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Heat and mass flows coupled with stress in a continuous medium

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Abstract—The present paper is concerned with the formulation of the generalization of theories describing heat and mass flows in a continuous medium. The considerations are based on the non-equilibrium thermodynamics. As a result the fundamental equations for the mass and heat fluxes and for the thermodynamic and mechanical fields, are obtained and the corresponding set of differential equations is formulated. Certain differences are pointed out between the general theories presented here and the thermodiffusion theory and the theory of mixtures. A thermodynamic variational principle is constructed. All the investigations concern only flows with a single temperature field. Copyright © 1996 Elsevier Science Ltd.

1. INTRODUCTION

Process of mass and heat transport in homo- and heterogeneous media have been the subject of intense investigation for several years. Some elements of mechanical processes in the theory of mixtures can be found in a paper written by Truesdell in 1957 [1]. He presented further results, which are based on contemporary thermodynamics, in refs. [2–4]. At present there are many publications on the theory of mixtures. Some of them are rather general (for instance the works of Atkin and Craine [5, 6] and Wilmanski [7]) and some concern its particular applications and aspects. There are also monographs concerning the theory of mixtures. In well-known works by Slattery [8] and Bowen [9] we find equations of balance and entropy inequalities for various problems of the theory of mixtures, and in addition a number of comments, and very comprehensive materials concerning those problems. In these books, as well as in the papers previously cited [5–7], there are extensive lists of references concerning the theory of mixtures. In this paper the list of references contains only certain chosen publications on this problem.

On the other hand there are numerous examples of single flows in a distinguished and dominant constituent, i.e. a skeleton, for instance fluids and gases permeating solids. These cases lead to the deformation of the body, its expansion and shrinkage. Thus, for example, filtration of hydrogen under pressure into steel results in appreciable deformations. Thin membranes permeated by hydrogen undergo bending or warping and the diffusion flows coupled with a stress field occur, often with conversion between body constituents.

The effect of heating the body during mass transport is equally important. An experiment proves that the distribution of humidity in a porous medium is substantially changed by changes of temperature fields [10, 11]. In order to accelerate the exit of a gas from a metal, heating of the body is used in such processes as the carbonation or decarbonation of steel which occur in a variable temperature field. These facts lead directly to the thermodiffusion description, and this theory involves the interactions between processes of mass transport, thermal processes described by temperature fields and the process of deformation of the body described by the displacement vector and the state of stress. (See for instance [12–16] in an elastic and [17–19] in a viscoelastic body.) These coupled thermal, mechanical and diffusion flows phenomena are typical not only for many capillary-porous media but one can also observe them in the majority of technological processes, where material structure rebuilding is concerned (i.e. recrystallization). Moreover one can describe new material constituent generation as a result of deformation processes, temperature changes, and mass flows, or to some extent of chemical reactions and phase changes in a solid [10].

The possibility of describing the processes described above is provided by two theories in general, i.e. either by the theory of mixtures for the multicomponent medium (which seems to be the most global) or by the thermodiffusion theory for single flows through the skeleton. However there are differences in the description of the process of mass transfer in these theories. While in the theory of mixtures the mass transport is characterized by the momentum of the particular particles [20–23], in the thermodiffusion

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NOMENCLATURE

a	the density of a scalar quantity per unit volume
$\mathbf{A}$	the density of a vector (tensor) quantity per unit volume
b	the region which is occupied at time t by an arbitrary material volume belonging to the volume $\mathscr{B}$ ($b \subset \mathscr{B}$)
c_α	concentration of the αth component
e	a trace of a deviator of a strain tensor (volume expansion) $e = \varepsilon_{ii}$
$\mathbf{e}_i$	basic vectors in a Cartesian coordinate system
e_{ij}	deviator of a strain tensor ε_{ij}
E	Young's modulus (of elasticity) in tension and compression
F	a scalar field of free (Helmholtz) energy density at time t per unit mass $[\rho F(\mathbf{x}, t) = \rho U(\mathbf{x}, t) - \rho T S(\mathbf{x}, t)]$
$\mathbf{F}$	volume distribution of body force per unit mass acting at time t ($\mathbf{F} = F_i \mathbf{e}_i$)
G	shear or rigidity modulus (of elasticity)
$\underset{\wedge}{\mathbf{j}}_a$	the density of the flow of the quantity A, per unit of surface $\partial\mathscr{B}$ and per unit of time
$\mathbf{j}^c_a$	the convection part of the flow $\underset{\wedge}{\mathbf{j}}_a$, which is equal to the scalar product $a\mathbf{v}$
$\hat{\mathbf{j}}_a$	the conduction (diffusion) part of the flow $\underset{\wedge}{\mathbf{j}}_a$
$\underset{\wedge}{\mathbf{j}}_s$	the global flow of the entropy
$\mathbf{j}^\alpha$	mass flux of the constituent α
$\mathbf{j}^{(\gamma)}$	a vector of thermodynamic fluxes
$\mathbf{j}$	mass flux of the total mixture (body)
M	chemical potential
$\mathbf{n}$	the unit vector normal to the surface $\partial\mathscr{B}$
$\underline{\mathbf{n}}$	the unit vector normal (external) to ∂b
$\mathbf{q}$	external energy flux across ∂b, due to heat flux only, per unit time and unit surface area $[\mathbf{q} = \mathbf{q}(\mathbf{x}, t)]$
r	a scalar field of external volumetric energy sources per unit mass and per unit time $[r = r(\mathbf{x}, t)]$
R^α	velocity with which mass is supplied to s_α from the other components per unit volume
S	scalar field of external volumetric production of entropy density at time t in each volume b in actual configuration per unit mass and per unit time $[S = S(\mathbf{x}, t)]$
$\mathbf{t}^\alpha$	vector of stress distribution $[\mathbf{t}^\alpha = \mathbf{t}^\alpha(\mathbf{x}, t, \underline{\mathbf{n}})]$; a stress vector acting on surface $x_i = \text{const.}$
t^α_{ij}	a stress tensor influencing the αth component as a result of the interaction of all the components
T	an absolute temperature $[T = T(\mathbf{x}, t)]$
U	a scalar field of internal energy density at time t per unit mass and unit time $[U = U(\mathbf{x}, t)]$
u_i	the vector of displacements
$\mathbf{u}^\alpha$	diffusive particle velocity (diffusive velocity of a particle) at time t
V	the volume of an arbitrary sub-body $\mathscr{B}$ cut out of the body $\mathscr{B}_0$ and bounded by the surface $\partial\mathscr{B}$
V_0	the volume of a body $\mathscr{B}_0$ bounded by the surface $\partial\mathscr{B}_0$
$\mathbf{v}$	the velocity of convection/mean velocity at time t
$\mathbf{v}^\alpha$	velocity vector at time t
$\mathbf{x}$	the spatial position $\mathbf{x} = \chi(\mathbf{X}, t)$ of particle X at moment of time t
X	a particle identified with its position $\mathbf{X}$
$\mathbf{X}$	a position of particle
$\mathbf{X}^{(\gamma)}$	a vector of thermodynamic forces.

Greek symbols

α	α-th component of the mixture
$\mathscr{B}$	a finite continuous body composed of particles $\mathbf{X}$
$\mathscr{B}_0$	a body occupying the volume V_0 bounded by the surface $\partial\mathscr{B}_0$
δ	the Gâteaux differential
δ_{ij}	the Kronecker delta-function
κ	a scalar describing the rate of global flow represented by conduction flow $\hat{\mathbf{j}}_a$
∂b	the boundary at time t of an arbitrary material volume occupying the region b
$\partial\mathscr{B}$	the boundary at time t of an arbitrary material volume occupying the volume $\mathscr{B}$
Σ_a	the intensity of the source, i.e. the density of the production of quantity A
Σ_s	the global source of the entropy (the rate of generation of entropy per unit volume and per unit time)
ε_{ij}	(or $\boldsymbol{\varepsilon}$) a strain tensor
χ	a vector function which defines a motion
μ, λ	Lame's functions (constants) $\mu = G$, $\lambda = \nu E/2(1+\nu)(1-\nu)$
ν	number of interacting components; each of them is understood as continuum/Poisson's ratio
ρ	total mass density (density of the total mixture) at time t
ρ_s	density of the skeleton
ρ_α	mass density of component s_α in position $\mathbf{x} = x_i \mathbf{e}_i$ at time t
$\cdot$	(a dot), a material (substantial) derivative with respect to the time t (Lagrangian derivative)
$\mathrm{d}/\mathrm{d}t$	a material (substantial) derivative with respect to the time t (Lagrangian derivative)
$\partial/\partial t$	a spatial (local) derivative with respect to the time t (Eulerian derivative)
∇	nabla operator
∇^2	Laplace operator ($\nabla^2 = \Delta$).

theory it is described by the gradient of either concentration or the chemical potential [12, 14, 15, 17, 19]. References [24–26] examine similarities and differences occurring in descriptions of heat and mass transport according to theory of mixtures and thermodiffusion. It is also shown there that there are several possibilities of transition from one description to another which are dependent on the assumptions made and kinematic or physical restrictions imposed. But in the majority of phenomena where mass transfer occurs, it is observed that the mass flow is more complicated. There exists a resultant flow between the flow generated by the gradient of concentration (or chemical potential) and the flow occurring because of the difference of momentum of particles in a multicomponent body (the skeleton and the fluid constituents). The constituent flows can have the same or opposite directions, i.e. the dominant flow will be either the gradient or the momentum flow. One of the evident examples of this phenomenon is, for instance, the water transport inside the walls of a sauna. There inside a lodging we can observe in the wall both water transport due to the differences of momentum of condensed water drops and the flow of moisture as a vapour which should be described by the generalized (replacement of the concentration by chemical potential) Fick law. Of course this phenomenon is very intricate because of phase transition, a temperature field, and possible flows of the filtration type in the capillary-porous materials. The situations become even more complicated if we consider the opposite case, i.e. the external side of the wall in different seasons and weather conditions. So during heavy rain for instance, there occurs a new flow into the building from the outside becoming larger as the momentum of water particles becomes larger and as the inlet angle approaches a right angle.

As another example of the previously mentioned mass transport phenomena one can consider the process of gas and oil subaqueous mining. However, despite all the above mentioned factors there is in every case a multicomponent medium and for this reason it is necessary to investigate the generalized theory of different type of flow mixtures.

As has been shown, there exists a need for a unified global theory containing the interactions between processes of mass transport characterized by concentration (or chemical potential) and momentum, thermal processes and the process of deformation of the body. We shall investigate the model of heat and mass transport described by the phenomenological laws. Later we shall consider some generalizations on the basis of the thermodynamics of irreversible processes.

Section 2 gives an introduction to some basic notations which are used through this paper. Then the rules of construction of the balance equations are provided. This concerns the rules for extensive scalar quantities and vector (tensor) quantities as well. In Section 3 the basic dynamic balances for a two component system are investigated. We discuss there the balances of mass, momentum, angular momentum, and internal energy. In the next section we consider Gibb's equation, as we need to introduce entropy in the most appropriate way. Subsequently the modern Gibbs' equation, thermodynamical forces and fluxes appear in Section 4. Then the set of constitutive equations for thermodynamic and mechanical quantities is laid down in Section 5. Finally, after linearization of the complete set of differential equations and making various simplifications, particular cases are presented and a variational principle of Gyarmati type is constructed in Section 6. The paper ends with a summary of its conclusions and list of references.

2. THE RULES OF BALANCE FOR TWO-COMPONENT SYSTEMS

We consider a two-component system consisting of one movable and one heavy species; a model of such a system is a gas dissolved in a metal or a fluid in a porous (elastic) medium. In our consideration the role of the frame of reference for diffusional flows will be played by the crystal lattice of the heavy component.

Consider a body b_0 occupying the volume V_0 bounded by the surface $\partial\mathscr{B}_0$. Let us separate out of the body b_0 an arbitrary sub-body b bounded by the surface $\partial\mathscr{B}$. For b we shall formulate the equation of balances for extensive quantities and for vector (tensor) quantities.

2.1. *Equation of balance for extensive scalar quantities*

The global balance of extensive quantity A for arbitrary body b we formulate according to the relation:

$$\frac{\partial A}{\partial t} = -\int_{\partial\mathscr{B}} \underset{\wedge}{\mathbf{j}}_a \cdot \mathbf{n}\,\mathrm{d}A + \int_{\mathscr{B}} \Sigma_a\,\mathrm{d}V \tag{1}$$

where the left-hand side of equation (1) represents the rate of changes of quantity A with respect to time; $\underset{\wedge}{\mathbf{j}}_a$ is the density of the flow of the scalar quantity $\hat{A}$, and it describes the amount of the scalar quantity considered which flows in unit time per unit surface $\partial\mathscr{B}$, $\mathbf{n}$ is the unit vector normal to the surface $\partial\mathscr{B}$ and Σ_a is the intensity of the source, i.e. the density of the production of quantity A. But the quantity A is represented by the integral

$$A = \int_{\mathscr{B}} a\,\mathrm{d}V \tag{2}$$

where a measures the density of the scalar quantity per unit volume. Substituting equation (2) into (1) we have

$$\int_{\mathscr{B}} \frac{\partial a}{\partial t}\mathrm{d}V = -\int_{\partial\mathscr{B}} \underset{\wedge}{\mathbf{j}}_a \cdot \mathbf{n}\,\mathrm{d}A + \int_{\mathscr{B}} \Sigma_a\,\mathrm{d}V. \tag{3}$$

Applying Green's transformation to the surface integral we have

$$\int_{\mathscr{B}} \frac{\partial a}{\partial t} \mathrm{d}V = \int_{\mathscr{B}} \left[-\mathrm{div}\, \underset{\wedge}{\mathbf{j}}_{\mathrm{a}} + \sum_{\mathrm{a}} \right] \mathrm{d}V. \tag{4}$$

In view of the assumed arbitrariness of the subvolume we obtain from (4) the local equation

$$\frac{\partial a}{\partial t} = -\mathrm{div}\, \underset{\wedge}{\mathbf{j}}_{\mathrm{a}} + \Sigma_{\mathrm{a}}. \tag{5}$$

In general we can divide the density of the flow $\underset{\wedge}{\mathbf{j}}_{\mathrm{a}}$, into two parts:

(a) the convection part $\mathbf{j}_{\mathrm{a}}^{\mathrm{c}}$ which is equal to the scalar product $a\mathbf{v}$ where $\mathbf{v}$ denotes the velocity of convection and

(b) the conduction (diffusion) flow which we will denote by $\kappa\hat{\mathbf{j}}_{\mathrm{a}}$, where κ is a scalar describing the rate at which the global flow is represented by conduction.

So, we have

$$\underset{\wedge}{\mathbf{j}}_{\mathrm{a}} = \mathbf{j}_{\mathrm{a}}^{\mathrm{c}} + \kappa\hat{\mathbf{j}}_{\mathrm{a}} \tag{6}$$

where

$$\mathbf{j}_{\mathrm{a}}^{\mathrm{c}} = a\mathbf{v}. \tag{7}$$

Substituting (6) and (7) into (5) we have

$$\begin{aligned}\frac{\partial a}{\partial t} &= -\mathrm{div}(\kappa\hat{\mathbf{j}}_{\mathrm{a}} + a\mathbf{v}) + \Sigma_{\mathrm{a}} \\ &= -\mathrm{div}\, \kappa\hat{\mathbf{j}}_{\mathrm{a}} - [a\, \mathrm{div}\, \mathbf{v} + \mathbf{v} \cdot \mathrm{grad}(a)] + \Sigma_{\mathrm{a}}.\end{aligned} \tag{8}$$

Thus we have two forms of general balance law in the Lagrange description for an arbitrary extensive scalar quantity in a continuous medium

$$\frac{\partial a}{\partial t} = -\mathrm{div}(\kappa\hat{\mathbf{j}}_{\mathrm{a}}) - \mathrm{div}(a\mathbf{v}) + \Sigma_{\mathrm{a}} \tag{9}$$

or

$$\frac{\mathrm{d}a}{\mathrm{d}t} = -\mathrm{div}(\kappa\hat{\mathbf{j}}_{\mathrm{a}}) - a\, \mathrm{div}\, \mathbf{v} + \Sigma_{\mathrm{a}} \tag{10}$$

where the notation for the Lagrange time operator

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \mathrm{grad} \tag{11}$$

has been used.

2.2. *Equation of balance for vector quantities*

We can obtain the general balance for vector quantities (and tensors as well) in a similar way to that shown above. If we denote the mentioned vector (tensor) by $\mathbf{A}$ in analogy to the equation (9) and (10) the balance equations are

$$\frac{\partial \mathbf{A}}{\partial t} = -\mathrm{div}(\kappa\hat{\mathbf{j}}_{\mathrm{a}}) - \mathrm{div}(\mathbf{A} \cdot \mathbf{v}) + \Sigma_{\mathrm{a}} \tag{12}$$

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = -\mathrm{div}(\kappa\hat{\mathbf{j}}_{\mathrm{a}}) - \mathbf{A} \cdot \mathrm{div}\, \mathbf{v} + \Sigma_{\mathrm{a}}. \tag{13}$$

3. BASIC DYNAMICAL BALANCES

3.1. *Equations of balance of mass*

We obtain the equations of balance of mass from equations (9) and (10) after replacing a by ρ_α, Σ_{a} by R^α and $\kappa\hat{\mathbf{j}}_{\mathrm{a}}$ by $\kappa\mathbf{j}_{\mathrm{a}}$. Let us change also the notation for velocity vector from $\mathbf{v}$ to $\mathbf{u}^\alpha$. This notation will be very useful in the following considerations connected with theory of mixtures ($\mathbf{u}^\alpha = \mathbf{v}^\alpha - \mathbf{v}$), thus in this particular case ($\mathbf{u}^\alpha = \mathbf{v}^\alpha = \mathbf{v}$) we have

$$\frac{\partial \rho_\alpha}{\partial t} = -\mathrm{div}(\kappa\mathbf{j}_{\mathrm{a}}) - \mathrm{div}(\rho_\alpha \mathbf{u}^\alpha) + R^\alpha$$

or

$$\frac{\mathrm{d}\rho_\alpha}{\mathrm{d}t} = -\mathrm{div}(\kappa\mathbf{j}_{\mathrm{a}}) - \rho_\alpha\, \mathrm{div}\, \mathbf{u}^\alpha + R^\alpha. \tag{14}$$

Sometimes it is useful to introduce the concentration c defined as the quantity of matter per unit volume, i.e. $c_\alpha = \rho_\alpha/\rho$. If we do this we will obtain

$$\frac{\partial \rho_\alpha}{\partial t} = \frac{\partial}{\partial t}(\rho c) = \rho\frac{\partial c}{\partial t} + c\frac{\partial \rho}{\partial t} = \rho\frac{\partial c}{\partial t}$$

$$\frac{\mathrm{d}\rho_\alpha}{\mathrm{d}t} = \rho\frac{\mathrm{d}c}{\mathrm{d}t} + c\frac{\partial \rho}{\partial t} = \rho\frac{\partial c}{\partial t} + c\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \mathrm{grad}\, \rho = \rho\frac{\partial c}{\partial t}$$

$$\begin{aligned}\mathrm{div}(\rho c\mathbf{u}^\alpha) &= \rho\, \mathrm{div}(c\mathbf{u}^\alpha) + c\mathbf{u}^\alpha \cdot \mathrm{grad}\, \rho \\ &= \rho\, \mathrm{div}(c\mathbf{u}^\alpha)\end{aligned} \tag{15}$$

and the alternative forms of balance of mass follow

$$\rho\frac{\partial c}{\partial t} = -\mathrm{div}(\kappa\mathbf{j}_{\mathrm{a}}) - \rho\, \mathrm{div}(c\mathbf{u}^\alpha) + R^\alpha$$

$$\rho\frac{\mathrm{d}c}{\mathrm{d}t} = -\mathrm{div}(\kappa\mathbf{j}_{\mathrm{a}}) - \rho c\, \mathrm{div}\, \mathbf{u}^\alpha + R^\alpha. \tag{16}$$

3.2. *Balance of linear momentum*

In the case of mass migration in the two-component body the equations of balance of linear momentum follow from the relations (12) and (13). Let us use the substitution

$$\begin{aligned}\mathbf{A} &= \rho\mathbf{v} \\ \kappa\hat{\mathbf{j}}_{\mathrm{a}} &= -\mathbf{P} \cdot \mathbf{n} = -\mathbf{t} \\ \Sigma_{\mathrm{a}} &= \rho\mathbf{F}.\end{aligned} \tag{17}$$

According to the formula

$$\mathrm{div}(\mathbf{ab}) = \mathbf{a} \cdot \mathrm{grad}\, \mathbf{b} + \mathbf{b}\, \mathrm{div}\, \mathbf{a} \tag{18}$$

the following relations can be written

$$\frac{\partial}{\partial t}(\rho\mathbf{v}) = \mathrm{div}\, \mathbf{t} - \mathrm{div}(\rho\mathbf{v} \cdot \mathbf{v}) + \rho\mathbf{F}$$

$$\rho\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\left(\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho\mathbf{v})\right) = \mathrm{div}\, \mathbf{t} + \rho\mathbf{F} - \rho\mathbf{v} \cdot \mathrm{grad}\, \mathbf{v}. \tag{19}$$

The relation in brackets on the left-hand side of equation (19) is the law of mass balance for the whole body, which says that the mass of the whole body remains unchanged.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathscr{B}}\rho\,\mathrm{d}V = 0 \quad \int_{\mathscr{B}}\left[\frac{\mathrm{d}}{\mathrm{d}t}(\rho)+\rho\operatorname{div}\mathbf{v}\right]\mathrm{d}V = 0$$

$$\left(\frac{\partial\rho}{\partial t}+\mathbf{v}\cdot\operatorname{grad}\rho\right)+\rho\operatorname{div}\mathbf{v} = 0$$

$$\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho\mathbf{v}) = 0. \tag{20}$$

Hence

$$\rho\frac{\partial\mathbf{v}}{\partial t} = \operatorname{div}\mathbf{t}+\rho\mathbf{F}-\rho\mathbf{v}\cdot\operatorname{grad}\mathbf{v}$$

or

$$\rho\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \operatorname{div}\mathbf{t}+\rho\mathbf{F}. \tag{21}$$

3.3. *Balance of angular momentum*

Substituting the following quantities:

$$\mathbf{A} = \mathbf{x}\times\rho\mathbf{v}$$

$$\kappa\hat{\mathbf{j}}_{\mathrm{a}} = -\mathbf{x}\times\mathbf{P}\cdot\mathbf{n} = -\mathbf{x}\times\mathbf{t}$$

$$\Sigma_{\mathrm{a}} = \mathbf{x}\times\rho\mathbf{F} \tag{22}$$

in equation (12) we find the relations

$$\frac{\partial}{\partial t}(\mathbf{x}\times\rho\mathbf{v}) = \operatorname{div}(\mathbf{x}\times t)-\operatorname{div}\left[(\mathbf{x}\times\rho\mathbf{v})\mathbf{v}\right]+\mathbf{x}\times\rho\mathbf{F}. \tag{23}$$

The relations

$$\frac{\partial}{\partial t}(\mathbf{x}\times\rho\mathbf{v}) = \rho\frac{\partial}{\partial t}(\mathbf{x}\times\mathbf{v})+\mathbf{x}\times\mathbf{v}\frac{\partial\rho}{\partial t}$$

$$= \rho\mathbf{x}\times\frac{\partial\mathbf{v}}{\partial t}+\rho\mathbf{v}\cdot\frac{\partial\mathbf{x}}{\partial t}+\mathbf{x}\times\mathbf{v}\frac{\partial\rho}{\partial t} \tag{24}$$

$$\operatorname{div}(\mathbf{x}\times t) = \mathbf{x}\times\operatorname{div}t+\mathbf{i}_1(t_{32}-t_{23})$$

$$+\mathbf{i}_2(t_{13}-t_{31})+\mathbf{i}_3(t_{21}-t_{12}) \tag{25}$$

lead to

$$\rho\frac{\partial}{\partial t}(\mathbf{x}\times\mathbf{v})+\mathbf{x}\times\mathbf{v}\frac{\partial\rho}{\partial t} = \operatorname{div}(\mathbf{x}\times\mathbf{t})$$

$$+\mathbf{x}\times\rho\mathbf{F}-\left[(\mathbf{x}\times\mathbf{v})\operatorname{div}(\rho\mathbf{v})+\rho\mathbf{v}\cdot\operatorname{grad}(\mathbf{x}\times\mathbf{v})\right] \tag{26}$$

$$(\mathbf{x}\times\mathbf{v})\left[\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho\mathbf{v})\right]+\rho\frac{\partial}{\partial t}(\mathbf{x}\times\mathbf{v})$$

$$= \operatorname{div}(\mathbf{x}\times\mathbf{t})+\mathbf{x}\times\rho\mathbf{F}-\rho\mathbf{v}\cdot\operatorname{grad}(\mathbf{x}\times\mathbf{v}) \tag{27}$$

$$\mathbf{x}\times\left[\rho\frac{\partial\mathbf{v}}{\partial t}+\rho\mathbf{v}\cdot\operatorname{grad}\mathbf{v}-\rho\mathbf{F}-\operatorname{div}\mathbf{t}\right]$$

$$= -\mathbf{v}\times\rho\frac{\partial\mathbf{x}}{\partial t}-\mathbf{v}\times\rho\mathbf{v}\operatorname{div}\mathbf{x}+\mathbf{i}_1(t_{32}-t_{23})$$

$$+\mathbf{i}_2(t_{13}-t_{31})+\mathbf{i}_3(t_{21}-t_{12}) \tag{28}$$

and finally we obtain

$$\mathbf{t} = \mathbf{t}^{\mathrm{T}}. \tag{29}$$

3.4. *Equation of balance of internal energy*

The internal energy is defined as the total energy minus the kinetic energy [7, 27, 28]; its density will be denoted by ρU. We define the quantity in equation (9) as follows:

$$a = \rho(U+\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v})$$

$$\kappa\hat{\mathbf{j}}_{\mathrm{a}} = -\mathbf{P}\cdot\mathbf{n}\cdot\mathbf{v}+\mathbf{q}$$

$$\Sigma_a = \rho\mathbf{F}\cdot\mathbf{v}+\rho r. \tag{30}$$

Hence the balance of energy takes the form

$$\frac{\partial}{\partial t}\left[\rho(U+\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v})\right] = \operatorname{div}\mathbf{t}\cdot\mathbf{v}-\operatorname{div}\mathbf{q}$$

$$-\operatorname{div}\left[\rho(U+\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v})\right]+\rho\mathbf{F}\cdot\mathbf{v}+\rho r. \tag{31}$$

Using the relations

$$\frac{\partial}{\partial t}\left[\rho\left(U+\frac{1}{2}\mathbf{v}\cdot\mathbf{v}\right)\right]=\left(U+\frac{1}{2}\mathbf{v}\cdot\mathbf{v}\right)\frac{\partial\rho}{\partial t}+\rho\frac{\partial U}{\partial t}+\rho\mathbf{v}\cdot\frac{\partial\mathbf{v}}{\partial t}$$

$$\operatorname{div}(\mathbf{t}\cdot\mathbf{v}) = \mathbf{v}\cdot\operatorname{div}\mathbf{t}+\mathbf{t}:\operatorname{grad}\mathbf{v}$$

$$\operatorname{div}\left[\rho(U+\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v})\right] = (U+\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v})\operatorname{div}(\rho\mathbf{v})$$

$$+\rho\mathbf{v}\cdot\operatorname{grad}(U+\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v}) = (U+\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v})\operatorname{div}(\rho\mathbf{v})$$

$$+\rho\mathbf{v}\cdot\operatorname{grad}(U)+\rho\mathbf{v}\cdot\operatorname{grad}\mathbf{v} \tag{32}$$

we easily obtain

$$\rho\frac{\partial U}{\partial t}+\left(U+\frac{1}{2}\mathbf{v}\cdot\mathbf{v}\right)\left[\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho\mathbf{v})\right]$$

$$= \mathbf{v}\cdot\left[\operatorname{div}\mathbf{t}+\rho\mathbf{F}-\rho\mathbf{v}\cdot\operatorname{grad}\mathbf{v}-\rho\frac{\partial\mathbf{v}}{\partial t}\right]$$

$$+\mathbf{t}:\operatorname{grad}\mathbf{v}-\rho\mathbf{v}\cdot\operatorname{grad}(U)-\operatorname{div}\mathbf{q}+\rho r \tag{33}$$

and on using the notation

$$\operatorname{grad}\mathbf{v} = \tfrac{1}{2}\operatorname{grad}\mathbf{v}+\tfrac{1}{2}\operatorname{grad}\mathbf{v}^{\mathrm{T}} = \boldsymbol{\varepsilon} \tag{34}$$

and balances of mass and linear momentum for the whole body we can write equation (33) in the form

$$\rho\frac{\partial U}{\partial t} = \rho r+\mathbf{t}:\boldsymbol{\varepsilon}-\operatorname{div}\mathbf{q}-\rho\mathbf{v}\cdot\operatorname{grad}(U) \tag{35}$$

or

$$\rho\frac{\mathrm{d}U}{\mathrm{d}t} = \rho r+\mathbf{t}:\boldsymbol{\varepsilon}-\operatorname{div}\mathbf{q}. \tag{36}$$

4. THE NEXT THERMODYNAMIC CONSIDERATION

4.1. *Entropy equation*

Let us introduce Gibbs' equation [11, 15, 29, 30, 31]:

$$T\mathrm{d}S = \mathrm{d}U - \mathbf{t} : \mathrm{d}\boldsymbol{\varepsilon} - M\,\mathrm{d}c. \tag{37}$$

In irreversible thermodynamics it is usually assumed that this equation is true for differential operators

$$T\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\mathrm{d}U}{\mathrm{d}t} - \mathbf{t} : \frac{\mathrm{d}\boldsymbol{\varepsilon}}{\mathrm{d}t} - M\frac{\mathrm{d}c}{\mathrm{d}t}. \tag{38}$$

Let us introduce the balance of internal energy (36) and the balance of mass (29) into the equation (38). The result is

$$T\rho\frac{\mathrm{d}S}{\mathrm{d}t} = \rho r - \operatorname{div}\mathbf{q} - M\frac{\mathrm{d}c}{\mathrm{d}t} \tag{39}$$

$$\rho\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\rho r}{T} - \frac{\operatorname{div}\mathbf{q}}{T} + \frac{M}{T}\operatorname{div}(\kappa\mathbf{j}_{\mathrm{a}}) + \frac{\rho c M}{T}\operatorname{div}\mathbf{u} - \frac{RM}{T} \tag{40}$$

but

$$\frac{M}{T}\operatorname{div}(\kappa\mathbf{j}_{\mathrm{a}}) = \operatorname{div}\left(\frac{\kappa M\mathbf{j}_{\mathrm{a}}}{T}\right) - \kappa\mathbf{j}_{\mathrm{a}}\operatorname{grad}\left(\frac{M}{T}\right) \tag{41}$$

$$\frac{\operatorname{div}\mathbf{q}}{T} = \operatorname{div}\left(\frac{\mathbf{q}}{T}\right) + \frac{1}{T^2}\mathbf{q}\cdot\operatorname{grad}T \tag{42}$$

$$\frac{\rho c M}{T}\operatorname{div}\mathbf{u} = \operatorname{div}\left(\frac{\rho M c\mathbf{u}}{T}\right) - \mathbf{u}\cdot\operatorname{grad}\left(\frac{\rho M c}{T}\right) \tag{43}$$

$$\mathbf{u}\cdot\operatorname{grad}\left(\frac{\rho M c}{T}\right) = \mathbf{u}c\cdot\operatorname{grad}\left(\frac{\rho M}{T}\right) + \frac{M}{T}\rho\mathbf{u}\cdot\operatorname{grad}(c). \tag{44}$$

Thus

$$\begin{aligned}\rho\frac{\mathrm{d}S}{\mathrm{d}t} = {} & -\operatorname{div}\left(\frac{\mathbf{q}}{T}\right) - \frac{1}{T^2}\mathbf{q}\cdot\operatorname{grad}(T) \\ & + \operatorname{div}\left(\frac{\kappa M\mathbf{j}_{\mathrm{a}}}{T}\right) - \kappa\mathbf{j}_{\mathrm{a}}\cdot\operatorname{grad}\left(\frac{M}{T}\right) \\ & + \operatorname{div}\left(\frac{\rho M c\mathbf{u}}{T}\right) - \mathbf{u}c\cdot\operatorname{grad}\left(\frac{\rho M}{T}\right) \\ & + \frac{M}{T}\rho\mathbf{u}\cdot\operatorname{grad}(c) + \frac{\rho r - RM}{T}.\end{aligned} \tag{45}$$

At each step we are going to obtain an equation of entropy balance in a form similar to the general equation (5) namely

$$\frac{\partial(\rho S)}{\partial t} = -\operatorname{div}\underset{\wedge}{\mathbf{j}}_{\mathrm{s}} + \Sigma_{\mathrm{s}} \tag{46}$$

where $\underset{\wedge}{\mathbf{j}}_{\mathrm{s}}$ denotes the global flow of the entropy, and Σ_{s} represents the global source of this quantity (the rate of generation of entropy per unit volume and per unit time due to irreversible processes).

If we introduce

$$\rho\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\mathrm{d}(\rho S)}{\mathrm{d}t} - S\frac{\mathrm{d}\rho}{\mathrm{d}t} \tag{47}$$

and use the equation of continuity ($\mathbf{u}^{\alpha} = \mathbf{v}$, or $\mathbf{u}^{\alpha} = \mathbf{v}^{\alpha}$)

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} - \rho\operatorname{div}\mathbf{v} = -\rho\operatorname{div}\mathbf{u} \tag{48}$$

then, in view of relation

$$\operatorname{div}(\rho S\mathbf{u}) = \rho S\operatorname{div}\mathbf{u} + \mathbf{u}\cdot\operatorname{grad}(\rho S),$$

we get

$$\begin{aligned}\rho\frac{\mathrm{d}S}{\mathrm{d}t} &= \frac{\mathrm{d}(\rho S)}{\mathrm{d}t} + \operatorname{div}(\rho S\mathbf{u}) - \mathbf{u}\cdot\operatorname{grad}(\rho S) \\ &= \frac{\partial(\rho S)}{\partial t} + \operatorname{div}(\rho S\mathbf{u}).\end{aligned} \tag{49}$$

With equation (49) we write equation (45) in the form appropriate to equation (46)

$$\begin{aligned}\frac{\partial(\rho S)}{\partial t} = {} & -\operatorname{div}\left(\rho S\mathbf{u} + \frac{\mathbf{q}}{T} - \frac{\kappa M\mathbf{j}_{\mathrm{a}}}{T} - \frac{\rho M(c\mathbf{u})}{T}\right) \\ & - \frac{\mathbf{q}}{T^2}\cdot\operatorname{grad}(T) - \kappa\mathbf{j}_{\mathrm{a}}\cdot\operatorname{grad}\left(\frac{M}{T}\right) \\ & - (c\mathbf{u})\cdot\operatorname{grad}\left(\frac{\rho M}{T}\right) + \frac{M}{T}\rho\mathbf{u}\cdot\operatorname{grad}(c) + \frac{\rho r - RM}{T}.\end{aligned} \tag{50}$$

The divergence operator acting on the global entropy flow in (50) as follows

$$\underset{\wedge}{\mathbf{j}}_{\mathrm{s}} = \rho S\mathbf{u} + \frac{\mathbf{q}}{T} - \frac{\kappa M\mathbf{j}_{\mathrm{a}}}{T} - \frac{\rho M(c\mathbf{u})}{T}. \tag{51}$$

We can distinguish here four contributions:

(1) the convective component of the entropy flow $\rho S\mathbf{u}$;

(2) the component $\mathbf{q}/T$ as a result of heat flow. This component describes entropy flow connected with heat flow in the closed (isolated) system, i.e. apart from the flow of components;

(3) the component due to the convection flow $\rho M(c\mathbf{u})/T$ and

(4) the part caused by the conduction (diffusion) flow of components $\kappa M\mathbf{j}_{\mathrm{a}}/T$.

Let us according to (46) introduce the rate of entropy production

$$\begin{aligned}\Sigma_{\mathrm{s}} = {} & -\frac{\mathbf{q}}{T^2}\cdot\operatorname{grad}(T) - \kappa\mathbf{j}_{\mathrm{a}}\cdot\operatorname{grad}\left(\frac{M}{T}\right) \\ & - (c\mathbf{u})\cdot\operatorname{grad}\left(\frac{\rho M}{T}\right) + \frac{M}{T}\rho\mathbf{u}\cdot\operatorname{grad}(c) \\ & + \frac{\rho r - RM}{T}.\end{aligned} \tag{52}$$

4.2. *Thermodynamical forces and fluxes*

The entropy source is connected with the causes of irreversible processes, i.e., with the intensive quantities called the thermodynamic force $\mathbf{X}^{(\gamma)}$. The entropy source is equal to the scalar product of the thermodynamic forces and the appropriate fluxes $\mathbf{j}^{(\gamma)}$ [32].

$$\Sigma_s = \frac{1}{T}\sum_\gamma \mathbf{j}^{(\gamma)}\cdot\mathbf{X}^{(\gamma)}. \tag{53}$$

We can rewrite equation (52) in the form

$$\Sigma_s = \frac{1}{T}\left\{\frac{-\mathbf{q}}{T}\cdot\operatorname{grad}(T) - \kappa\mathbf{j}_a T\cdot\operatorname{grad}\left(\frac{M}{T}\right)\right.$$
$$\left. - (c\mathbf{u})\cdot\left[T\operatorname{grad}\left(\frac{\rho M}{T}\right) + \frac{\rho M}{c}\operatorname{grad}(c)\right]\right\}$$
$$+\frac{\rho r - RM}{T} \geqslant 0. \tag{54}$$

Thus in view of (53) one can write

$$\Sigma_s = \frac{1}{T}\{\mathbf{q}\cdot\mathbf{X}^q + \kappa\mathbf{j}_a\cdot\mathbf{X}^a + \mathbf{j}_c\cdot\mathbf{X}^c\}. \tag{55}$$

The comparison between (54) and (55) yields

$$\mathbf{X}^q = -\frac{1}{T}\operatorname{grad}(T) \quad \mathbf{X}^a = -T\operatorname{grad}\left(\frac{M}{T}\right)$$
$$\mathbf{X}^c = -\left[T\operatorname{grad}\left(\frac{\rho M}{T}\right) + \frac{\rho M}{c}\operatorname{grad}(c)\right]. \tag{56}$$

On the other hand there are in general nonlinear relations between the vectors of fluxes and the thermodynamic forces

$$\mathbf{j}^{(\gamma)} = \mathbf{j}^{(\gamma)}(\mathbf{X}^{(\gamma)}) \quad \Rightarrow$$
$$\mathbf{q} = \mathbf{q}(\mathbf{X}^q, \mathbf{X}^a, \mathbf{X}^c) \quad \kappa\mathbf{j}_a = \kappa\mathbf{j}_a(\mathbf{X}^q, \mathbf{X}^a, \mathbf{X}^c)$$
$$\mathbf{j}_c = \mathbf{j}_c(\mathbf{X}^q, \mathbf{X}^a, \mathbf{X}^c). \tag{57}$$

For laminar flows we assume that the above relations are linear

$$\begin{cases} \mathbf{q} = L_{qq}\mathbf{X}^q + L_{qa}\mathbf{X}^a + L_{qc}\mathbf{X}^c \\ \kappa\mathbf{j}_a = L_{aq}\mathbf{X}^q + L_{aa}\mathbf{X}^a + L_{ac}\mathbf{X}^c. \\ \rho\mathbf{u} = L_{cq}\mathbf{X}^q + L_{ca}\mathbf{X}^a + L_{cc}\mathbf{X}^c \end{cases} \tag{58}$$

The relations (58) are phenomenological. The quantities L_{ij} here are constant and satisfy the reciprocity (Onsager's) conditions $L_{qa} = L_{aq}$, $L_{qc} = L_{cq}$ and $L_{ac} = L_{ca}$. Moreover, the conditions (54) imply that

$$L_{cc} > 0 \quad L_{aa}L_{cc} - L_{cc}^2 > 0$$
$$L_{qq}L_{aa}L_{cc} + 2L_{qa}L_{ac}L_{qc}$$
$$- L_{qc}^2L_{aa} - L_{ac}^2L_{qq} - L_{qa}^2L_{cc} > 0. \tag{59}$$

Using the relation

$$\operatorname{grad}\left(\frac{\rho M}{T}\right) = \rho\operatorname{grad}\left(\frac{M}{T}\right) + \frac{M}{T}\operatorname{grad}(\rho) = \rho\operatorname{grad}\left(\frac{M}{T}\right) \tag{60}$$

one can rewrite the equations (58) in the form

$$\begin{cases} \mathbf{q} = -\dfrac{L_{qq}}{T}\operatorname{grad}(T) - (L_{qa} + \rho L_{qc})T\operatorname{grad}\left(\dfrac{M}{t}\right) \\ \qquad -\dfrac{\rho M}{c}L_{qc}\operatorname{grad}(c) \\ \kappa\mathbf{j}_a = -\dfrac{L_{qa}}{T}\operatorname{grad}(T) - (L_{aa} + \rho L_{ac})T\operatorname{grad}\left(\dfrac{M}{T}\right) \\ \qquad -\dfrac{\rho M}{c}L_{ac}\operatorname{grad}(c) \\ c\mathbf{u} = -\dfrac{L_{qc}}{T}\operatorname{grad}(T) - (L_{ac} + \rho L_{cc})T\operatorname{grad}\left(\dfrac{M}{T}\right) \\ \qquad -\dfrac{\rho M}{c}L_{cc}\operatorname{grad}(c). \end{cases} \tag{61}$$

With relation

$$T\operatorname{grad}\left(\frac{M}{T}\right) = \operatorname{grad}(M) - \frac{M}{T}\operatorname{grad}(T) \tag{62}$$

we can find from the set of equations in (61), the following equations

$$c\mathbf{u} + \kappa\mathbf{j}_a = \mathbf{j} = -\frac{1}{T}\{L_{qa} + L_{qc} - L_{aa}$$
$$+ L_{ac} + \rho(L_{cc} + L_{ac})M\}\operatorname{grad}(T)$$
$$- L_{aa} + L_{ac} + \rho(L_{cc} + L_{ac})\operatorname{grad}(M)$$
$$-\frac{\rho M}{c}(L_{cc} + L_{ac})\operatorname{grad}(c) \tag{63}$$

$$\mathbf{q} = -\frac{1}{T}\left\{L_{qq} - L_{qa}\frac{L_{qc}}{L_{ac}} + \left(L_{qa} - L_{aa}\frac{L_{qc}}{L_{ac}}\right)M\right\}\operatorname{grad}(T)$$
$$-\left(L_{qa} - L_{aa}\frac{L_{qc}}{L_{ac}}\right)\operatorname{grad}(M) + \frac{L_{qc}}{L_{ac}}\kappa\mathbf{j}_a \tag{64}$$

$$c\mathbf{u} = -\frac{1}{T}\left\{L_{qc} - L_{qq}\frac{L_{cc}}{L_{qc}} + \left(L_{ac} - L_{qa}\frac{L_{cc}}{L_{qc}}\right)M\right\}\operatorname{grad}(T)$$
$$-\left(L_{ac} - L_{qa}\frac{L_{cc}}{L_{qc}}\right)\operatorname{grad}(M) + \frac{L_{cc}}{L_{qc}}\mathbf{q} \tag{65}$$

$$\mathbf{q} = -\frac{1}{T}\left\{L_{qq} - L_{qc}\frac{L_{qc}}{L_{cc}} + \left(L_{qa} - L_{ac}\frac{L_{qc}}{L_{cc}}\right)M\right\}\operatorname{grad}(T)$$
$$-\left(L_{qa} - L_{ac}\frac{L_{qc}}{L_{cc}}\right)\operatorname{grad}(M) + \frac{L_{qc}}{L_{cc}}c\mathbf{u} \tag{66}$$

$$\kappa\mathbf{j}_{\mathrm{a}} = -\frac{1}{T}\left\{L_{\mathrm{qa}} - L_{\mathrm{qc}}\frac{L_{\mathrm{ac}}}{L_{\mathrm{cc}}} + \left(L_{\mathrm{aa}} - L_{\mathrm{ac}}\frac{L_{\mathrm{ac}}}{L_{\mathrm{cc}}}\right)M\right\}\mathrm{grad}(T)$$
$$-\left(L_{\mathrm{aa}} - L_{\mathrm{ac}}\frac{L_{\mathrm{ac}}}{L_{\mathrm{cc}}}\right)\mathrm{grad}(M) + \frac{L_{\mathrm{qc}}}{L_{\mathrm{cc}}}c\mathbf{u} \tag{67}$$

$$c\mathbf{u} = -\frac{1}{T}\left\{L_{\mathrm{ac}} - L_{\mathrm{qa}}\frac{L_{\mathrm{cc}}}{L_{\mathrm{qc}}} + (L_{\mathrm{ac}}^2 - L_{\mathrm{cc}}L_{\mathrm{aa}})\frac{M}{L_{\mathrm{qc}}}\right\}\mathrm{grad}(T)$$
$$-\frac{1}{L_{\mathrm{qc}}}(L_{\mathrm{ac}}^2 - L_{\mathrm{cc}}L_{\mathrm{aa}})\,\mathrm{grad}(M) + \frac{L_{\mathrm{cc}}}{L_{\mathrm{qc}}}\kappa\mathbf{j}_{\mathrm{a}} \tag{68}$$

$$\kappa\mathbf{j}_{\mathrm{a}} = -\frac{1}{T}\{L_{\mathrm{qa}} - (L_{\mathrm{aa}} + \rho L_{\mathrm{ac}})M\}\,\mathrm{grad}(T)$$
$$-(L_{\mathrm{aa}} + \rho L_{\mathrm{ac}})\,\mathrm{grad}(M) - \frac{\rho M}{c}L_{\mathrm{ac}}\,\mathrm{grad}(c). \tag{69}$$

Let us now return to Gibbs' equation (38)

$$\dot{U} = \mathbf{t}:\dot{\boldsymbol{\varepsilon}} + T\dot{S} + M\dot{c}. \tag{70}$$

But on the other hand dU is a total differential so we have

$$\dot{U} = \frac{\partial U}{\partial \varepsilon}\dot{\boldsymbol{\varepsilon}} + \frac{\partial U}{\partial S}\dot{S} + \frac{\partial U}{\partial c}\dot{c}. \tag{71}$$

Hence after simple comparison we have

$$\mathbf{t} = \frac{\partial U}{\partial \boldsymbol{\varepsilon}} \quad T = \frac{\partial U}{\partial S} \quad M = \frac{\partial U}{\partial c}. \tag{72}$$

The Taylor series of the function $U(\varepsilon_{ij}, S, c)$ in the vicinity of the natural state ($\varepsilon_{ij} = 0, S = 0, c = c_0$) for the isotropic and homogenious medium has the form

$$U(\varepsilon_{ij}, S, c) = U_0(0, 0, c_0) + \frac{\partial U_0}{\partial \varepsilon_{ij}}\varepsilon_{ij} + \frac{\partial U_0}{\partial S}S$$
$$+\frac{\partial U_0}{\partial c}(c - c_0) + \frac{1}{2}\frac{\partial^2 U_0}{\partial \varepsilon_{kl}\,\partial \varepsilon_{kl}}\varepsilon_{ij}\varepsilon_{ij}$$
$$+\frac{1}{2}\frac{\partial^2 U_0}{\partial \varepsilon_{\mathrm{pp}}\,\partial \varepsilon_{\mathrm{qq}}}\varepsilon_{kk}\varepsilon_{ll} + \frac{1}{2}\frac{\partial^2 U_0}{\partial S^2}S^2$$
$$+\frac{1}{2}\frac{\partial^2 U_0}{\partial c^2}(c - c_0)^2 + \frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial S}\varepsilon_{ij}S$$
$$+\frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial c}\varepsilon_{ij}(c - c_0) + \frac{\partial^2 U_0}{\partial S\,\partial c}S(c - c_0) + \cdots. \tag{73}$$

Let us assume as in [15] that $U(0, 0, c_0) = 0$ and let us neglect the first three parts in the series (73) because for $\varepsilon_{ij} = 0$, $S = 0$, $c = 0$ it should be that $t_{ij} = 0$, $T = T_0$ and $M = 0$. Using the notation

$$c = c - c_0 \quad \Theta = T - T_0$$

in view of relations (71) we get

$$t_{ij} = \frac{\partial U}{\partial \varepsilon_{ij}} = \frac{\partial^2 U_0}{\partial \varepsilon_{kl}\,\partial \varepsilon_{kl}}\varepsilon_{ij}$$
$$+\frac{\partial^2 U_0}{\partial \varepsilon_{\mathrm{pp}}\,\partial \varepsilon_{\mathrm{qq}}}\varepsilon_{kk}\,\delta_{ij} + \frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial S}S + \frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial c}c$$

$$\Theta = \frac{\partial U}{\partial S} = \frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial S}\varepsilon_{ij} + \frac{\partial^2 U_0}{\partial S^2}S + \frac{\partial^2 U_0}{\partial S\,\partial c}c$$
$$M = \frac{\partial U}{\partial c} = \frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial c}\varepsilon_{ij} + \frac{\partial^2 U_0}{\partial S\,\partial c}S + \frac{\partial^2 U_0}{\partial c^2}c. \tag{74}$$

Let us now introduce the notation

$$\frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial \varepsilon_{ij}} = 2\mu' \quad \frac{\partial^2 U_0}{\partial \varepsilon_{kk}\,\partial \varepsilon_{ll}} = \lambda'$$
$$\frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial S} = -\gamma_{\mathrm{s}}'\,\delta_{ij} \quad \frac{\partial^2 U_0}{\partial \varepsilon_{ij}\,\partial c} = -\gamma_{\mathrm{c}}'\,\delta_{ij}$$
$$\frac{\partial^2 U_0}{\partial S^2} = m' \quad \frac{\partial U_0}{\partial c^2} = n' \quad \frac{\partial^2 U_0}{\partial S\,\partial c} = -l' \tag{75}$$

and now we can write the set of constitutive relations as

$$t_{ij} = \frac{\partial U}{\partial \varepsilon_{ij}} = 2\mu'\varepsilon_{ij} + (\lambda'\varepsilon_{kk} - \gamma_{\mathrm{s}}'S - \gamma_{\mathrm{c}}')\,\delta_{ij}$$
$$\Theta = \frac{\partial U}{\partial S} = -\gamma_{\mathrm{s}}'\varepsilon_{kk} + m'S + l'c$$
$$M = \frac{\partial U}{\partial c} = -\gamma_{\mathrm{c}}'\varepsilon_{kk} - l'S + n'c. \tag{76}$$

Let us introduce the free energy $F = U - ST$ [31, 32]. Taking into account the relation (70) we have for its derivative

$$\dot{F} = \mathbf{t}:\dot{\boldsymbol{\varepsilon}} - S\dot{T} + M\dot{c}. \tag{77}$$

Using similar notations to these in relation (75)

$$\frac{\partial^2 F_0}{\partial \varepsilon_{ij}\,\partial \varepsilon_{ij}} = 2\mu \quad \frac{\partial^2 F_0}{\partial \varepsilon_{kk}\,\partial \varepsilon_{ll}} = \lambda$$
$$\frac{\partial^2 F_0}{\partial \varepsilon_{ij}\,\partial \Theta} = -\gamma_{\mathrm{T}}\,\delta_{ij} \quad \frac{\partial^2 F_0}{\partial \varepsilon_{ij}\,\partial c} = -\gamma_{\mathrm{c}}\,\delta_{ij}$$
$$\frac{\partial^2 F_0}{\partial \Theta^2} = -m \quad \frac{\partial F_0}{\partial c^2} = n \quad \frac{\partial^2 F_0}{\partial \Theta\,\partial c} = -l. \tag{78}$$

In a similar way to that shown above we get the following form of the Taylor series of the function $F(\varepsilon_{ij}, \Theta, c)$ in the vicinity of the natural state ($\varepsilon_{ij} = 0, T = T_0, c = 0$) which for the isotropic and homogeneous medium has the form

$$F(\varepsilon_{ij}, \Theta, c) = F_0(0, \Theta_0, 0) + \frac{\partial F_0}{\partial \varepsilon_{ij}}\varepsilon_{ij} + \frac{\partial F_0}{\partial \Theta}\Theta$$
$$+\frac{\partial F_0}{\partial c}c + \mu\varepsilon_{ij}\varepsilon_{ij} + \frac{\lambda}{2}\varepsilon_{kk}\varepsilon_{ll} + \frac{m}{2}\Theta^2 + \frac{n}{2}c^2$$
$$-\gamma_{\mathrm{T}}\varepsilon_{kk}\Theta - \gamma_{\mathrm{c}}\varepsilon_{kk}c - l\Theta c. \tag{79}$$

In view of (76) we have the second set of constitutive relations

$$\mathbf{t}_{ij} = \frac{\partial F}{\partial \varepsilon_{ij}} = 2\mu\varepsilon_{ij} + (\lambda\varepsilon_{kk} - \gamma_{\mathrm{T}}\Theta - \gamma_{\mathrm{c}}c)\,\delta_{ij}$$

$$S = \frac{\partial F}{\partial T} = \gamma_{\mathrm{T}}\varepsilon_{kk} + m\Theta + lc \quad \gamma_{\mathrm{T}} = (2\mu + 3\lambda)\alpha_{\mathrm{T}}$$

$$m = c_{\mathrm{s}}/T_0 \quad M = \frac{\partial F}{\partial c} = -\gamma_{\mathrm{c}}\varepsilon_{kk} - l\Theta + nc \quad T = \Theta. \tag{80}$$

Let us now return to the equations (64)–(69). Substituting into these equations the quantity M from equation (80) we find

$$\kappa\mathbf{j}_{\mathrm{a}} = -D\,\mathrm{grad}(c) - D_\varepsilon\,\mathrm{grad}(\varepsilon_{kk}) - D_{\mathrm{T}}\,\mathrm{grad}(\Theta) \tag{81}$$

where

$$D = \underline{n(L_{\mathrm{aa}}} + \rho L_{\mathrm{ac}}) + \frac{\rho}{c} L_{\mathrm{ac}}(\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc)$$

$$D_\varepsilon = \underline{-\gamma_{\mathrm{c}}(L_{\mathrm{aa}}} + \rho L_{\mathrm{ac}})$$

$$D_{\mathrm{T}} = \underline{\frac{1}{T_0}[L_{\mathrm{qa}}} - \underline{lT_0(L_{\mathrm{aa}}} + \rho L_{\mathrm{ac}})$$

$$- (\underline{L_{\mathrm{aa}}} + \rho L_{\mathrm{ac}})(\underline{\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc})] \tag{82}$$

where the underlined parts appear in the classical thermodiffusion theory [11, 12, 15]. After linearization of equation $(82)_1$ and $(82)_3$ we get

$$D = \underline{n(L_{\mathrm{aa}}} + \rho L_{\mathrm{ac}})$$

$$D_\varepsilon = \underline{-\gamma_{\mathrm{c}}(L_{\mathrm{aa}}} + \rho L_{\mathrm{ac}})$$

$$D_{\mathrm{T}} = \left[\underline{\frac{1}{T_0}L_{\mathrm{qa}}} - \underline{lT_0(L_{\mathrm{aa}}} + \rho L_{\mathrm{ac}})\right]. \tag{83}$$

In the same way we get

$$\mathbf{q} = -k\,\mathrm{grad}(\Theta) - k_\varepsilon\,\mathrm{grad}(\varepsilon_{kk}) - k_{\mathrm{c}}\,\mathrm{grad}(c) \tag{84}$$

where

$$k = \frac{1}{T_0}\left[L_{\mathrm{qq}} - lT_0\left(L_{\mathrm{qa}} + \rho L_{\mathrm{qc}} - 2L_{\mathrm{aa}}\frac{L_{\mathrm{qc}}}{L_{\mathrm{ac}}}\right)\right]$$

$$- (L_{\mathrm{qa}} + \rho L_{\mathrm{qc}})(\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc)$$

$$k_\varepsilon = -\gamma_{\mathrm{c}}(L_{\mathrm{qa}} + \rho L_{\mathrm{qc}})$$

$$k_{\mathrm{c}} = n(L_{\mathrm{qa}} + \rho L_{\mathrm{qc}}) + \frac{\rho}{c} L_{\mathrm{qc}}(\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc). \tag{85}$$

After linearization of equation $(85)_1$ and $(85)_3$ we have

$$k = \frac{1}{T_0}\left[L_{\mathrm{qq}} - lT_0\left(L_{\mathrm{qa}} + \rho L_{\mathrm{qc}} - 2L_{\mathrm{aa}}\frac{L_{\mathrm{qc}}}{L_{\mathrm{ac}}}\right)\right]$$

$$k_\varepsilon = -\gamma_{\mathrm{c}}(L_{\mathrm{qa}} + \rho L_{\mathrm{qc}})$$

$$k_{\mathrm{c}} = n(L_{\mathrm{qa}} + \rho L_{qc}) \tag{86}$$

and the next quantity

$$c\mathbf{u} = -\underset{\sim}{D}\,\mathrm{grad}(c) - \underset{\sim}{D}_\varepsilon\,\mathrm{grad}(\varepsilon_{kk}) - \underset{\sim}{D}_{\mathrm{T}}\,\mathrm{grad}(\Theta) \tag{87}$$

where

$$\underset{\sim}{D} = n(L_{\mathrm{ac}} + \rho L_{\mathrm{cc}}) + \frac{\rho}{c} L_{\mathrm{cc}}(\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc)$$

$$\underset{\sim}{D}_\varepsilon = -\gamma_{\mathrm{c}}(L_{\mathrm{ac}} + \rho L_{\mathrm{cc}})$$

$$\underset{\sim}{D}_{\mathrm{T}} = \frac{1}{T_0}\left[L_{\mathrm{qc}} - lT_0\left(L_{\mathrm{ac}} + \rho L_{\mathrm{cc}} - 2L_{\mathrm{qa}}\frac{L_{\mathrm{cc}}}{L_{\mathrm{qc}}} + 2L_{\mathrm{aa}}\frac{L_{\mathrm{cc}}}{L_{\mathrm{ac}}}\right)\right.$$

$$\left. - (L_{\mathrm{ac}} + \rho L_{\mathrm{cc}})(\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc)\right]. \tag{88}$$

After linearization of equation $(88)_1$ and $(88)_3$ we get

$$\underset{\sim}{D} = n(L_{\mathrm{ac}} + \rho L_{\mathrm{cc}})$$

$$D_\varepsilon = -\gamma_{\mathrm{c}}(L_{\mathrm{ac}} + \rho L_{\mathrm{cc}})$$

$$\underset{\sim}{D}_{\mathrm{T}} = \frac{1}{T_0}\left[L_{\mathrm{qc}} - lT_0\left(L_{\mathrm{ac}} + \rho L_{\mathrm{cc}}\right.\right.$$

$$\left.\left. - 2L_{\mathrm{qa}}\frac{L_{\mathrm{cc}}}{L_{\mathrm{qc}}} + 2L_{\mathrm{aa}}\frac{L_{\mathrm{cc}}}{L_{\mathrm{ac}}}\right)\right] \tag{89}$$

and finally we get

$$\kappa\mathbf{j}_{\mathrm{a}} + c\mathbf{u} = \mathbf{j} = -\hat{D}\,\mathrm{grad}(c) - \hat{D}_\varepsilon\,\mathrm{grad}(\varepsilon_{kk})$$

$$-\hat{D}_{\mathrm{T}}\,\mathrm{grad}(\Theta) \tag{90}$$

where

$$\hat{D} = \underline{n[L_{\mathrm{aa}}} + L_{\mathrm{ac}} + \rho(L_{\mathrm{ac}} + L_{\mathrm{cc}})]$$

$$- \frac{\rho}{c}(L_{\mathrm{ac}} + L_{\mathrm{cc}})(\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc)$$

$$\hat{D}_\varepsilon = \underline{-\gamma_{\mathrm{c}}[L_{\mathrm{aa}}} + L_{\mathrm{ac}} + \rho(L_{\mathrm{ac}} + L_{\mathrm{cc}})]$$

$$\hat{D}_{\mathrm{T}} = \underline{\frac{1}{T_0}\Big\{L_{\mathrm{qa}}} + L_{\mathrm{qc}} - \underline{lT_0\Big[(L_{\mathrm{aa}}} + L_{\mathrm{ac}})$$

$$- \rho(L_{\mathrm{ac}} + L_{\mathrm{cc}}) + 2L_{\mathrm{cc}}\left(\frac{L_{\mathrm{aa}}}{L_{\mathrm{cc}}} - \frac{L_{\mathrm{qa}}}{L_{\mathrm{qc}}}\right)\Big]$$

$$- [\underline{L_{\mathrm{aa}}} + L_{\mathrm{ac}} + \rho(L_{\mathrm{ac}} + L_{\mathrm{cc}})](\underline{\gamma_{\mathrm{c}}\varepsilon_{kk} + l\Theta - nc})\Big\} \tag{91}$$

where as before the underlined parts appear in the classical thermodiffusion theory [11, 12, 15]. After linearization of equation $(91)_1$ and $(91)_3$ we have

$$\hat{D} = \underline{n[L_{\mathrm{aa}}} + L_{\mathrm{ac}} + \rho(L_{\mathrm{ac}} + L_{\mathrm{cc}})]$$

$$\hat{D}_\varepsilon = \underline{-\gamma_{\mathrm{c}}[L_{\mathrm{aa}}} + L_{\mathrm{ac}} + \rho(L_{\mathrm{ac}} + L_{\mathrm{cc}})]$$

$$\hat{D}_{\mathrm{T}} = \underline{\frac{1}{T_0}\Big\{L_{\mathrm{qa}}} + L_{\mathrm{qc}} - \underline{lT_0\Big[(L_{\mathrm{aa}}} + L_{\mathrm{ac}}) - \rho(L_{\mathrm{ac}} + L_{\mathrm{cc}})$$

$$+ 2L_{\mathrm{cc}}\left(\frac{L_{\mathrm{aa}}}{L_{\mathrm{cc}}} - \frac{L_{\mathrm{qa}}}{L_{\mathrm{qc}}}\right)\Big]\Big\}. \tag{92}$$

5. THE SET OF EQUATIONS AND SIMPLIFICATIONS

5.1. *The complete set of the differential equations*

Let us return to the balance of entropy (39)

$$\rho T\dot{S} = \rho r - \operatorname{div}\mathbf{q} - M(-\operatorname{div}(\kappa\mathbf{j}_a) - \rho c \operatorname{div}\mathbf{u} + R) \tag{93}$$

where the balance of mass (29) has been used. Substituting into this equation for the quantity $\mathbf{q}$ from equation (83) we have

$$\begin{aligned}\rho T\dot{S} = {} & k \operatorname{div}\operatorname{grad}(\Theta) + k_\varepsilon \operatorname{div}\operatorname{grad}(\varepsilon_{kk}) \\ & + k_c \operatorname{div}\operatorname{grad}(c) - M(-\operatorname{div}(\kappa\mathbf{j}_a) \\ & - \rho c \operatorname{div}\mathbf{u} + R) + \rho r.\end{aligned} \tag{94}$$

There are nonlinear terms in the part $M(-\operatorname{div}(\kappa\mathbf{j}_a) - \rho c \operatorname{div}\mathbf{u} + R)$. These parts may be neglected by comparison with the first three parts on the left-hand side of equation (94). Thus

$$\rho T\dot{S} \simeq k\nabla^2\Theta + k_\varepsilon\nabla^2\varepsilon_{kk} + k_c\nabla^2 c + \rho r. \tag{95}$$

Introducing into the left-hand side of this equation the quantity S from the constitutive relation (79) we obtain after linearization (we assume that $\Theta/T_0 \ll 0$)

$$\begin{aligned}& k\nabla^2\Theta + k_\varepsilon\nabla^2\varepsilon_{kk} + k_c\nabla^2 c \\ & - \rho T_0(\gamma_T\dot{\varepsilon}_{kk} + m\dot{\Theta} + l\dot{c}) = -\rho r\end{aligned} \tag{96}$$

$$\begin{aligned}& (k\nabla^2 - m\underset{\sim}{\partial}_t)\Theta + (k_\varepsilon\nabla^2 - \rho T_0\gamma_T\underset{\sim}{\partial}_t)\operatorname{div}(\mathbf{u}) \\ & + (k_c\nabla^2 - \rho T_0 l\underset{\sim}{\partial}_t)c = -\rho r.\end{aligned} \tag{97}$$

Let us now substitute equation (89) into the principle of mass conservation (16)

$$\begin{aligned}\rho\dot{c} = {} & -\operatorname{div}(-\hat{D}\operatorname{grad}(c) - \hat{D}_\varepsilon\operatorname{grad}(\varepsilon_{kk}) \\ & - \hat{D}_T\operatorname{grad}(\Theta) - c\mathbf{u}) - \rho c \operatorname{div}\mathbf{u} + R.\end{aligned} \tag{98}$$

Because $\operatorname{div}(c\mathbf{u}) - \rho c \operatorname{div}\mathbf{u} = c(1-\rho)\operatorname{div}\mathbf{u} + \mathbf{u}\cdot\operatorname{grad}(c)$ we easily obtain

$$\begin{aligned}\rho\dot{c} = {} & (\hat{D}\nabla^2 + \mathbf{u}\nabla)c + (\hat{D}_\varepsilon\nabla^2 \\ & + c(1-\rho))\operatorname{div}\mathbf{u} + \hat{D}_T\nabla^2\Theta + R\end{aligned} \tag{99}$$

$$\begin{aligned}& (\hat{D}\nabla^2 + \mathbf{u}\nabla - \rho\underset{\sim}{\partial}_t)c + (\hat{D}_\varepsilon\nabla^2 \\ & + c(1-\rho))\operatorname{div}\mathbf{u} + \hat{D}_T\nabla^2\Theta = -R.\end{aligned} \tag{100}$$

Let us rewrite equations (97) and (100) according to the notation

$$\underset{\sim}{\partial}_t(\cdot) = \frac{\mathrm{d}(\cdot)}{\mathrm{d}t} = \partial_t(\cdot) + \mathbf{u}\cdot\nabla(\cdot). \tag{101}$$

The result is

$$\begin{aligned}& (k\nabla^2 - \mathbf{u}m\nabla - m\underset{\sim}{\partial}_t)\Theta + (k_\varepsilon\nabla^2 - \mathbf{u}\rho T_0\gamma_T\nabla \\ & - \rho T_0\gamma_T\partial_t)\operatorname{div}(\mathbf{u}) + (k_c\nabla^2 - \mathbf{u}\cdot\rho T_0 l\nabla \\ & - \rho T_0 l\partial_t)c = -\rho r\end{aligned} \tag{102}$$

$$\begin{aligned}& \hat{D}\nabla^2 + \mathbf{u}(1-\rho)\cdot\nabla - \rho\underset{\sim}{\partial}_t)c + (\hat{D}_\varepsilon\nabla^2 \\ & + c(1-\rho))\operatorname{div}(\mathbf{u}) + \hat{D}_T\nabla^2\Theta = -R.\end{aligned} \tag{103}$$

Equation (103) is the diffusion equation. It can take two forms. The first possibility is that we express the mass flux using equation (90). Then we obtain equation (99).

However, we can proceed in a different manner. Let us determine c from the third relation of (80) and substitute the result into the left-hand side of equation (99) and into equation (102). Hence (102) and (103) take the form

$$\begin{aligned}& [(k + \underline{l}k_c)\nabla^2 - \mathbf{u}(m + \underline{l}l)\rho T_0\cdot\nabla \\ & - \rho T_0(m + \underline{l}l)\underset{\sim}{\partial}_t]\Theta + [(k_\varepsilon + k_c\underline{\gamma_c})\nabla^2 \\ & - \mathbf{u}(\gamma_T + \underline{\gamma_c}l)\rho T_0\cdot\nabla - \rho T_0(\gamma_T + \underline{\gamma_c}l)\underset{\sim}{\partial}_t]\operatorname{div}(\mathbf{u}) \\ & + [k_c\underline{n}\nabla^2 - \mathbf{u}\cdot\rho T_0 l\underline{n}\nabla - \rho T_0 l\underline{n}\underset{\sim}{\partial}_t]M = -\rho r\end{aligned} \tag{104}$$

$$\begin{aligned}& [(\hat{D}_T + \underline{l}\hat{D})\nabla^2 - \mathbf{u}(1-\rho)\underline{l}\cdot\nabla - \rho\underline{l}\underset{\sim}{\partial}_t]\Theta + [(\hat{D}_\varepsilon + \underline{\gamma_c}\hat{D})\nabla^2 \\ & + \mathbf{u}(1-\rho)\underline{\gamma_c}\cdot\nabla - \rho\underline{\gamma_c}\underset{\sim}{\partial}_t + \\ & + (1-\rho)(\underline{n}M + \underline{\gamma_c}\varepsilon_{kk} + \underline{l}\Theta)]\operatorname{div}(\mathbf{u}) \\ & + [\hat{D}\underline{n}\nabla^2 + \mathbf{u}(1-\rho)\underline{n}\cdot\nabla + \rho\underline{n}\underset{\sim}{\partial}_t]M = -R\end{aligned} \tag{105}$$

where

$$\underline{l} = \frac{l}{n} \quad \underline{n} = \frac{l}{n} \quad \underline{\gamma_c} = \frac{\gamma_c}{n}. \tag{106}$$

After linearization on the sets of equations (102) and (103) or (104) and (105) we arrive at the system of equations

$$\begin{aligned}& (k\nabla^2 - m\underset{\sim}{\partial}_t)\Theta + (\underline{k_\varepsilon\nabla^2} - \rho T_0\gamma_T\partial_t)\operatorname{div}(\mathbf{u}) \\ & + (\underline{k_c\nabla^2} - \rho T_0 l\partial_t)c = -\rho r(\hat{D}\nabla^2 - \rho\underset{\sim}{\partial}_t)c \\ & + \hat{D}_\varepsilon\nabla^2\operatorname{div}(\mathbf{u}) + \hat{D}_T\nabla^2\Theta = -R\end{aligned} \tag{107}$$

or

$$\begin{aligned}& [(k + \underline{l}k_c)\nabla^2 - \rho T_0(m + \underline{l}l)\underset{\sim}{\partial}_t]\Theta \\ & + [\underline{(k_\varepsilon + k_c\underline{\gamma_c})\nabla^2} - \rho T_0(\gamma_T + + \underline{\gamma_c}l)\underset{\sim}{\partial}_t]\operatorname{div}(\mathbf{u}) \\ & + [\underline{k_c\underline{n}\nabla^2} - \rho T_0 l\underline{n}\underset{\sim}{\partial}_t]M = -\rho r\end{aligned}$$

$$\begin{aligned}& [\underline{(\hat{D}_T + \underline{l}\hat{D})\nabla^2} - \rho\underline{l}\underset{\sim}{\partial}_t]\Theta + [\underline{(\hat{D}_\varepsilon + \underline{\gamma_c}\hat{D})\nabla^2} \\ & - \rho\underline{\gamma_c}\underset{\sim}{\partial}_t]\operatorname{div}(\mathbf{u}) + [\hat{D}\underline{n}\nabla^2 + \rho\underline{n}\underset{\sim}{\partial}_t]M = -R\end{aligned} \tag{108}$$

where we underline the new terms which appear in comparison with the "classical" linear thermodiffusion theory [11–14].

Introducing now into the equation of motion

$$t_{ij,j} + \rho F_i = \rho\ddot{u}_i \tag{109}$$

the stresses given by the first constitutive relation of (79) and making use of the definition of strain

$$2\varepsilon_{ij} = u_{i,j}+u_{j,i} \tag{110}$$

we obtain the system of equations in displacements

$$\mu\nabla^2 u_i+(\lambda+\mu)u_{j,ji}+\rho F_i = \rho\ddot{u}_i+\gamma_{\mathrm{T}}\Theta_{,i}+\gamma_{\mathrm{c}}c_{,i}. \tag{111}$$

Using the equation for concentration $(80)_3$ we arrive at the relation

$$\mu\nabla^2 u_i+(\lambda+\mu-\underline{\gamma_{\mathrm{c}}}\gamma_{\mathrm{c}})u_{j,ji}+\rho F_i$$

$$= \rho\ddot{u}_i+(\gamma_{\mathrm{T}}+\underline{\gamma_{\mathrm{c}}}l)\Theta_{,i}+\underline{n}\gamma_{\mathrm{c}}M_{,i} \tag{112}$$

or in the vector notation

$$\mu\nabla^2\mathbf{u}+(\lambda+\mu-\underline{\gamma_{\mathrm{c}}}\gamma_{\mathrm{c}})\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F}$$

$$= \rho\ddot{\mathbf{u}}+(\gamma_{\mathrm{T}}+\underline{l}\gamma_{\mathrm{c}})\,\mathrm{grad}\,\Theta+\underline{n}\gamma_{\mathrm{c}}\,\mathrm{grad}\,M. \tag{113}$$

Equations (107) and (111) or (108) and (113) constitute the complete set of the equations of heat and mass transfer in a solid.

The final system of equations is as follows

$$D_1 c+\hat{D}_\varepsilon\nabla^2\,\mathrm{div}(\mathbf{u})+\hat{D}_{\mathrm{T}}\nabla^2\Theta = -R$$

$$D_2\Theta+D_3\,\mathrm{div}(\mathbf{u})+D_4 c = -\rho r$$

$$\mu\nabla^2\mathbf{u}+(\lambda+\mu)\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F}$$

$$= \rho\mathbf{u}+\gamma_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{c}}\,\mathrm{grad}(c) \tag{114}$$

or

$$\underset{\wedge}{D}_1 M+\underset{\wedge}{D}_\varepsilon\nabla^2\,\mathrm{div}(\mathbf{u})+\underset{\wedge}{D}_{\mathrm{T}}\nabla^2\Theta = -R$$

$$\underset{\wedge}{D}_2\Theta+\underset{\wedge}{D}_3\,\mathrm{div}(\mathbf{u})+\underset{\wedge}{D}_4 M = -\rho r$$

$$\mu\nabla^2\mathbf{u}+(\lambda+\mu-\underset{\wedge}{\gamma}_{\mathrm{M}})\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F}$$

$$= \rho\mathbf{u}+\underset{\wedge}{\gamma}_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{M}}\,\mathrm{grad}\,M \tag{115}$$

where

$$D_1 = \hat{D}\nabla^2-\rho\underset{\cdot}{\partial}_{\mathrm{t}} \quad D_2 = k\nabla^2-m\underset{\cdot}{\partial}_{\mathrm{t}}$$

$$D_3 = k_\varepsilon\nabla^2-\rho T_0\gamma_{\mathrm{T}}\,\partial_{\mathrm{t}} \quad D_4 = k_{\mathrm{c}}\nabla^2-\rho T_0 l\,\partial_{\mathrm{t}}$$

$$\underset{\wedge}{D}_1 = \hat{D}\underline{n}\nabla^2+\rho\underline{n}\,\underset{\cdot}{\partial}_{\mathrm{t}} \quad \underset{\wedge}{D}_\varepsilon = (\hat{D}_\varepsilon+\underline{\gamma_{\mathrm{c}}}\hat{D})\nabla^2-\rho\underline{\gamma_{\mathrm{c}}}\,\underset{\cdot}{\partial}_{\mathrm{t}}$$

$$\underset{\wedge}{D}_{\mathrm{T}} = (\hat{D}_{\mathrm{T}}+\underline{l}\hat{D})\nabla^2 \quad \underset{\wedge}{D}_2 = (k+\underline{l}k_{\mathrm{c}})\nabla^2-\rho T_0(m+\underline{l}l)\,\underset{\cdot}{\partial}_{\mathrm{t}}$$

$$\underset{\wedge}{D}_3 = (k_\varepsilon+k_{\mathrm{c}}\underline{\gamma_{\mathrm{c}}})\nabla^2-\rho T_0(\gamma_{\mathrm{T}}+\underline{\gamma_{\mathrm{c}}}l)\,\underset{\cdot}{\partial}_{\mathrm{t}}$$

$$\underset{\wedge}{D}_4 = k_{\mathrm{c}}\underline{n}\nabla^2-\rho T_0 l\underline{n}\,\underset{\cdot}{\partial}_{\mathrm{t}} \quad \underset{\wedge}{\gamma}_{\mathrm{M}} = \underline{\gamma_{\mathrm{c}}}\gamma_{\mathrm{c}}$$

$$\underset{\wedge}{\gamma}_{\mathrm{T}} = \gamma_{\mathrm{T}}+\underline{l}\gamma_{\mathrm{c}} \quad \gamma_{\mathrm{M}} = \underline{n}\gamma_{\mathrm{c}}. \tag{116}$$

Finally in this section we are going to introduce thermodynamical inequalities in the same manner as that shown in [11]. Considering the equation of the internal energy (73)

$$2U = 2\mu' e_{ij}e_{ij}+\left(\frac{2\mu'}{3}+\lambda'\right)e^2-2\gamma'_{\mathrm{s}}Se$$

$$-2\gamma'_{\mathrm{s}}ce+m'S^2+n'c^2-2l'Sc \tag{117}$$

where e_{ij} is the deviator of the strain tensor

$$e_{ij} = \varepsilon_{ij}-\tfrac{1}{3}\delta_{ij}\varepsilon_{kk} = \varepsilon_{ij}-\tfrac{1}{3}\delta_{ij}e \quad e_{ii} = 0 \tag{118}$$

and constitutive equations for a concentration and an entropy obtained from the relations $(76)_{1,2}$

$$c = \frac{1}{n'm'-l'^2}[l'\Theta+m'M+(\gamma'_{\mathrm{c}}m'+\gamma'_{\mathrm{s}}l')e]$$

$$S = \frac{1}{n'm'-l'^2}[n'\Theta+l'M+(\gamma'_{\mathrm{c}}l'+\gamma'_{\mathrm{s}}n')e] \tag{119}$$

one can get

$$2U = 2\mu' e_{ij}e_{ij}+e^2\left[\frac{2\mu'}{3}+\lambda'\right.$$

$$\left.-\frac{1}{n'm'-l'^2}(\gamma_{\mathrm{s}}'^2 n'+\gamma_{\mathrm{c}}'^2 m'+2\gamma'_{\mathrm{s}}\gamma'_{\mathrm{c}}l')\right]$$

$$+\frac{1}{n'm'-1'^2}(n'\Theta^2+m'M^2+2l'M\Theta). \tag{120}$$

The internal energy however is defined as a quadratic function which is nonnegative. Following now the consideration presented by Nowacki [11] we get similar final inequalities for the coefficients which occur in the constitutive equations (76). These inequalities are as follows:

$$\mu' > 0 \quad \frac{2\mu'}{3}+\lambda' > 0 \quad \gamma'_{\mathrm{s}} > 0; \quad \gamma'_{\mathrm{c}} > 0$$

$$m' > 0; \quad n' > 0; \quad n'm'-l'^2 > 0. \tag{121}$$

5.2. *Simplifications—particular cases*

The final set of linearized equations (114) and (115) of mass and heat flows coupled with mechanical field is very complicated. However one can make some simplifications. In a similar manner to the cases of thermodiffusion [12] or coupled thermoelasticity [13] we can neglect here the term $\nabla^2\mathrm{div}(\mathbf{u})$ in the mass equations and the terms $\nabla^2\,\mathrm{div}(\mathbf{u})$ and $\mathrm{div}\,\dot{\mathbf{u}}$ in the heat equations. Then we arrive at the set of relations

$$(k\nabla^2-m\underset{\cdot}{\partial}_{\mathrm{t}})\Theta+(k_{\mathrm{c}}\nabla^2-\rho T_0 l\,\partial_{\mathrm{t}})c = -\rho r$$

$$(\hat{D}\nabla^2-\rho\underset{\cdot}{\partial}_{\mathrm{t}})c+\hat{D}_{\mathrm{T}}\nabla^2\Theta = -R$$

$$\mu\nabla^2\mathbf{u}+(\lambda+\mu)\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F}$$

$$= \rho\mathbf{u}+\gamma\,\underset{T}{\mathrm{grad}}\,\Theta+\gamma\,\underset{\mathrm{c}}{\mathrm{grad}}(c) \tag{122}$$

or

$$\begin{aligned}
&[(k+\underline{l}k_{\mathrm{c}})\nabla^2-\rho T_0(m+\underline{l}l)\,\underset{\cdot}{\partial}_{\mathrm{t}}]\Theta \\
&\qquad +[k_{\mathrm{c}}\underline{n}\nabla^2-\rho T_0 l\underline{n}\,\underset{\cdot}{\partial}_{\mathrm{t}}]M = -\rho r \\
&[\hat{D}\underline{n}\nabla^2+\rho\underline{n}\,\underset{\cdot}{\partial}_{\mathrm{t}}]M+[(\hat{D}_{\mathrm{T}}+\underline{l}\hat{D})\nabla^2-\rho\underline{l}\,\underset{\cdot}{\partial}_{\mathrm{t}}]\Theta = -R \\
&\mu\nabla^2\mathbf{u}+(\lambda+\mu-\underset{\wedge}{\gamma}_{\mathrm{M}})\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F} \\
&\qquad = \rho\mathbf{u}+\underset{\wedge}{\gamma}_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{M}}\,\mathrm{grad}\,M. \qquad (123)
\end{aligned}$$

Here the equations of heat conduction and mass are coupled. After solving this set of equations the functions Θ and c or Θ and M appear in equations $(114)_3$ or $(115)_3$ as known. With these equations which are analogous to the equations of the theory of heat stresses we can determine the influence of heat and mass flow on the strain of the body. On the other hand we cannot determine the influence of strain on the mass and heat flow because there are no appropriate terms in these equations.

If we do not examine the influence of mechanical vibration on the heat and mass transport then we can neglect the terms $\mathrm{div}\,\dot{\mathbf{u}}$ in the given sets of final relations. Thus

$$\begin{aligned}
&(k\nabla^2-m\underset{\cdot}{\partial}_{\mathrm{t}})\Theta+k_{\varepsilon}\nabla^2\,\mathrm{div}(\mathbf{u})+(k_{\mathrm{c}}\nabla^2-\rho T_0 l\,\partial_{\mathrm{t}})c = -\rho r \\
&(\hat{D}\nabla^2-\rho\underset{\cdot}{\partial}_{\mathrm{t}})c+\hat{D}_{\varepsilon}\nabla^2\,\mathrm{div}(\mathbf{u})+\hat{D}_{\mathrm{T}}\nabla^2\Theta = -R \\
&\mu\nabla^2\mathbf{u}+(\lambda+\mu)\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F} \\
&\qquad = \rho\mathbf{u}+\gamma_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{c}}\,\mathrm{grad}(c) \qquad (124)
\end{aligned}$$

or

$$\begin{aligned}
&[(k+\underline{l}k_{\mathrm{c}})\nabla^2-\rho T_0(m+\underline{l}l)\,\underset{\cdot}{\partial}_{\mathrm{t}}]\Theta+(k_{\varepsilon}+k_{\mathrm{c}}\underline{\gamma_{\mathrm{c}}})\nabla^2\,\mathrm{div}(\mathbf{u}) \\
&\qquad +[k_{\mathrm{c}}\underline{n}\nabla^2-\rho T_0 l\underline{n}\,\underset{\cdot}{\partial}_{\mathrm{t}}]M = -\rho r \\
&[\hat{D}\underline{n}\nabla^2+\rho\underline{n}\,\underset{\cdot}{\partial}_{\mathrm{t}}]M+(\hat{D}_{\varepsilon}+\underline{\gamma_{\mathrm{c}}}\hat{D})\nabla^2\,\mathrm{div}(\mathbf{u}) \\
&\qquad +[(\hat{D}_{\mathrm{T}}+\underline{l}\hat{D})\nabla^2-\rho\underline{l}\,\underset{\cdot}{\partial}_{\mathrm{t}}]\Theta = -R \\
&\mu\nabla^2\mathbf{u}+(\lambda+\mu-\gamma_{\mathrm{M}})\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F} \\
&\qquad = \rho\mathbf{u}+\gamma_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{M}}\,\mathrm{grad}\,M. \qquad (125)
\end{aligned}$$

In the quasi-stationary cases the time derivatives disappear in relations (114) or (115). Then we obtain the set of equations

$$\begin{aligned}
&k\nabla^2\Theta+k_{\varepsilon}\nabla^2\,\mathrm{div}(\mathbf{u})+k_{\mathrm{c}}\nabla^2 c = -\rho r \\
&\hat{D}\nabla^2 c+\hat{D}_{\varepsilon}\nabla^2\,\mathrm{div}(\mathbf{u})+\hat{D}_{\mathrm{T}}\nabla^2\Theta = -R \\
&\mu\nabla^2\mathbf{u}+(\lambda+\mu)\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F} \\
&\qquad = \gamma_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{c}}\,\mathrm{grad}(c) \qquad (126)
\end{aligned}$$

or

$$\begin{aligned}
&(k+\underline{l}k_{\mathrm{c}})\nabla^2\Theta+(k_{\varepsilon}+k_{\mathrm{c}}\underline{\gamma_{\mathrm{c}}})\nabla^2\,\mathrm{div}(\mathbf{u})+k_{\mathrm{c}}\underline{n}\nabla^2 M = -\rho r \\
&\hat{D}\underline{n}\nabla^2 M+(\hat{D}_{\varepsilon}+\gamma_{\mathrm{c}}\hat{D})\nabla^2\,\mathrm{div}(\mathbf{u})+(\hat{D}_{\mathrm{T}}+\underline{l}\hat{D})\nabla^2\Theta = -R \\
&\mu\nabla^2\mathbf{u}+(\lambda+\mu-\underset{\wedge}{\gamma}_{\mathrm{M}})\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F} \\
&\qquad = \underset{\wedge}{\gamma}_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{M}}\,\mathrm{grad}\,M. \qquad (127)
\end{aligned}$$

Finally, when we neglect the influence of strain on the mass and heat flow in the quasi-stationary cases, we arrive at the system of equations

$$\begin{aligned}
&k\nabla^2\Theta+k_{\mathrm{c}}\nabla^2 c = -\rho r \\
&\hat{D}\nabla^2 c+\hat{D}_{\mathrm{T}}\nabla^2\Theta = -R \\
&\mu\nabla^2\mathbf{u}+(\lambda+\mu)\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F} \\
&\qquad = \gamma_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{c}}\,\mathrm{grad}(c) \qquad (128)
\end{aligned}$$

or

$$\begin{aligned}
&(k+\underline{l}k_{\mathrm{c}})\nabla^2\Theta+(k_{\varepsilon}+k_{\mathrm{c}}\underline{\gamma_{\mathrm{c}}})\nabla^2\,\mathrm{div}(\mathbf{u}) \\
&\qquad +k_{\mathrm{c}}\underline{n}\nabla^2 M = -\rho r \\
&\hat{D}\underline{n}\nabla^2 M+(\hat{D}_{\mathrm{T}}+\underline{l\hat{D}})\nabla^2\Theta = -R \\
&\mu\nabla^2\mathbf{u}+(\lambda+\mu-\underset{\wedge}{\gamma}_{\mathrm{M}})\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}+\rho\mathbf{F} \\
&\qquad = \underset{\wedge}{\gamma}_{\mathrm{T}}\,\mathrm{grad}\,\Theta+\gamma_{\mathrm{M}}\,\mathrm{grad}\,M. \qquad (129)
\end{aligned}$$

6. VARIATION FORMULATIONS

The object of this section is to emphasize a few features involved in the construction of variational principles for the theory considered in this paper. Firstly, we are going to present the integral variational principle of Gyarmati. Secondly we will supply an extension of this principle which is more appropriate to the approach which was made in the previous sections. Finally, we will apply this generalization to a theory. This problem consists of finding a 'state', i.e. thermodynamical quantities which satisfies the governing field equations in a given region of space and meets certain boundary conditions and kinematic equations for the thermodynamic forces and equations for the appropriate fluxes.

Let us denote by V the volume of an arbitrary body $\mathscr{B}$ of three-dimensional (3D) Euclidean space and bounded by the surface $\partial\mathscr{B}$.

6.1. *Gyarmati variational formulation*

Let us consider the variational principle formulated by Gyarmati [33, 34] and described by him as "universal":

$$\delta\int_V \mathscr{F}_{\mathrm{G}}\,\mathrm{d}V = \delta\int_V [\boldsymbol{\Sigma}-(\psi+\varphi)]\,\mathrm{d}V = 0 \qquad (130)$$

where

$$\boldsymbol{\Sigma} = \mathbf{j}_i\cdot\mathbf{X}_i \quad \mathbf{X}_i = \nabla\boldsymbol{\Gamma}_i \qquad (131)$$

$$\psi = \tfrac{1}{2}L_{ik}\mathbf{X}_i\cdot\mathbf{X}_k \qquad (132)$$

$$\varphi = \tfrac{1}{2}R_{ik}\mathbf{j}_i\cdot\mathbf{j}_k \qquad (133)$$

so the Lagrangian potential is a function of forces and fluxes

$$\mathscr{F}_{\mathrm{G}} = \mathscr{F}_{\mathrm{G}}(\Gamma_i, \nabla\Gamma_i, \mathbf{j}_i) \tag{134}$$

and Γ_i and $\mathbf{j}_i$ are the quantities for which the variations should be calculated. The functional (130) leads to the following equations given in the form of the Euler equations

$$\nabla\cdot\frac{\partial\mathscr{F}_{\mathrm{G}}}{\partial\nabla\Gamma_i} - \frac{\partial\mathscr{F}_{\mathrm{G}}}{\partial\Gamma_i} = 0$$

$$\frac{\partial\mathscr{F}_{\mathrm{G}}}{\partial\mathbf{j}_i} = 0 \tag{135}$$

which gives:

(i) the balance equations

$$\rho\dot{a}_i + \nabla\cdot L_{ik}\nabla\Gamma_k - r_i = 0 \quad x\in\mathscr{B} \tag{136}$$

(ii) the kinematic equations for $\mathbf{X}$

$$\mathbf{X}_i = \nabla\Gamma_i = R_{ik}\mathbf{j}_i \quad x\in\mathscr{B} \tag{137}$$

(iii) and the boundary conditions

$$\mathbf{j}_i = \hat{\mathbf{j}}_i = L_{ik}\nabla\Gamma_k \quad x\in\partial\mathscr{B}. \tag{138}$$

Moreover from the balance equations the relations for the fluxes results

$$\mathbf{j}_i = L_{ik}\nabla\Gamma_k \quad x\in\mathscr{B}. \tag{139}$$

6.2. *A certain generalization—the variational principle of Gyarmati type*

A simple comparison of (131) and (54) shows that there is a need to extend the Gyarmati variational principle for these cases where the potential Σ or at least one part of it is of the type

$$\Sigma = \mathbf{j}_i\cdot s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})} \quad \text{(no sum on (b))} \tag{140}$$

as the thermodynamical forces $\mathbf{X}_i$ should be expressed by (56). Some calculations show also that this leads to the modification of the Gyarmati principle. In particular the "local, dissapative potentials" Σ, ψ and φ should be modified. Thus we are led to the following extension of the Gyarmati principle.

We shall let $U = U(\mathscr{B}, \partial\mathscr{B}, s^{(\mathrm{b})}, \Gamma_i^{(\mathrm{b})}, \nabla\Gamma_i^{(\mathrm{b})}, \mathbf{j}_i)$ denote the foregoing problem for the case in which the governing equations are following:

(i) the balance equations

$$\rho\dot{a}_i + \nabla\cdot s^{(\mathrm{b})}L_{ik}\nabla\Gamma_k^{(\mathrm{b})} - r_i = 0 \quad x\in\mathscr{B} \quad \text{(no sum on (b))} \tag{141}$$

(ii) the kinematic equations

$$s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})} = R_{ik}\mathbf{j}_k \quad x\in\mathscr{B} \quad \text{(no sum on (b))} \tag{142}$$

(iii) the constitutive equations for the fluxes

$$\mathbf{j}_i = s^{(\mathrm{b})}L_{ik}\nabla\Gamma_k^{(\mathrm{b})} \quad x\in\mathscr{B} \quad \text{(no sum on (b))} \tag{143}$$

(iv) and the boundary conditions

$$\mathbf{j}_i = \hat{\mathbf{j}}_i = s^{(\mathrm{b})}L_{ik}\nabla\Gamma_k^{(\mathrm{b})} \quad x\in\partial\mathscr{B} \quad \text{(no sum on (b))}. \tag{144}$$

Theorem. Let $u\in U$ and let $\mathscr{F}(u)$ have a linear Gâteaux differential at every u, where $\mathscr{F}$ is the functional defined by

$$\mathscr{F}(u) = \mathscr{F}(s^{(\mathrm{b})}, \Gamma_i^{(\mathrm{b})}, \nabla\Gamma_i^{(\mathrm{b})}, \mathbf{j}_i) = \int_V [\Sigma - (\psi + \varphi - \vartheta)]\,\mathrm{d}V \tag{145}$$

where

$$\Sigma = \mathbf{j}_i\cdot\mathbf{X}_i = \mathbf{j}_i\cdot\nabla s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})} = \Sigma' + \Sigma'' = \mathbf{j}_i\cdot(\mathbf{X}_i' + \mathbf{X}_i'')$$

$$= \mathbf{j}_i\cdot s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})} + \mathbf{j}_i\Gamma_i^{(\mathrm{b})}\cdot\nabla s^{(\mathrm{b})}$$

$$\mathbf{X}_{\mathrm{i}}' = s^{(\mathrm{b})}\,\nabla\Gamma_i^{(\mathrm{b})} \quad \mathbf{X}_i'' = \Gamma_i^{(\mathrm{b})}\cdot\nabla s^{(\mathrm{b})} \quad \text{(no sum on (b))} \tag{146}$$

$$\psi = \tfrac{1}{2}L_{ik}\mathbf{X}_i\cdot\mathbf{X}_k = \tfrac{1}{2}L_{ik}\nabla s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\cdot\nabla s^{(\mathrm{t})}\Gamma_i^{(\mathrm{t})} \quad \text{(no sum on (b) and (t))} \tag{147}$$

$$\varphi = \tfrac{1}{2}R_{ik}\mathbf{j}_i\cdot\mathbf{j}_k \tag{148}$$

$$\vartheta = \tfrac{1}{2}L_{ik}(\mathbf{X}_i - \mathbf{X}_i')(\mathbf{X}_k - \mathbf{X}_k') = \tfrac{1}{2}L_{ik}\mathbf{X}_i''\cdot\mathbf{X}_k''$$

$$= \tfrac{1}{2}L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})} \quad \text{(no sum on (b) and (t)).} \tag{149}$$

Then

$$\delta\mathscr{F}(u) = 0 \quad \text{over } U \tag{150}$$

if and only if u is a solution of a boundary problem consisting of equations (141)–(144)

Proof. Let u be an arbitrary element in U. We are going to calculate the Gâteaux differential of $\mathscr{F}$.
Let us start from insertion of (146)–(149) into (145). The result is

$$\mathscr{F}(u) = \mathscr{F}(s^{(\mathrm{b})}, \Gamma_i^{(\mathrm{b})}, \nabla\Gamma_i^{(\mathrm{b})}, \mathbf{j}_i) = \int_V \{\mathbf{j}_i\cdot\nabla s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})} - \tfrac{1}{2}[L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\Gamma_k^{(\mathrm{t})}\cdot\nabla s^{(\mathrm{t})} + R_{ik}\mathbf{j}_i\cdot\mathbf{j}_k - L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})}]\}\,\mathrm{d}V. \tag{151}$$

Using the identity

$$\mathbf{j}_i\cdot\nabla s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})} = \nabla\cdot(\mathbf{j}_i s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}) - s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\nabla\cdot\mathbf{j}_i \tag{152}$$

and applying Green's theorem we have

$$\mathscr{F}(u) = \int_V \{-s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\cdot\nabla\mathbf{j}_i - \tfrac{1}{2}[L_{ik}\nabla s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\cdot\nabla s^{(\mathrm{t})}\Gamma_i^{(\mathrm{t})} + R_{ik}\mathbf{j}_i\cdot\mathbf{j}_k - L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})}]\}\,\mathrm{d}V + \int_A \{(\mathbf{j}_i s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\mathbf{n}\}\,\mathrm{d}A \tag{153}$$

where A denotes the surface bounding a medium. Taking the general balance equations into account

$$\rho\dot{a}_i-r_i = -\nabla\mathbf{j}_i \tag{154}$$

we can rewrite (153) as

$$\begin{aligned}\mathscr{F}(u) = \int_V &\{(\rho\dot{a}_i-r_i)s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\\ &-\tfrac{1}{2}[L_{ik}\nabla s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\cdot\nabla s^{(\mathrm{t})}\Gamma_i^{(\mathrm{t})}+R_{ik}\mathbf{j}_i\cdot\mathbf{j}_k\\ &-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})}]\}\,\mathrm{d}V\\ &+\int_A\{(\mathbf{j}_i s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\mathbf{n}\}\,\mathrm{d}A.\end{aligned} \tag{155}$$

Now according to the assumptions concerning calculations of variation in the universal principle of the Gyarmati type we are varying, concurrently and independently each of other, $s^{(\mathrm{b})}$, $\Gamma_i^{(\mathrm{b})}$, $\nabla\Gamma_i^{(\mathrm{b})}$ and $\mathbf{j}_i$, respectively. Then the Gâteaux differential of $\mathscr{F}$ is as follows:

$$\begin{aligned}\delta\mathscr{F}(u) &= \langle\mathrm{grad}\,\mathscr{F}(u)\rangle = \frac{\mathrm{d}}{\mathrm{d}\alpha}(\mathscr{F}(u+\alpha u)|_{\alpha=0})\\ &= \int_V\{\delta[(\rho\dot{a}_i-r_i)s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}]\\ &\quad-\tfrac{1}{2}\delta[L_{ik}\nabla(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})]\\ &\quad-\tfrac{1}{2}\delta[R_{ik}\mathbf{j}_i\cdot\mathbf{j}_k]+L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &\quad-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\delta(s^{(\mathrm{t})}\cdot\nabla\Gamma_k^{(\mathrm{t})})\}\,\mathrm{d}V\\ &\quad+\delta\int_A\{\mathbf{j}_i s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\}\mathbf{n}\,\mathrm{d}A\end{aligned} \tag{156}$$

where the relation

$$\begin{aligned}&\tfrac{1}{2}\delta[L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})}] = \tfrac{1}{2}[L_{ik}\,\delta(\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})})\cdot\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})}\\ &\quad+L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta(\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})}) = L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta(\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})})\\ &\quad+[L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta(s^{(\mathrm{t})}\nabla\Gamma_k^{(\mathrm{t})})-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta(s^{(\mathrm{t})}\nabla\Gamma_k^{(\mathrm{t})})]\\ &\quad= \Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}L_{ik}\cdot\delta(s^{(\mathrm{t})}\nabla\Gamma_k^{(\mathrm{t})})+\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}L_{ik}\cdot\delta(\Gamma_k^{(\mathrm{t})}\nabla s^{(\mathrm{t})})\\ &\quad-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta(s^{(\mathrm{t})}\nabla\Gamma_k^{(\mathrm{t})}) = L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\nabla\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &\quad-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta(s^{(\mathrm{t})}\nabla\Gamma_k^{(\mathrm{t})})\end{aligned} \tag{157}$$

has been used. With the formula

$$\begin{aligned}&\tfrac{1}{2}\delta[L_{ik}\nabla(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})]\\ &\qquad= L_{ik}\nabla\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})}\end{aligned} \tag{158}$$

equation (156) becomes

$$\begin{aligned}\delta\mathscr{F}(u) = \int_V &\{\delta[(\rho\dot{a}_i-r_i)s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}]\\ &-\delta[L_{ik}\nabla(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})]\\ &-R_{ik}\mathbf{j}_i\cdot\delta\mathbf{j}_k+L_{ik}\nabla\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &+L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\,\delta(s^{(\mathrm{t})}\cdot\nabla\Gamma_k^{(\mathrm{t})})\}\,\mathrm{d}V\\ &+\delta\int_A\{\mathbf{j}_i s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\}\mathbf{n}\,\mathrm{d}A.\end{aligned} \tag{159}$$

Thus in view of equation

$$\begin{aligned}&\delta[L_{ik}\nabla(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})]\\ &\quad= L_{ik}\nabla\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &\quad+L_{ik}\nabla(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &\quad= L_{ik}\nabla\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\cdot\nabla(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &\quad+L_{ik}s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &\quad+L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\end{aligned} \tag{160}$$

one can write

$$\begin{aligned}\delta\mathscr{F}(u) = \int_V &\{\delta[(\rho\dot{a}_i-r_i)s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}]\\ &-L_{ik}s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})-R_{ik}\mathbf{j}_i\cdot\delta\mathbf{j}_k\\ &-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\,\delta(s^{(\mathrm{t})}\cdot\nabla\Gamma_k^{(\mathrm{t})})\}\,\mathrm{d}V\\ &+\delta\int_A\{\mathbf{j}_i s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\}\mathbf{n}\,\mathrm{d}A.\end{aligned} \tag{161}$$

The following relations arose from the equations of balance

$$s^{(\mathrm{b})}\,\delta(\rho\dot{a}_i-r_i) = -s^{(\mathrm{b})}\,\delta\nabla\cdot\mathbf{j}_i = -\nabla s^{(\mathrm{b})}\,\delta\mathbf{j}_i+\nabla s^{(\mathrm{b})}\cdot\delta\mathbf{j}_i \tag{162}$$

so the equation (161) may now be written

$$\begin{aligned}\delta\mathscr{F}(u) = \int_V &\{(\rho\dot{a}_i-r_i)\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\\ &-s^{(\mathrm{b})}L_{ik}\nabla\Gamma_i^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &-\Gamma_i^{(\mathrm{b})}\nabla\cdot s^{(\mathrm{b})}\,\delta\mathbf{j}_i+\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta\mathbf{j}_i-R_{ik}\mathbf{j}_i\cdot\delta\mathbf{j}_k\\ &-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\,\delta(s^{(\mathrm{t})}\cdot\nabla\Gamma_k^{(\mathrm{t})})\}\,\mathrm{d}V\\ &+\int_A\mathbf{j}_i\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})+s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\,\delta\mathbf{j}_i\}\mathbf{n}\,\mathrm{d}A.\end{aligned} \tag{163}$$

This formula may be expressed by the relation

$$\begin{aligned}\delta\mathscr{F}(u) = \int_V &\{(\rho\dot{a}_i-r_i)\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\\ &-s^{(\mathrm{b})}L_{ik}\nabla\Gamma_i^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\\ &+s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})}\cdot\delta\mathbf{j}_i+\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta\mathbf{j}_i-R_{ik}\mathbf{j}_i\cdot\delta\mathbf{j}_k\\ &-L_{ik}\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\,\delta(s^{(\mathrm{t})}\cdot\nabla\Gamma_k^{(\mathrm{t})})\}\,\mathrm{d}V\\ &-\int_V\{\nabla\cdot(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\,\delta\mathbf{j}_i)\}\,\mathrm{d}V\\ &+\int_A\{\mathbf{j}_i\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})+s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\,\delta\mathbf{j}_i\}\mathbf{n}\,\mathrm{d}A\end{aligned} \tag{164}$$

where the identity

$$-\Gamma_i^{(\mathrm{b})}\nabla\cdot s^{(\mathrm{b})}\,\delta\mathbf{j}_i = -\nabla\cdot(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}\,\delta\mathbf{j}_i)+s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})}\cdot\delta\mathbf{j}_i \tag{165}$$

has been used.

Introducing now the relationship

$$\begin{aligned}-s^{(\mathrm{b})}L_{ik}\nabla\Gamma_i^{(\mathrm{b})}\cdot\nabla\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})}) &= -\nabla\cdot[s^{(\mathrm{b})}L_{ik}\nabla\Gamma_i^{(\mathrm{b})}\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})}) \\ &\quad +(\nabla\cdot s^{(\mathrm{b})}L_{ik}\nabla\Gamma_i^{(\mathrm{b})})\,\delta(s^{(\mathrm{t})}\Gamma_k^{(\mathrm{t})})\end{aligned} \tag{166}$$

and applying the divergence theorem we finally obtain, after some calculations, the relation

$$\begin{aligned}\delta\mathscr{F}(u) = \int_V &\{(\rho\dot{a}_i+\nabla\cdot s^{(\mathrm{t})}L_{ik}\nabla\Gamma_k^{(\mathrm{t})}-r_i)\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})}) \\ &+(s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})}-R_{ik}\mathbf{j}_k) \\ &\cdot\delta\mathbf{j}_k+\Gamma_i^{(\mathrm{b})}\nabla s^{(\mathrm{b})}\cdot\delta(\mathbf{j}_i-s^{(\mathrm{t})}L_{ik}\nabla\Gamma_k^{(\mathrm{t})})\}\,\mathrm{d}V \\ &+\int_A\{(\mathbf{j}_i-s^{(\mathrm{t})}L_{ik}\nabla\Gamma_k^{(\mathrm{t})})\,\delta(s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})})\}\mathbf{n}\,\mathrm{d}A.\end{aligned} \tag{167}$$

One first proves sufficiency. Suppose that $u\in U$ is a solution of equations (141)–(144). Then relation (167) becomes

$$(\operatorname{grad}\mathscr{F}(u))_U = 0 \quad \text{over } U \tag{168}$$

and point $u\in U$ is a critical point of the functional $\mathscr{F}(u)$. This implies equation (150).

To prove necessity, let us assume that equation (150) holds. In view of Lemmas 1–4 [35], one can see that

$$\operatorname{grad}\mathscr{F}(u) = N(u) \equiv 0 \tag{169}$$

which completes the proof of the theorem.

The functional derived herein gives, when varied, the governing equations including the boundary conditions in form of the Euler equations.

6.3. *Applying to the constructed theory*

Let us now use in (145) the following substitutions according to the relations (54) and (56) in Section 4.2.

$$\mathbf{j}_1 = \mathbf{q} \quad s^{(1)} = -\frac{1}{T} \quad \mathbf{X}_1' = -\frac{1}{T}\nabla T$$

$$\mathbf{X}_1'' = T\nabla\left(-\frac{1}{T}\right) \quad \mathbf{X}_1 = \nabla\left(-\frac{1}{T}T\right) \quad \mathbf{j}_2 = \kappa\mathbf{j}_\mathrm{a}$$

$$s^{(2)} = -T \quad \mathbf{X}_2' = -T\nabla\frac{M}{T} \quad \mathbf{X}_2'' = \frac{M}{T}\nabla(-T)$$

$$\mathbf{X}_2 = \nabla\left(-T\frac{M}{T}\right) \quad \mathbf{j}_3 = c\mathbf{u} \quad s_{\mathrm{I}}^{(3)} = -T$$

$$s_{\mathrm{II}}^{(3)} = -\frac{\rho M}{c} \quad \mathbf{X}_3^{\mathrm{I}'} = -T\nabla\left(\frac{\rho M}{T}\right) \quad \mathbf{X}_3^{\mathrm{I}''} = \frac{\rho M}{T}\nabla(-T)$$

$$\mathbf{X}_3^{\mathrm{I}} = \nabla\left(-T\frac{\rho M}{T}\right) \quad \mathbf{X}_3^{\mathrm{II}'} = -\frac{\rho M}{c}\nabla c$$

$$\mathbf{X}_3^{\mathrm{II}''} = c\nabla\left(-\frac{\rho M}{c}\right) \quad \mathbf{X}_3^{\mathrm{II}} = \nabla\left(-\frac{\rho M}{c}c\right) \tag{170}$$

where the quantity Σ, $\mathbf{X}_i'$ and $\mathbf{j}_i$ we have taken appropriate to equations (54) and (56).

$$\begin{aligned}\Sigma' = \mathbf{j}_i\cdot\mathbf{X}_i' = \mathbf{j}_i\cdot s^{(\mathrm{b})}\nabla\Gamma_i^{(\mathrm{b})} &= \mathbf{q}\cdot\left[-\frac{1}{T}\nabla T\right]+\kappa\mathbf{j}_\mathrm{a}\cdot\left[-T\nabla\frac{M}{T}\right] \\ &\quad +c\mathbf{u}\cdot\left[-T\nabla\left(\frac{\rho M}{T}\right)-\frac{\rho M}{c}\nabla c\right]\end{aligned} \tag{171}$$

$$\begin{aligned}\Sigma'' = \mathbf{j}_i\cdot\mathbf{X}_i'' = \mathbf{j}_i\Gamma_i^{(\mathrm{b})}\cdot\nabla s^{(\mathrm{b})} &= \mathbf{q}\left[T\cdot\nabla\left(-\frac{1}{T}\right)\right]+\kappa\mathbf{j}_\mathrm{a}\left[\frac{M}{T}\cdot\nabla(-T)\right] \\ &\quad +c\mathbf{u}\left[-\frac{\rho M}{T}-\cdot\nabla(T)-c\cdot\nabla\left(\frac{\rho M}{c}\right)\right]\end{aligned} \tag{172}$$

$$\begin{aligned}\boldsymbol{\Sigma} = \mathbf{j}_i\cdot\mathbf{X}_i = \mathbf{j}_i\cdot\nabla s^{(\mathrm{b})}\Gamma_i^{(\mathrm{b})} &= \mathbf{q}\cdot\nabla\left(-\frac{1}{T}T\right)+\kappa\mathbf{j}_\mathrm{a}\cdot\nabla\left(-T\frac{M}{T}\right) \\ &\quad +c\mathbf{u}\cdot\left[-\nabla\left(T\frac{\rho M}{T}-\right)-\nabla\left(\frac{\rho M}{c}c\right)\right].\end{aligned} \tag{173}$$

Analogously to eqs (147)–(149) we have

$$\begin{aligned}\psi = \frac{1}{2}\bigg\{&L_{\mathrm{qq}}\nabla\left(\frac{1}{T}T\right)\nabla\left(\frac{1}{T}T\right)+L_{\mathrm{aa}}\nabla\left(T\frac{M}{T}\right)\nabla\left(T\frac{M}{T}\right) \\ &+L_{\mathrm{cc}}\left[\nabla\left(T\frac{\rho M}{T}\right)+\nabla\left(\frac{\rho M}{c}c\right)\right]\left[\nabla\left(T\frac{\rho M}{T}\right)\right. \\ &\left.+\nabla\left(\frac{\rho M}{c}c\right)\right]+2L_{\mathrm{qa}}\nabla\left(\frac{1}{T}T\right)\nabla\left(T\frac{M}{T}\right) \\ &+2L_{\mathrm{qc}}\nabla\left(T\frac{\rho M}{T}\right)\left[\nabla\left(T\frac{\rho M}{T}\right)+\nabla\left(\frac{\rho M}{c}c\right)\right] \\ &+2L_{\mathrm{ac}}\nabla\left(T\frac{M}{T}\right)\left[\nabla\left(T\frac{\rho M}{T}\right)+\nabla\left(\frac{\rho M}{c}c\right)\right]\bigg\}\end{aligned} \tag{174}$$

$$\begin{aligned}\varphi = \tfrac{1}{2}\{&R_{\mathrm{qq}}\mathbf{q}\cdot\mathbf{q}+R_{\mathrm{aa}}\kappa\mathbf{j}_\mathrm{a}\cdot\kappa\mathbf{j}_\mathrm{a}+R_{\mathrm{cc}}c\mathbf{u}\cdot c\mathbf{u}+2R_{\mathrm{qa}}\mathbf{q}\cdot\kappa\mathbf{j}_\mathrm{a} \\ &+2R_{\mathrm{qc}}\mathbf{q}\cdot c\mathbf{u}+2R_{\mathrm{ac}}\kappa\mathbf{j}_\mathrm{a}\cdot c\mathbf{u}\}\end{aligned} \tag{175}$$

$$\begin{aligned}\vartheta = \vartheta &= \frac{1}{2}L_{ik}(\mathbf{X}_i-\mathbf{X}_i')(\mathbf{X}_k-\mathbf{X}_k') \\ &= \frac{1}{2}L_{ik}\mathbf{X}_i''\cdot\mathbf{X}_k'' = \frac{1}{2}\bigg\{L_{\mathrm{qq}}T^2\nabla^2\left(\frac{1}{T}\right)+L_{\mathrm{aa}}\left(\frac{M}{T}\right)^2\nabla^2(T)\end{aligned}$$

$$+L_{\mathrm{cc}}\left[\frac{\rho M}{T}-\nabla(T)+c\nabla\left(\frac{\rho M}{c}\right)\right]\cdot\left[\frac{\rho M}{T}\nabla(T)\right.$$
$$\left.+c\nabla\left(\frac{\rho M}{c}\right)\right]+2L_{\mathrm{qa}}T\frac{M}{T}\nabla\left(\frac{1}{T}\right)\nabla(T)$$
$$+2L_{\mathrm{qc}}T\nabla\left(\frac{1}{T}\right)\cdot\left[\frac{\rho M}{T}\nabla(T)+c\nabla\left(\frac{\rho M}{c}\right)\right]$$
$$\left.+2L_{\mathrm{ac}}\frac{M}{T}\nabla(T)\cdot\left[\frac{\rho M}{T}\nabla(T)+c\nabla\left(\frac{\rho M}{c}\right)\right]\right\} \quad (176)$$

where the matrixes L_{ik} and R_{ik} are inverses of each other and Onsager's conditions have been used ($L_{ij} = L_{ji}; R_{ij} = R_{ji}$). In equations (154) and (162) we have taken respectively:
entropy equation (39) (the second reduced energy equation)

$$T\rho\dot{S} = \rho r-\nabla\cdot\mathbf{q}-M\dot{c} \Rightarrow -\nabla\cdot\mathbf{q} = T\rho\dot{S}+M\dot{c}-\rho r \quad (177)$$

balances of mass (16)

$$\rho\dot{c} = -\nabla\cdot\kappa\mathbf{j}_{\mathrm{a}}-\rho c\nabla\mathbf{u}+R \Rightarrow -\nabla\cdot\kappa\mathbf{j}_{\mathrm{a}} = \rho\dot{c}+\rho c\nabla\mathbf{u}-R \quad (178)$$

$$\rho\frac{\partial c}{\partial t} = -\nabla\cdot\kappa\mathbf{j}_{\mathrm{a}}-\rho\nabla\cdot(c\mathbf{u})+R$$
$$\Rightarrow -\nabla\cdot(c\mathbf{u}) = \frac{1}{\rho}\left(\rho\frac{\partial c}{\partial r}+\nabla\cdot\kappa\mathbf{j}_{\mathrm{a}}-R\right). \quad (179)$$

Hence following step by step all the calculations from Section 6.2 in place of relations (141)–(144) which are the Euler equations of $\mathscr{F}(u)$ (solutions of relation (167)) we obtain:

(i) the balance equations

$$T\rho\dot{S}+\nabla\cdot\left(-\frac{1}{T}L_{\mathrm{qq}}\nabla T-TL_{\mathrm{qa}}\nabla\left(\frac{M}{T}\right)\right.$$
$$\left.+L_{\mathrm{qc}}\left[-T\nabla\left(\frac{\rho M}{T}\right)-\frac{\rho M}{c}\nabla c\right]\right)$$
$$+M\dot{c}-\rho r = 0 \quad x\in\mathscr{B} \quad (180)$$

$$\rho\dot{c}+\nabla\cdot\left(-\frac{1}{T}L_{\mathrm{qa}}\nabla T-TL_{\mathrm{aa}}\nabla\left(\frac{M}{T}\right)+L_{\mathrm{ac}}\left[-T\nabla\left(\frac{\rho M}{T}\right)\right.\right.$$
$$\left.\left.-\frac{\rho M}{c}\nabla c\right]\right)+\rho c\nabla\mathbf{u}-R = 0 \quad x\in\mathscr{B} \quad (181)$$

$$\rho\frac{\partial c}{\partial t}+\nabla\cdot\left(-\frac{1}{T}L_{\mathrm{qc}}\nabla T-TL_{\mathrm{ac}}\nabla\left(\frac{M}{T}\right)\right.$$
$$\left.+L_{\mathrm{cc}}\left[-T\nabla\left(\frac{\rho M}{T}\right)-\frac{\rho M}{c}\nabla c\right]\right)+\nabla\cdot\kappa\mathbf{j}_{\mathrm{a}}-R = 0$$
$$x\in\mathscr{B} \quad (182)$$

(ii) the kinematic equations for $\mathbf{X}_i'$

$$-\frac{1}{T}\nabla T = R_{\mathrm{qq}}\mathbf{q}+R_{\mathrm{qa}}\kappa\mathbf{j}_{\mathrm{a}}+R_{\mathrm{qc}}c\mathbf{u} \quad x\in\mathscr{B}$$
$$-T\nabla\frac{M}{T} = R_{\mathrm{aa}}\kappa\mathbf{j}_{\mathrm{a}}+R_{\mathrm{aq}}\mathbf{q}+R_{\mathrm{ac}}c\mathbf{u} \quad x\in\mathscr{B}$$
$$-T\nabla\left(\frac{\rho M}{T}\right)-\frac{\rho M}{c}\nabla c = R_{\mathrm{cc}}c\mathbf{u}+2R_{\mathrm{ca}}\kappa\mathbf{j}_{\mathrm{a}}+R_{\mathrm{cq}}\mathbf{q}$$
$$x\in\mathscr{B} \quad (183)$$

(iii) the boundary conditions

$$\mathbf{q}-\left(-\frac{1}{T}L_{\mathrm{qq}}\nabla T-TL_{\mathrm{qa}}\nabla\left(\frac{M}{T}\right)+L_{\mathrm{qc}}\left[-T\nabla\left(\frac{\rho M}{T}\right)\right.\right.$$
$$\left.\left.-\frac{\rho M}{c}\nabla c\right]\right) = 0 \quad x\in\partial\mathscr{B}$$

$$\kappa\mathbf{j}_{\mathrm{a}}-\left(-\frac{1}{T}L_{\mathrm{qa}}\nabla T-TL_{\mathrm{aa}}\nabla\left(\frac{M}{T}\right)+L_{\mathrm{ac}}\left[-T\nabla\left(\frac{\rho M}{T}\right)\right.\right.$$
$$\left.\left.-\frac{\rho M}{c}\nabla c\right]\right) = 0 \quad x\in\partial\mathscr{B}$$

$$c\mathbf{u}-\left(-\frac{1}{T}L_{\mathrm{qc}}\nabla T-TL_{\mathrm{ac}}\nabla\left(\frac{M}{T}\right)+L_{\mathrm{cc}}\left[-T\nabla\left(\frac{\rho M}{T}\right)\right.\right.$$
$$\left.\left.-\frac{\rho M}{c}\nabla c\right]\right) = 0 \quad x\in\partial\mathscr{B} \quad (184)$$

(iv) and as at the previous time the equations for the fluxes result from the balance equations

$$\mathbf{q} = \left(-\frac{1}{T}L_{\mathrm{qq}}\nabla T-TL_{\mathrm{qa}}\nabla\left(\frac{M}{T}\right)+L_{\mathrm{qc}}\left[-T\nabla\left(\frac{\rho M}{T}\right)\right.\right.$$
$$\left.\left.-\frac{\rho M}{c}\nabla c\right]\right) \quad x\in\mathscr{B}$$

$$\kappa\mathbf{j}_{\mathrm{a}} = \left(-\frac{1}{T}L_{\mathrm{qa}}\nabla T-TL_{\mathrm{aa}}\nabla\left(\frac{M}{T}\right)+L_{\mathrm{ac}}\left[-T\nabla\left(\frac{\rho M}{T}\right)\right.\right.$$
$$\left.\left.-\frac{\rho M}{c}\nabla c\right]\right) \quad x\in\mathscr{B}$$

$$c\mathbf{u} = \left(-\frac{1}{T}L_{\mathrm{qc}}\nabla T-TL_{\mathrm{ac}}\nabla\left(\frac{M}{T}\right)+L_{\mathrm{cc}}\left[-T\nabla\left(\frac{\rho M}{T}\right)\right.\right.$$
$$\left.\left.-\frac{\rho M}{c}\nabla c\right]\right) \quad x\in\mathscr{B}. \quad (185)$$

So the functional defined by (145)–(149) gives, as the Euler equations the entropy equations (39), balances of mass (16) the boundary conditions in fluxes and constitutive equations for them. It is easy to show by using (60) that equations (185) are the same to the (61) which results from thermodynamical considerations.

7. CONCLUSIONS

The system of equations (114) or (115) obtained in this paper together with the equations for heat and mass fluxes given by (81), (84), (87) and (90) are the basis for solving different initial-boundary problems in solid bodies. The variational formulation presented here could be also convenient in particular cases.

After consideration of this work we would like to underline that whereas in thermodiffusion the mass migration is described by the gradient of concentration, and in the theory of mixtures one treats all the components with equal rank, in the present paper the mass flux is generalized and links both types of flows, i.e. this is characterized by the momentum of migrating particles, and this is described by the gradient of either concentration or the chemical potential. Such a resultant flow is given by the relation (90). The present theory retains the interactions among processes of mass transport, thermal processes and the processes of deformation of the body; as in the coupled thermodiffusion theory.

However the proposal for the description of mass and heat flows coupled with a stress field shown here is valid only while the single mass component flow occurs. So there is a need to construct such a theory for multicomponents flows. There are opportunities to do this on the basis of considerations presented here and the theory of mixtures. One can also observe that, in the majority of phenomena of heat and mass transport, in technological processes where material structure rebuilding is concerned, and in numerous examples of flows in capillary-porous media, the macroscopic state of the system depends not only on the state at a given time but on previous states as well. These facts lead us to make the attempt to extend the investigations presented in this paper into the viscoelastic nature of materials.

Such problems as well as the generalization of the variational formulation shown here will be a matter for future investigation.

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