \frac{\delta_m \psi_\sigma}{\delta t} - \nabla_\sigma \cdot \mathbf{\Phi}_\sigma - \gamma p_\sigma + \left[\!\!\left[\varrho(\psi_v - \psi_\sigma)(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{\Phi}_v \right]\!\!\right] \mathbf{n} = 0.$$

For such mathematical models we write balance laws by using general balance law (6.18) and Table 2.

Ta	ble	2.

ψ	ψ_{σ}	Φ_{σ}	p_{σ}
momentum	ż	S	\mathbf{f}_{σ}
moment of momentum	$\mathbf{x} imes \dot{\mathbf{x}}$	$\mathbf{x} imes \mathbf{S}$	$\mathbf{x} imes \mathbf{f}_{\sigma}$
energy	$\frac{1}{2}\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}+\varepsilon_{\sigma}$	$\mathbf{S}\dot{\mathbf{x}}+\mathbf{q}_{\sigma}$	$\mathbf{f}_{\sigma}\cdot\dot{\mathbf{x}}+h_{\sigma}$
entropy	η_{σ}	\mathbf{s}_{σ}	$h_{\sigma}/ heta$

Here,

 $\mathbf{S} = S^{i\alpha} \mathbf{g}_i \otimes \mathbf{a}_{\alpha}$ – surface stress,

 \mathbf{f}_{σ} – external body force per unit mass of material surface,

 ε_{σ} – specific internal surface energy,

 $\mathbf{q}_{\sigma} = q_{\sigma}^{\alpha} \mathbf{a}_{\alpha}$ – surface heat flux vector,

 η_{σ} – surface entropy density,

 $\mathbf{s}_{\sigma} = s^{\alpha} \mathbf{a}_{\alpha}$ – surface entropy flux vector,

 h_{σ}/θ – surface entropy production.

It is also $\mathbf{x} \times \mathbf{S} = \varepsilon_{ijk} x^j S^{k\alpha} \mathbf{g}^i \otimes \mathbf{a}_{\alpha}$.

Next, by substituting corresponding quantities from Table 2 into (6.18) we get the following balance laws for material interface:

(c) Balance of momentum of material interface

(6.19)
$$\gamma \ddot{\mathbf{x}} - \nabla_{\sigma} \cdot \mathbf{S} - \gamma \mathbf{f}_{\sigma} + \left[\!\!\left[\varrho(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) \otimes (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{T}\right]\!\!\right] \mathbf{n} = -\hat{\gamma} \dot{\mathbf{x}},$$

(d) Balance of moment of momentum of material interface

(6.20)
$$\varepsilon_{ijk} x^i_{,\alpha} S^{j\alpha} \mathbf{g}^k = -\hat{\gamma} \mathbf{x} \times \dot{\mathbf{x}} +$$

(e) Balance of energy of material interface

(6.21)
$$\gamma \dot{\varepsilon}_{\sigma} - \operatorname{tr} \mathbf{S}^{T} (\nabla_{\sigma} \dot{\mathbf{x}}) - \nabla_{\sigma} \mathbf{q}_{\sigma} - \gamma h_{\sigma}$$
$$+ \left[\left[\varrho \left[\frac{1}{2} (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}})^{2} + (\varepsilon_{v} - \varepsilon_{\sigma}) \right] (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{T}^{T} (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{q} \right] \right] \cdot \mathbf{n}$$
$$= -\hat{\gamma} \left(\varepsilon_{\sigma} - \frac{1}{2} \dot{\mathbf{x}} \dot{\mathbf{x}} \right),$$

(f) Balance of entropy of material interface

(6.22)
$$\gamma \dot{\eta}_{\sigma} - \nabla_{\sigma} \cdot s_{\sigma} - \gamma \frac{h_{\sigma}}{\theta} + \left[\!\left[\varrho(\eta - \eta_{\sigma}) \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}\right) - \mathbf{s}\right]\!\right] \cdot \mathbf{n} = -\hat{\gamma}\eta_{\sigma}.$$

Remark. In the special case when the mathematical model is nonpolar continuum, where influence of nonlocality is disregarded, that is, when $\hat{\gamma} = 0$, balance laws of material interface (6.16), (6.19), (6.20), (6.21) and (6.22) become (see Moekel [30])

(6.23)

$$\frac{\partial \gamma}{\partial t} + \nabla_{\sigma}(\gamma \dot{\mathbf{u}}) - 2\gamma u K_{M} + \llbracket \varrho(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) \rrbracket \mathbf{n} = 0, \\
\gamma \ddot{\mathbf{x}} - \nabla_{\sigma} \mathbf{S} - \gamma \mathbf{f}_{\sigma} + \llbracket \varrho(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) \otimes (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) - \mathbf{T} \rrbracket \mathbf{n} = 0, \\
\varepsilon_{ijk} x_{,\alpha}^{i} S^{j\alpha} \mathbf{g}^{k} = 0,$$

$$\gamma \dot{\varepsilon}_{\sigma} - \operatorname{tr} \mathbf{S}^{T} (\nabla_{\sigma} \dot{\mathbf{x}}) - \nabla_{\sigma} \cdot \mathbf{q}_{\sigma} - \gamma h_{\sigma} + \left[\left[\varrho \left[\frac{1}{2} \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}} \right)^{2} + \left(\varepsilon_{v} - \varepsilon_{\sigma} \right) \right] \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}} \right) - \mathbf{T}^{T} \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}} \right) - \mathbf{q} \right] \mathbf{n} = 0, \gamma \dot{\eta}_{\sigma} - \nabla_{\sigma} \mathbf{S}_{\sigma} - \gamma \frac{h_{\sigma}}{\theta} + \left[\left[\varrho (\eta - \eta_{\sigma}) \left(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}} \right) - \mathbf{s} \right] \right] \mathbf{n} = 0.$$

Relation (6.23) is significantly simplified by decomposing the stress tensor on normal and tangential components $S^{j\alpha} = S^{\alpha}n^j + S^{\beta\alpha}x^j_{\ \beta}$. Then (6.23) is reduced to $S^{\alpha} = 0$, $\varepsilon_{\alpha\beta}S^{\alpha\beta} = 0$. Thus, surface stress $\mathbf{S} = S^{\alpha\beta}\mathbf{a}_{\alpha} \otimes \mathbf{a}_{\beta}$ is a symmetrical tensor.

These balance laws are valid for the most general class of material surfaces which allow mass transport of the bulk material through it, i.e., when

(6.24)
$$(\boldsymbol{\xi} - \dot{\mathbf{x}}) \cdot \mathbf{n} \neq 0.$$

Such material surfaces are said to be *permeable*.

In some cases material surfaces allow transport of just one kind of a bulk material. For that material, which we are going to denote by α , (6.24) is valid in the form $(\dot{\boldsymbol{\xi}}_{\alpha} - \dot{\mathbf{x}}) \cdot \mathbf{n} \neq 0$. Then the condition of impermeability for the bulk material β reads $(\dot{\boldsymbol{\xi}}_{\beta} - \dot{\mathbf{x}}) \cdot \mathbf{n} = 0$. Such material surfaces are said to be *semi-permeable*.

6.3.2. Impermeable Material Surface. It is the most restricted class of material surfaces. In that case the particles of the bulk material do not pass through surface. Mathematically, it is equivalent to the condition $(\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) \cdot \mathbf{n} = 0$. Then balance *laws of the impermeable material surface* reads

$$\frac{\partial \gamma}{\partial t} + \nabla_{\sigma} \cdot (\gamma \dot{\mathbf{u}}) - 2u\gamma K_M = 0, \gamma \ddot{\mathbf{x}} - \nabla_{\sigma} \cdot \mathbf{S} - \gamma \mathbf{f}_{\sigma} - [[\mathbf{T}]] \mathbf{n} = 0,$$

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$$\gamma \dot{\varepsilon}_{\sigma} - \operatorname{tr} \mathbf{S}^{T} \left(\nabla_{\sigma} \dot{\mathbf{x}} \right) - \nabla_{\sigma} \cdot \mathbf{q}_{\sigma} - \gamma h_{\sigma} - \left[\left[\mathbf{T}^{T} (\dot{\boldsymbol{\xi}} - \dot{\mathbf{x}}) + \mathbf{q} \right] \right] \cdot \mathbf{n} = 0,$$

$$\gamma \dot{\eta}_{\sigma} - \nabla_{\sigma} \cdot \mathbf{s}_{\sigma} - \gamma \frac{h_{\sigma}}{\theta} + \left[\left[\mathbf{s} \right] \right] \cdot \mathbf{n} = 0.$$

6.4. Balance Laws for a Mixture. In single-components systems (or pure substances), which has been considered, up to now, the chemical composition in all phases is the same. But, in many areas within the field of continuum physics it is necessary to use the fact that the material being described may be composed of several different constituents.

Such multicomponents systems are called *mixtures*. In these systems the chemical composition of a given phase changes in response to pressure and temperature and these compositions are not the same in all phases.

The constituents of mixture, generally, may react with each other to produce new constituents. Such a general material will be called a *heterogeneous reacting continuum* or simply a *reacting continuum*. If the constituents composing the material do not react, then it will be called a *heterogeneous continuum*. An example of a reacting continuum is a dissociating and ionizing gas. Liquid helium II, an electrically conducting plasma and a suspension of solid particles in a fluid are examples of heterogeneous continua.

Most of the literature on reacting continua, and on heterogeneous continua deals with chemically reacting fluids. This literature has been unified and generalized by Truesdell and Toupin [20], who presented the differential balance equations for a mixture of chemically reacting continua. He does not restrict the continuum to be a solid, liquid or gas.

Thus, the theory of mixture is more complicated than the theory of a single body but not different in kind.

The approach presented here is an extension of the program started by Truesdell [37] to the problem of nonlocal heterogeneous continuum.

Modeling of the behaviour of multicomponents systems can be done using several methods and looking at the problem at different spatial scales. Eringen and his coworkers have developed the micromorphic theory of mixture of several constituents in anticipation of the possible application, for example, to crystal lattices in which the lattice sites are regularly occupied by two or more different ions or molecules, to granular or polycrystalline mixture, to composite materials, or to fluid suspensions (Twiss and Eringen [38], [39]).

For derivation of complete theory we refer the reader to the above papers and literature cited in them. Because of that here we give the basic concepts and expressions which are going to be used in what follows.

In order to treat motion of physical mixtures possibly undergoing chemical changes, Fick [40] and Stefan [41] suggested that each place \mathbf{x} may be regarded as occupied simultaneously by several different particles \mathbf{X}_{α} , $\alpha = 1, 2, \ldots, k$, one for each constituent α . The mixture is thus represented as a superposition of α continuous media, each of which follows its own individual motion

(6.25)
$$\mathbf{x} = \mathbf{x}_{\alpha}(\mathbf{X}_{\alpha}, t),$$

Henceforth media whose motion is described by (6.25) will be called *heterogeneous* if $\alpha > 1$; if $\alpha = 1$, they will be called *simple*. In considering kinematics of heterogenous systems we follow Truesdel and Toupin [20].

Then the *constituent* (individual) velocity \mathbf{v}_{α} is defined by

$$\mathbf{v}_{\alpha} \equiv \frac{\partial \mathbf{x}}{\partial t}\Big|_{\mathbf{X}_{\alpha} = \text{const}}, \quad \text{or} \quad v_{a}^{k} \equiv \frac{\partial x^{k}}{\partial t}\Big|_{\mathbf{X}_{\alpha} = \text{const}}$$

Further, since each constituent has its individual density ρ_{α} , we define the total density ρ by

(6.26)
$$\varrho = \sum_{\alpha=1}^{k} \varrho_{\alpha}$$

The concentration c_{α} of the constituent α is defined by $c_{\alpha} = \rho_{\alpha}/\rho$, so that (6.26) is equivalent to $\sum_{\alpha=1}^{k} c_{\alpha} = 1$. The *mean velocity* **v** of the mixture is defined by the requirement that the total

mass flow is the sum of the individual mass flows:

(6.27)
$$\boldsymbol{\varrho}\mathbf{v} = \sum_{\alpha=1}^{k} \boldsymbol{\varrho}_{\alpha}\mathbf{v}_{\alpha}, \quad \text{or} \quad \mathbf{v} = \sum_{\alpha=1}^{k} c_{\alpha}\mathbf{v}_{\alpha}.$$

The diffusion velocity, or peculiar velocity of the constituent α is its velocity

relative to the mean velocity: $\mathbf{u}_{\alpha} = \mathbf{v}_{a} - \mathbf{v}$. From (6.27) it follows $\sum_{\alpha=1}^{k} \varrho_{\alpha} \mathbf{u}_{\alpha} = 0$, and $\sum_{\alpha=1}^{k} c_{\alpha} \mathbf{u}_{\alpha} = 0$. That is to say, the mean velocity has been defined in such a way that the total mass flow of the diffusive motions is zero.

We now introduce two different material derivatives $\dot{\psi}$ and $\dot{\psi}$; the former, which coincides with that used for simple media, follows the mean motion, while the latter follows the individual motion of the constituent α :

(6.28)
$$\dot{\psi} = \frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \operatorname{grad} \psi, \qquad \dot{\psi} = \frac{\partial \psi}{\partial t} + \mathbf{v}_{\alpha} \cdot \operatorname{grad} \psi.$$

Hence $\dot{\psi} - \dot{\psi} = \mathbf{u}_{\alpha} \cdot \operatorname{grad} \psi$, so that the two derivatives coincide, in the case when ψ is a non-constant scalar, if and only if (iff) the diffusion velocity of the constituent α is tangent to the surface $\psi = \text{const.}$

Further, we set

(6.29)
$$\varrho \psi \equiv \sum_{\alpha} \varrho_{\alpha} \psi_{\alpha}$$

and then, making use of (6.28), we obtain the following fundamental identity

(6.30)
$$\sum_{\alpha} \varrho_{\alpha} \dot{\psi}_{\alpha} = \varrho \dot{\psi} + \psi \left[\frac{\partial \varrho}{\partial t} + \operatorname{div} \left(\varrho \mathbf{v} \right) \right] \\ + \sum_{\alpha} \operatorname{div} \left(\varrho_{\alpha} \psi_{\alpha} \mathbf{u}_{\alpha} \right) - \sum_{\alpha} \psi_{\alpha} \left[\frac{\partial \varrho_{\alpha}}{\partial t} + \operatorname{div} \left(\varrho_{\alpha} \mathbf{v}_{\alpha} \right) \right],$$

or

$$\begin{split} \sum_{\alpha} \varrho_{\alpha} \dot{\psi}_{\alpha} &= \varrho \dot{\psi} + \psi \left[\frac{\partial \varrho}{\partial t} + \left(\varrho v^{k} \right)_{,k} \right] \\ &+ \sum_{\alpha} \left(\varrho_{\alpha} \psi_{\alpha} u^{k}_{\alpha} \right)_{,k} - \sum_{\alpha} \psi_{\alpha} \left[\frac{\partial \varrho_{\alpha}}{\partial t} + \left(\varrho_{\alpha} v^{k}_{\alpha} \right)_{,k} \right]. \end{split}$$

Upon this identity, which relates the material derivative of the mean value (6.29) to the mean value of the material derivatives, all our proofs of equations of balance in a heterogeneous medium are founded.

Then, the general balance laws can be written in the form:

$$\left(\int_{v} \psi_{\alpha} \, dv\right)' = \int_{\partial v} \boldsymbol{\phi}_{\alpha} \mathbf{n} \, da + \int_{v} p_{\alpha} \, dv.$$

Since this holds for all v, however small, a classical argument yields the differential form of the general balance:

(6.31)
$$\hat{\psi}_{\alpha} + \psi_{\alpha} \operatorname{div} \mathbf{v}_{\alpha} - \operatorname{div} \boldsymbol{\phi}_{\alpha} - p_{\alpha} = \hat{p}_{\alpha}$$

(6.32)
$$\llbracket \psi_{\alpha}(\mathbf{v}_{\alpha} - \mathbf{u}) - \boldsymbol{\phi}_{\alpha} \rrbracket \mathbf{n} = \hat{\tilde{p}}_{\alpha},$$

where

$$\int_{v-\sigma} \hat{p}_{\alpha} \, dv + \int_{\sigma} \hat{\tilde{p}}_{\alpha} \, da = 0.$$

Remark. It is very important to underline that \hat{p}_{α} and \hat{p}_{α} contain both influences: nonlocality and chemical reactions of the constituents. Very general theory of mixture for micromorphic material with chemical reactions can be found in Cvetković [42]. Here we follow this approach, which is based on Eringen's paper [43]. Also we make use of their notations. Note that these papers contain only parts of \hat{p}_{α} and $\hat{\tilde{p}}_{\alpha}$ i.e., the influence of a chemical reactions. In other words, they did not take into account the effects of nonlocality. Here we underline that the influence of nonlocality will be taken into account through the constitutive equations.

By using arguments quite similar to those presented in Section 16, we derive constituent balance equations for mixture. We start with

i) the balance of mass; In this case $\psi_{\alpha} = \varrho_{\alpha}$, $\phi_{\alpha} = 0$, $p_{\alpha} = 0$, and $\hat{p}_{\alpha} = \varrho \hat{\beta}_{\alpha}$. Then from (6.31) and (6.32) we obtain

(6.33)
$$\hat{\varrho}_{\alpha} + \varrho_{\alpha} \operatorname{div} \mathbf{v}_{\alpha} = \varrho \hat{\beta}_{\alpha}, \quad \text{or} \quad \frac{\partial \varrho_{\alpha}}{\partial t} + \operatorname{div}(\varrho_{\alpha} \mathbf{v}_{\alpha}) = \varrho \hat{\beta}_{\alpha},$$

(6.34)
$$\left\| \varrho_{\alpha} (\mathbf{v}_{\alpha} - \mathbf{u}) \right\| \mathbf{n} = 0.$$

In order to simplify further calculation, particularly having in mind (6.30), we need the expression $\partial \rho / \partial t + \operatorname{div}(\rho \mathbf{v})$. This can be achieved by summing (6.33) and (6.34) over all constituents. In this way we obtain the local balance equation of mass of mixture

(6.35)
$$\frac{\partial \varrho}{\partial t} + \operatorname{div}(\varrho \mathbf{v}) = 0, \quad \sum_{\alpha} \hat{\beta}_{\alpha} = 0,$$

as a consequence of the assumption that the mass of mixture does not change.

Making use of (6.33) and (6.35) in (6.30) we reduced the fundamental identity to the form

$$\sum_{\alpha} \varrho_{\alpha} \acute{\psi}_{\alpha} = \varrho \dot{\psi} + \sum_{\alpha} \operatorname{div}(\varrho_{\alpha} \psi_{\alpha} \mathbf{u}_{\alpha}) - \sum_{\alpha} \varrho \hat{\beta}_{\alpha} \psi_{\alpha}.$$

Also, we write

(6.36)
$$\psi_{\alpha} \to \varrho_{\alpha}\psi_{\alpha}, \quad p_{\alpha} \to \varrho_{\alpha}p_{\alpha}, \quad \hat{p}_{\alpha} \to \varrho\hat{p}_{\alpha}$$

Then, in view of (6.31), (6.32), (6.33) and (6.36) we obtain

$$\begin{aligned} \operatorname{div} \boldsymbol{\phi}_{\alpha} + \varrho_{\alpha}(p_{\alpha} - \psi_{\alpha}') &= \varrho \big(\hat{\beta}_{\alpha} \psi_{\alpha} - \hat{p}_{\alpha} \big), \\ & [\![\varrho_{\alpha} \psi_{\alpha}(\mathbf{v}_{\alpha} - \mathbf{u}) - \boldsymbol{\phi}_{\alpha}]\!]\mathbf{n} = \hat{\tilde{p}}_{\alpha}. \end{aligned}$$

These relations are fundamental in obtaining the local form of *constituent balance* equations for mixture. In order to derive them, we can use tables 1a and 1b for a constituent of mixture. In this way, we obtain

ii) the constituent local balance equations for momentum:

(6.37)
$$\mathbf{t}_{\alpha,k}^{k} + \varrho_{\alpha}(\mathbf{f}_{\alpha} - \dot{\mathbf{v}}_{\alpha}) = \varrho \hat{\beta}_{\alpha} \mathbf{v}_{\alpha},$$

(6.38) $\left[\!\left[\mathbf{t}_{\alpha}^{k}-\varrho_{\alpha}\mathbf{v}_{\alpha}\left(\boldsymbol{v}_{\alpha}^{k}-\boldsymbol{u}^{k}\right)\right]\!\right]\boldsymbol{n}_{k}=0.$

Further, we need

iii) the constituent local balance equations for moment of momentum:

(6.39)
$$\mathbf{t}_{\alpha,k}^{kl} + \mathbf{t}_{\alpha}^{l} - \tilde{\mathbf{t}}_{\alpha}^{l} + \varrho_{\alpha} \mathbf{f}_{\alpha}^{l} = \varrho \hat{\beta}_{\alpha}^{l} \mathbf{v}_{\alpha},$$

(6.40)
$$\llbracket \mathbf{t}_{\alpha}^{kl} \rrbracket n_k = 0.$$

We do not need the *constituent local balance laws of energy and entropy*. Again, we refer the reader to the original literature if needed (see for instance Cvetković [42]).

The mixture local balance of momentum and moment of momentum and the jump conditions are obtained by summing (6.37) through (6.40) over all constituents. The results are:

(a) the balance of momentum

$$\mathbf{t}_{,k}^{k} + \varrho(\mathbf{f} - \dot{\mathbf{v}}) = 0,$$
$$[\mathbf{t}^{k} - \varrho \mathbf{v} (v^{k} - u^{k})] n_{k} = 0,$$

where $\rho \mathbf{f} = \sum_{\alpha} \rho_{\alpha} \mathbf{f}_{\alpha}, \, \mathbf{t}^{k} = \sum_{\alpha} \left(\mathbf{t}_{\alpha}^{k} - \rho_{\alpha} \mathbf{u}_{\alpha} u_{\alpha}^{k} \right);$ (b) the balance of moment of momentum

$$\mathbf{t}^{km}_{,k} + \mathbf{t}^m - \bar{\mathbf{t}}^m + \varrho \mathbf{f}^m = \varrho \mathbf{v} \sum_{\alpha} \hat{\beta}^m_{\alpha}$$

under the conditions $\sum_{\alpha} \hat{\beta}^m_{\alpha} = 0$. Also, by definition,

$$\mathbf{t}^{km} = \sum_{\alpha} \mathbf{t}^{km}_{\alpha}, \quad \mathbf{t}^m - \bar{\mathbf{t}}^m = \sum_{\alpha} \left(\mathbf{t}^m_{\alpha} - \bar{\mathbf{t}}^m_{\alpha} \right), \quad \varrho \mathbf{f}^m = \sum_{\alpha} \mathbf{f}^m_{\alpha}, \quad [\![\mathbf{t}^{kl}]\!] n_k = 0.$$

7. Conclusion

Motion, stress, energy, entropy, and electromagnetism are the concepts upon which field theories are constructed. Laws of conservation or balance are laid down as relating these quantities in all cases. These basic principles, which are in integral form, in regions where the variables change sufficiently smoothly are equivalent to differential field equations; at surfaces of discontinuity, to jump conditions.

The field equations and jump conditions form an undetermined system, insufficient to yield specific answers unless further equations are supplied.

The balance laws of continuum physics make no reference to the constitution of the body. Material bodies of the same mass and geometry respond to the same external effects in different ways. Internal constitution of matter is responsible for these differences. From a continuum point of view we may develop equations which reflect the nature of the material and the constitution of the body. Such a set of the equations are known as constitutive equations. Thus, the characterization of particular materials is brought within the framework of continuum physics through the formulation of constitutive equations (or equation of state).

From theoretical point of view, constitutive equations define an ideal material.

Mathematically the purpose of these relations is to support connections between kinematic, mechanical and thermal fields which are compatible with the field equations and which, in conjunction with them, yield a theory capable of providing solutions correctly set problems.

Each field of continuum mechanics deals with certain continuous media including fluids, which are liquids or gases (such as water, oil, air etc.) and solids (such as rubber, metal, ceramics, wood, living tissue etc.). If the constitutive equations are valid for physical objects such as fluids we call the field of continuum mechanics fluid mechanics. Another important field in which constitutive equations are valid for solids is known as solid mechanics.

Physically, constitutive equations represent various forms of idealized material response which serve as model of the behaviour of actual substances. The predictive value of models, as assessed experimentally over particular ranges of physical conditions, affords justification for the special continuum the mentioned above.

Since the constitutive theory is very broad and specific subject, and because of the limited space here we refer the reader to the following excellent reference books: Truesdell and Noll [44], Eringen [31], Gurtin [33], Chadwik [32] and Holzapfel [34].

In this way the theoretical approach is completed. Then, the particulary problems of bulk material and interfaces can be considered and solved.

Thus, the constitutive equations and field equations together, along with the jump conditions and boundary condition, should lead to a definite theory, predicting specific answers to particular problems.

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