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Viscoelasticity and Thermodiffusion in Electric Field

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Basic equations for description and modelling of electric, thermal and diffusion processes in multicomponent viscoelactic structures under presence of the external electric field are presented. The corresponding constitutive relations are analyzed.

Key words: multicomponent continua, constitutive equations, mechano-thermo-diffusion, electric field, viscoelasticity

Introduction. We shall analyze a multicomponent continuous medium in which diffusive transport takes place being caused by both chemical potential gradient and by the action of electric field.

In the medium there is a skeleton component of the mass density ρ^0 which is one order higher than that for the remaining components $\rho^0 >> \rho^\alpha$, $\alpha = \overline{1,n}$. We shall treat this skeleton, as a viscoelastic body. The medium analyzed is in an electric field which generates ionization of the particular components of the medium and diffusive flow. Thus, the sources of mass appear as a result of the ionization and recombination processes. We shall also assume that the skeleton of the body is dielectric while the remaining components are the ions which diffuse with respect to this skeleton.

The model of the medium assumed in this paper can serve, among others, for describing the transport of electrolyte, electrodiffusion in a body with capillary-porous structure, and in the description of electrochemical corrosion of reinforced concrete or the mass transfer processes in the plastics [4, 10, 11].

The starting point of our consideration is the system of balances for multicomponent mixture which is in the electric field. Within this range, we analyze the balance of mass, momentum, energy and inequality of entropy increase.

The interaction of electric field generates Lorentz's force and electric polarization which appear consequently as an additional body forces in the balance of momentum and energy. As the final result we obtain residual inequality which determines the trend of evolution of the electrodiffusive process.

Taking into consideration the constitutive assumption we shall obtain the sought physical equations describing the process of thermal-electrodiffusion in viscoelastic body.

1. Balances of the process

The equations of multicomponent simple mixture in the electromagnetic field are the starting point of our consideration.

In these equations each component is cinematically equivalent, as opposed to diffusion, in which the migration of components in relation to the solid $(\alpha = 0)$ generally takes place; at the same time the mass density of the skeleton is one order higher than that of the migrating component ρ^{α}, $\alpha = \overline{1,n}$.

The fields describing processes are as follows [1, 9]:

$\vec{x} = \vec{\chi}^{\alpha}(\vec{X}^{\alpha}, t)$ is function of motion of the particle $\vec{X}^{\alpha}$;

$\vec{x} = \vec{\chi}(\vec{X}, t)$ is function of motion of the solid component in reference configuration ($x_k = \chi_k(X_K, t)$; $k, K = \overline{1,3}$);

$\vec{v}^{\alpha} = \dfrac{\partial \vec{\chi}^{\alpha}(\vec{X}^{\alpha}, t)}{\partial t}$ is velocity of particle $\vec{X}^{\alpha}$;

$\vec{v}^{0} = \dfrac{\partial \vec{\chi}(\vec{X}, t)}{\partial t} = \dfrac{\partial \vec{\chi}(\vec{\chi}^{-1}(\vec{x}, t), t)}{\partial t} = \vec{v}^{0}(\vec{x}, t)$ is Eulerian velocity of the solid component. (1)

The mean velocity of the mixture and diffusion velocities are defined respectively as

$$w_i = \frac{1}{\rho}\sum_{\alpha=0}^{n} \rho^{\alpha} v_i^{\alpha} \approx v_i^{0}, \quad u_i^{\alpha} = v_i^{\alpha} - w_i, \quad i = \overline{1,3}. \tag{2}$$

In the classical notations the balance laws have the forms:

- Conservation of mass

$$\frac{\partial \rho^{\alpha}}{\partial t} + (\rho^{\alpha} v_i^{\alpha})_{,i} = R^{\alpha}, \tag{3}$$

where R^{α} is the mass supply of the constituent α. An index following a comma denotes the partial derivation and repeated Latin indicates are summed but not Greek indices.

Let us sum up the components of the mixture considered. Then from (3) we obtain

$$\frac{\partial \rho}{\partial t} + (\rho w_i)_{,i} = 0, \quad \sum_{\alpha} R^{\alpha} = 0. \tag{4}$$

If we introduce the mass concentration of the α-th constituent c^{α} defined as $c^{\alpha} = \rho^{\alpha}/\rho$, we will obtain another version of (3)

$$\rho \dot{c}^{\alpha} = R^{\alpha} - j_{i,i}^{\alpha}. \tag{5}$$

In the above equation, $j_i^{\alpha} = \rho^{\alpha} u_i^{\alpha}$ denotes mass flux of the constituent α and $(\circ) = \dfrac{\partial(\circ)}{\partial t} + \vec{w} \cdot grad(\circ)$ indicates material derivative following the motion $\vec{w}$.

- Balance of momentum [1, 2]

$$\frac{\partial}{\partial t}(\rho^{\alpha} v_i^{\alpha}) + (\rho^{\alpha} v_i^{\alpha} v_j^{\alpha})_{,\,j} = \phi_i^{\alpha} + \rho^{\alpha} F_i^{\alpha} + \rho^{\alpha} e^{\alpha} E_i + \sigma_{ij,\,j}^{\alpha}, \quad \alpha = \overline{1, n};$$

$$\frac{\partial}{\partial t}(\rho^{0} v_i^{0}) + (\rho^{0} v_i^{0} v_j^{0})_{,\,j} = \phi_i^{0} + \rho^{0} F_i^{0} + E_{i,\,j} P_j + \sigma_{ij,\,j}^{0}, \tag{6}$$

where $\rho^{\alpha} e^{\alpha}$ is the charge density of α-th component, ϕ_i^{α} is the momentum supply, F_i^{α} is body force density acting for the α-th constituent, σ_{ij}^{α} is partial stress tensor, P_i is electric polarization per unit volume and E_i is electric field. The terms $\rho^{\alpha} e^{\alpha} E_i$ and $E_{i,j} P_j$ on the right-hand side of this equation are the volume electric force.

After summing up we obtain [6, 7]

$$\rho \dot{w}_k = \rho F_k + \sigma_{kl,\,l} + \sum_{\alpha} \rho^{\alpha} e^{\alpha} E_k + E_{k,\,j} P_j\,. \tag{7}$$

Here $\rho F_k = \sum_{\alpha} \rho^{\alpha} F_k^{\alpha}$, $\sigma_{kl} = \sum_{\alpha} \sigma_{kl}^{\alpha}$.

- Balance of energy [1, 2].

$$\rho \dot{U} = \rho r - q_{i,\,i} + \sigma_{ij} w_{i,\,j} + \sum_{\alpha=1}^{n} \rho M^{\alpha} \dot{c} - \sum_{\alpha=1}^{n} j_i^{\alpha} M_{,\,i}^{\alpha} - h_e\,. \tag{8}$$

In the above equation U is specific internal energy, q_i is the heat flux, r is the heat supply, M^{α} is chemical potential for the α-th constituent. The quantity h_e is the electric energy source [2] given by

$$h_e = \sum_{\alpha} J_i^{\alpha} E_i + \rho E_i \dot{\pi}_i\,, \tag{9}$$

where π_i is polarization per unit mass $\pi_i = P_i / \rho$.

The complete set of balances of the process closes the inequality of the entropy increase. This inequality proposed in [2, 8] is taken in the following form

$$\rho \dot{S} - \frac{q_{i,\,i}}{T} - \frac{T_{,i}}{T^2} q_i - \frac{\rho r}{T} \geq 0\,. \tag{10}$$

2. Residual inequality

Making use of the balance of energy (8) and inequality of entropy (10) we shall obtain the following residual inequality

$$\rho T \dot{S} - \rho \dot{U} + \sigma_{ij} w_{i,\,j} + \sum_{\alpha=1}^{n} \rho M^{\alpha} \dot{c}^{\alpha} - \sum_{\alpha=1}^{n} j_i^{\alpha} M_{,\,i}^{\alpha} +$$

$$+ \frac{T_{,\,i}}{T} q_i + \rho \dot{\pi}_i E_i + \sum_{\alpha=1}^{n} J_i^{\alpha} E_i \geq 0\,. \tag{11}$$

In further considerations it is convenient to make use of function

$A = U - ST - E_k P_k / \rho$.

Then residual inequality has the form

$$-\rho \dot{T} S - \rho \dot{A} + \sigma_{ij} w_{i,j} + \sum_{\alpha=1}^{n} \rho M^{\alpha} \dot{c}^{\alpha} - \sum_{\alpha=1}^{n} j_i^{\alpha} M_{,i}^{\alpha} +$$

$$+ \frac{T_{,i}}{T} q_i - P_i \dot{E}_i + \sum_{\alpha=1}^{n} J_i^{\alpha} E_i \geq 0 \qquad (12)$$

Although descriptions of the coupled flow phenomena of interest are naturally posed in current configuration, numerical solutions of governing equations are more conveniently carried out on a fixed Lagrangian reference configuration. It is, therefore necessary to define the following material tensor field [3]

$$T_{KL} = J X_{K,k} X_{L,i} \sigma_{ki}, \qquad Q_K = J X_{K,k} q_k,$$

$$\Pi_K = J X_{K,k} P_k, \qquad J_K^{\alpha} = J X_{K,k} J_k^{\alpha},$$

$$C_{KL} = x_{k,K} x_{k,L}, \qquad T_{,K} = T_{,k} x_{k,K},$$

$$E_K = E_k x_{k,K}, \qquad J = \det x_{k,K},$$

$$j_K^{\alpha} = J X_{K,k} j_k^{\alpha}, \qquad M_{,K} = M_{,k} x_{k,K}. \qquad (13)$$

The residual inequality in terms of the material field can be written as

$$-\rho_0 (\dot{A} + S\dot{T}) + \frac{1}{2} {}_E T_{KL} \dot{C}_{KL} + \frac{1}{T} Q_K T_{,K} + \sum_{\alpha=1}^{n} \rho M^{\alpha} \dot{c}^{\alpha} -$$

$$- \sum_{\alpha=1}^{n} j_K^{\alpha} M_{,K}^{\alpha} - \Pi_K \dot{E}_K + \sum_{\alpha=1} J_K^{\alpha} E_K \geq 0, \qquad (14)$$

where ${}_E T_{KL} = J X_{K,k} X_{L,l} \, {}_E \sigma_{kl}$, ${}_E \sigma_{kl} = \sigma_{kl} + P_k E_k$.

Inequality (14) is the significant importance for defining physical equations of thermo-diffusion.

3. Constitutive equations

Let us now define the process by history Λ

$$\Lambda^T = \left\{ \Theta(s), \quad E_K(s), \quad E_{KJ}(s), \quad c^{\alpha}(s) \right\}$$

$$\Theta = T - T_0, \quad c^{\alpha} = c^{\alpha} - c_0^{\alpha}.$$

Here $E_{KJ} = (C_{KL} - \delta_{KL})/2$ is the Lagrangian tensor deformation, Θ and c denotes the increment of the temperature and of the concentration, respectively.

We make the following constitutive assumptions

$$\rho A = \rho \underset{s=0}{\overset{\infty}{\mathbf{A}}} \left[\Lambda(t-s); \Lambda(t) \right] \qquad (15)$$

from which we obtain physical equations

$$
{}_{E}T_{IJ} = \mathop{\mathbf{J}_{IJ}}_{s=0}^{\infty}\left[\Lambda(t-s);\Lambda(t)\right], \qquad S = \mathop{\mathbf{G}}_{s=0}^{\infty}\left[\Lambda(t-s);\Lambda(t)\right],
$$

$$
\Pi_I = \mathop{\mathbf{D}_{Ii}}_{s=0}^{\infty}\left[\Lambda(t-s);\Lambda(t)\right], \qquad q_i = \mathop{\mathbf{Q}_i}_{s=0}^{\infty}\left[\nabla T(t-s)\right],
$$

$$
j_i^{\alpha} = \mathop{\mathbf{J}_i^{\alpha}}_{s=0}^{\infty}\left[\nabla M^{\alpha}(t-s)\right], \qquad J_i = \sum_{\alpha} e^{\alpha} j_i^{\alpha} \,. \tag{16}
$$

Then the present set of equations has the form partly close to the equations of viscoelasticity and thermodiffusion.

Changes appear, however, when defining the flux of mass. In the simplest case, the flux of ions is defined by equation

$$
J_i^{\alpha} = e^{\alpha} \mathop{\mathbf{J}_i^{\alpha}}_{s=0}^{\infty}\left(\nabla M^{\alpha}(t-s)\right) \approx -D_{ij}^{\alpha} e^{\alpha} M_{,j}^{\alpha}, \quad J_i = \sum_{\alpha} J_i^{\alpha} = -\sum_{\alpha} D_{ij}^{\alpha} e^{\alpha} M_{,j}^{\alpha}, \tag{17}
$$

or in an isotropic case

$$
J_i^{\alpha} = -D^{\alpha} e^{\alpha} M_{,i}^{\alpha}, \quad J_i = \sum_{\alpha} J_i^{\alpha} = -\sum_{\alpha} D^{\alpha} e^{\alpha} M_{,i}^{\alpha} \,. \tag{18}
$$

Confining ourselves to the linear problems, we approximate the functional ρA only by the linear and square functionals of the form [5]

$$
\begin{aligned}
\rho A = {} & \rho A_0 + \int_{-\infty}^{t} L_{KL}^{1}(t-\tau)\frac{\partial E_{KL}(\tau)}{\partial \tau} d\tau - \int_{-\infty}^{t} L^{2}(t-\tau)\frac{\partial \Theta(\tau)}{\partial \tau} d\tau + \\
& + \sum_{\alpha} \int_{-\infty}^{t} L^{3\alpha}(t-\tau)\frac{\partial c(\tau)}{\partial \tau} d\tau + \int_{-\infty}^{t} L_{I}^{4}(t-\tau)\frac{\partial E_{I}(\tau)}{\partial \tau} d\tau + \\
& + \frac{1}{2}\int_{-\infty}^{t}\int_{-\infty}^{t} G_{IJKL}(t-\tau, t-n)\frac{\partial E_{KL}(\tau)}{\partial \tau}\frac{\partial E_{KL}(\eta)}{\partial \eta} d\tau\, d\eta - \\
& - \int_{-\infty}^{t}\int_{-\infty}^{t} \Phi_{IJ}(t-\tau, t-\eta)\frac{\partial E_{IJ}(\tau)}{\partial \tau}\frac{\partial \Theta(\eta)}{\partial \eta} d\tau\, d\eta + \\
& - \sum_{\alpha}\int_{-\infty}^{t}\int_{-\infty}^{t} \psi_{IJ}^{\alpha}(t-\tau, t-\eta)\frac{\partial E_{IJ}(\tau)}{\partial \tau}\frac{\partial c^{\alpha}(\eta)}{\partial \eta} d\tau\, d\eta - \\
& - \int_{-\infty}^{t}\int_{-\infty}^{t} A_{IJK}(t-\tau, t-\eta)\frac{\partial E_{IJ}(\tau)}{\partial \tau}\frac{\partial E_{K}(\eta)}{\partial \eta} d\tau\, d\eta + \\
& - \frac{1}{2}\int_{-\infty}^{t}\int_{-\infty}^{t} m(t-\tau, t-\eta)\frac{\partial \Theta(\tau)}{\partial \tau}\frac{\partial \Theta\ (\eta)}{\partial \eta} d\tau\, d\eta -
\end{aligned}
$$

$$-\sum_{\alpha}\int_{-\infty}^{t}\int_{-\infty}^{t} l^{\alpha}(t-\tau, t-\eta)\frac{\partial\Theta\ (\tau)}{\partial\tau}\frac{\partial c^{\alpha}(\eta)}{\partial\eta}d\tau\, d\eta +$$

$$-\int_{-\infty}^{t}\int_{-\infty}^{t} R_K(t-\tau, t-\eta)\frac{\partial\Theta(\tau)}{\partial\tau}\frac{\partial E_K(\eta)}{\partial\eta}d\tau\, d\eta -$$

$$+\frac{1}{2}\sum_{\alpha}\int_{-\infty}^{t}\int_{-\infty}^{t} n^{\alpha}(t-\tau, t-\eta)\frac{\partial c^{\alpha}(\tau)}{\partial\tau}\frac{\partial c^{\alpha}(\eta)}{\partial\eta}d\tau\, d\eta +$$

$$+\sum_{\alpha}\int_{-\infty}^{t}\int_{-\infty}^{t} C_K^{\alpha}(t-\tau, t-\eta)\frac{\partial c^{\alpha}(\tau)}{\partial\tau}\frac{\partial E_K(\eta)}{\partial\eta}d\tau\, d\eta +$$

$$+\frac{1}{2}\int_{-\infty}^{t}\int_{-\infty}^{t} W_{KL}(t-\tau, t-\eta)\frac{\partial E_K(\tau)}{\partial\tau}\frac{\partial E_L(\eta)}{\partial\eta}d\tau\, d\eta + 0(\varepsilon^2)\,. \qquad (19)$$

Here $L_{IJ}^{1}(\tau)$, $L^{2}(\tau)$, $L^{3\alpha}(\tau)$, $L_{I}^{4}(\tau)$, $G_{IJKL}(\tau,\eta)$, $\Phi_{IJ}(\tau,\eta)$, $\psi_{IJ}(\tau,\eta)$, $A_{IJK}(\tau,\eta), m(\tau,\eta)$, $l^{\alpha}(\tau,\eta)$, $R_I(\tau,\eta), C_I^{\alpha}(\tau,\eta), n^{\alpha}(\tau,\eta), W_{KL}(\tau,\eta)$ are the relaxation functions, which determine physical properties of the material. These functions are continuous for $\tau \ge 0$, $\eta \ge 0$ and disappear for $\tau < 0$ and $\eta < 0$.

Let us introduce the functional (19) into the inequality (16). After transformation we obtain the following set of the constitutive equations for:

- stress tensor

$$_{E}T_{IJ}(t) = L_{IJ}^{1}(0) + \int_0^t G_{IJKL}(t-\tau,0)\dot{E}_{KL}(\tau)\,d\tau - \int_0^t \Phi_{IJ}(0,t-\tau)\dot{\Theta}(\tau)\,d\tau -$$

$$-\sum_{\alpha}\int_0^t \psi_{IJ}^{\alpha}(0,t-\tau)\dot{c}^{\alpha}(\tau)\,d\tau - \int_0^t \Lambda_{IJK}(0,t-\tau)\,\dot{E}_K(\tau)\,d\tau\,; \qquad (20)$$

- entropy

$$S(t) = L^{2}(0) + \int_0^t m(t-\tau,0)\Theta(\tau)\,d\tau + \int_0^t \Phi_{IJ}(t-\tau,0)\,\dot{E}_{IJ}(\tau)\,d\tau +$$

$$+\sum_{\alpha}\int_0^t l^{\alpha}(0,t-\tau)\,\dot{c}^{\alpha}(\tau)\,d\tau + \int_0^t R_I(0,t-\tau)\,\dot{E}_I(\tau)\,d\tau\,; \qquad (21)$$

- chemical potential

$$M^{\alpha}(t) = L^{3}(0) + \int_0^t n^{\alpha}(t-\tau,0)\dot{c}^{\alpha}(\tau)\,d\tau + \int_0^t \psi_{IJ}(t-\tau,0)\dot{E}_{IJ}(\tau)\,d\tau -$$

$$-\int_0^t l^{\alpha}(t-\tau,0)\,\dot{\Theta}(\tau)\,d\tau + \int_0^t C_I^{\alpha}(0,t-\tau)\,\dot{E}_I(\tau)\,d\tau\,; \qquad (22)$$

- electric polarization

$$\Pi_I(t) = 4\Pi L_I^4(0) + \int_0^t W_{IJ}(t-\tau,0)\dot{E}_J(\tau)\,d\tau - \int_0^t A_{IJK}(t-\tau,0)\,\dot{E}_{JK}(\tau)\,d\tau -$$

$$-\int_0^t R\ (t-\tau,0)\,\dot{\Theta}(\tau)\,d\tau + \sum_\alpha \int_0^t C^\alpha(t-\tau,0)\,\dot{c}^\alpha(\tau)\,d\tau\,. \qquad (23)$$

The suggested set of equations is the simplest description of the diffusive flows in the electric field.

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В’язкопружність і термодифузія в електричному полі

Ядвіґа Єнджейчик-Кубік

Сформульовано вихідні рівняння модельного опису електротермодифузійних процесів у n-компонентних в’язкопружних структурах за наявності зовнішнього електричного поля. Проведено аналіз отриманих визначальних співвідношень.

Вязкоупругость и термодиффузия в электрическом поле

Ядвига Єнджейчык-Кубик

Сформулированы исходные уравнения модельного описания электротермодиффузионных процессов в n-компонентных вязкоупругих структурах при наличии внешнего электрического поля. Проведен анализ полученных определяющих соотношений.

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