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Generalization of Hamilton's principle for the problem of coupled thermodiffusion

Uogólnienie zasady Hamiltona na zagadnienie termodyfuzji sprzężonej

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Abstract. Variables in time of temperature field and concentration of diffusion substance field cause deformation of the solid. There is also a reverse process, i.e., deformation of the solid causes thermal energy (and its conduction) and mass flow. The mentioned processes are coupled together and thermodiffusion deals with the study of this coupling. In the paper the problem of initial – boundary of the continuous center with moderate temperature change and moderate change in concentration of diffusion substance was considered. Such an issue can be written with conjugate differential equations, extended thermal, diffusion and the theory of elasticity equations supplemented with boundary and initial conditions. It is possible to describe such an issue by the integral form using for this purpose the above differential equations and the equation of a virtual power in the space–time domain. It has been shown in the work that the equation of a virtual power, derived from the above differential equations, actually leads to the generalized Hamilton's principle. The equation of a virtual power and Hamilton's principle in the form shown in the work cannot be expressed as a minimum of a well-defined functional. It is known, that such formulation allows the use of direct methods. It is easy to show that the elasticity, thermal conductivity and diffusion equations can be obtained from the presented variation principle.

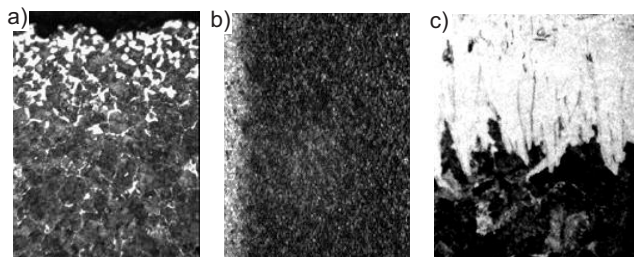
Keywords: Hamilton's principle; coupled thermodiffusion; mechanics of continuous medium; thermodynamics of irreversible processes.

Streszczenie. Zmienna w czasie temperatura i stężenie substancji dyfundującej powodują deformację ciała stałego. Istnieje również proces odwrotny, czyli odkształcenie ciała stałego powoduje wytworzenie energii cieplnej oraz przepływ masy. Wymienione procesy są ze sobą sprzężone, a badaniem tego sprzężenia zajmuje się termodyfuzja. W artykule rozpatrzono zagadnienie początkowo-brzegowe ośrodka ciągłego, geometrycznie i fizycznie liniowego, przy umiarkowanej zmianie temperatury i stężenia substancji dyfuzyjnej. Zagadnienie takie można opisać za pomocą sprzężonych równań różniczkowych, rozszerzonego równania przewodnictwa cieplnego, rozszerzonego równania dyfuzji i równań teorii sprężystości uzupełnionych o warunki brzegowe i początkowe. W artykule wykazano, że równanie czasopracy wirtualnej, wyprowadzone na bazie równań różniczkowych, prowadzi do uogólnienia zasady Hamiltona. Równania czasopracy wirtualnej i zasady Hamiltona nie da się wyrazić w postaci minimum dobrze zdefiniowanego funkcjonału. Wiadomo, że takie sformułowanie pozwala na zastosowanie metod bezpośrednich. Łatwo wykazać, że z przedstawionej zasady wariacyjnej można wyprowadzić równania sprężystości, przewodnictwa cieplnego i dyfuzji.

Słowa kluczowe: zasada Hamiltona; sprzężona termodyfuzja; mechanika ośrodków ciągłych; termodynamika procesów nieodwracalnych.

Hamilton's principle is a generalization of the principle of minimum potential energy in the case of linear dynamics [1]. This generalisation is essentially based on building a functional and then on demanding that this functional meets the required minimum conditions. However, it is possible to omit the stage of building the functional using, by analogy, the virtual power principle, also called the principle of virtual time-work [1, 2]. Moreover, the subject of extended Hamilton's principle was discussed in other papers, i.e. [3 – 7].

Thermodiffusion, as a branch of solid mechanics, includes studies on the coupling of the deformation field, the temperature and concentration of the diffusion substance. In the area of civil engineering, many phenomena in the scope of thermodiffusion can be distinguished. Practical examples include thermochemical surface treatments such as nitriding,



The progress of various thermo-chemical treatment processes; diffusion layer composed of: carbon (a); nitrogen (b); iron boride (c) obtained on a steel plate [<http://www.labmat.pw.plock.pl>]

Przebieg różnych procesów obróbki cieplno-chemicznej; warstwa dyfuzyjna złożona z: węgla (a); azotu (b); borków żelaza (c) uzyskana na płycie stalowej [<http://www.labmat.pw.plock.pl>]

carburising or boriding (see the photo below). Under elevated temperature conditions, unilateral thermodiffusion occurs, i.e. diffusion of the gas into the solid. Various types of coatings are also used for the surface treatment of metals. Then, the process of interdiffusion takes place. In both cases,

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understanding the complex transport processes allows for better surface properties of the protective layer. This enables the optimisation of the mechanical and chemical parameters of these materials, as well as the prediction of their durability.

In construction, a significant group of thermodiffusion phenomena are thermo-humidity processes, which are the domain of building physics. In the era of rationalisation of energy consumption, the flow of moisture and heat through the building envelope is one of the main design and execution concerns of civil engineers. The diffusive flow of water vapour can cause many unfavourable effects, such as biological and chemical corrosion, which significantly deteriorates the physical and mechanical properties of materials.

Knowledge of the complex processes of mass and heat flow also makes it possible to model the behaviour of structures in emergency situations such as fire, flood or nuclear failure. The response of structural elements to increasing ambient temperatures is also important when assessing their fire resistance. The fluctuating temperature range affects the physical characteristics of the material and water (or water vapour). In porous materials, the internal pore structure can undergo modifications resulting in a change in its basic properties. In the case of concrete, it is additionally subject to dehydration, which is manifested in heat bleed and free water sources.

Uncontrolled thermodiffusion can have very negative effects. An example is the behaviour of wood in an atmosphere with dynamically changing humidity. As the material dries, it shrinks, and the consequence of inhomogeneous moisture distribution within the element is the development of deformations and stresses. However, if the diffusion occurs slowly, the moisture distribution inside the element can be considered uniform and the material is free of internal drying stresses. Modelling the moisture distribution in the dried material or simulating the phenomena occurring during the drying process makes it possible to identify the drying phases in which undesirable consequences may occur.

In this paper, Hamilton's principle is generalised to the case of coupled thermodiffusion in deformable solids. It has been shown that the virtual time-work equation leads to a generalization of Hamilton's principle.

The issue of initial-boundary thermodiffusion in solids

The subject under consideration is a solid occupying area B with boundary surface ∂B . The motion was studied in the time interval $t \in < 0, \infty$). The solid in a non-deformed and strain-free conditions is at a constant temperature $T_0 = T(\mathbf{X}, 0)$ and is characterised by a constant concentration of the diffusion substance $C_0 = C(\mathbf{X}, 0)$. Under the influence of external and/or internal forces, the solid will undergo displacements $u_i(\mathbf{X}, t)$, deformations $\varepsilon_{ij}(\mathbf{X}, t)$, stress will arise $\sigma_{ij}(\mathbf{X}, t)$, and the temperature will change by $\theta(\mathbf{X}, t)$, while the diffusion substance's concentration will be altered by $c(\mathbf{X}, t)$. A continuous medium is analysed under small changes in temperature and the diffusion substance concentration.

In order to derive the equations describing the issue under consideration, the Helmholtz free energy function was developed into a in the natural state environment and then differentiated with respect to the deformations:

$$\begin{aligned} \frac{\partial F(\varepsilon_{ij}, T, C)}{\partial \varepsilon_{ij}} &= \frac{\partial F(0, T_0, C_0)}{\partial \varepsilon_{ij}} + \frac{\partial^2 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \varepsilon_{kl} + \\ &+ \frac{\partial^2 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial T} (T - T_0) + \frac{\partial^2 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial C} (C - C_0) + \\ &+ \frac{1}{2} \left[\frac{\partial^3 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial \varepsilon_{kl} \partial \varepsilon_{mn}} \varepsilon_{kl} \varepsilon_{mn} + \frac{\partial^3 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial T^2} (T - T_0)^2 + \right. \\ &+ \left. \frac{\partial^3 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial C^2} (C - C_0)^2 + 2 \frac{\partial^3 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial \varepsilon_{kl} \partial T} \varepsilon_{kl} (T - T_0) + \right. \\ &+ 2 \frac{\partial^3 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial \varepsilon_{kl} \partial C} \varepsilon_{kl} (C - C_0) + \\ &+ \left. 2 \frac{\partial^3 F(0, T_0, C_0)}{\partial \varepsilon_{ij} \partial C \partial T} (C - C_0) (T - T_0) \right] + \dots \end{aligned} \quad (1)$$

Taking into account the assumptions made in the natural state (stresses and strains equal zero) and introducing the applied symbols, the following formula is obtained:

$$\frac{\partial F(\varepsilon_{ij}, \theta, c)}{\partial \varepsilon_{ij}} = C_{ijkl} \varepsilon_{kl} - \alpha_{ij} \theta - \beta_{ij} c + \dots \quad (2)$$

Due to the assumption of infinitesimal deformations, a small relative temperature increment and a small increment in the concentration of the diffusion substance, the higher-order quantities can be omitted in expression (2), obtaining the following form of the constitutive thermodiffusion equation:

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} - \alpha_{ij} \theta - \beta_{ij} c \quad (3)$$

where:

C_{ijkl} – component of the tensor describing material parameters related to mechanical properties of the material;

α_{ij} – component of the tensor describing material parameters related to mechanical and thermal properties of the material;

β_{ij} – component of the tensor describing material parameters related to the mechanical and diffusional properties of the material.

It is worth noting that in the case of a homogeneous isotropic solid, the formula (3), after taking into account the aforementioned assumptions, will take the following form:

$$\sigma_{ij} = 2\mu \varepsilon_{ij} + (\lambda e - \gamma_T \theta - \gamma_C c) \delta_{ij} \quad (4)$$

gdzie:

μ [N/m²], λ [N/m²], γ_T [N/m²], γ_C [Nm/kg] – material constants;

δ_{ij} – Kronecker delta.

The equilibrium equations, describing the relation between stresses, mass forces, and inertia forces can be expressed as follows:

$$\sigma_{ij,i} + \rho f_j - \rho \ddot{u}_j = 0 \quad (5)$$

where:

ρ – volumetric density of the solid [kg/m³].

Using the first and second principle of thermodynamics, the entropy balance equation and Onsager's relationships for laminar thermodynamic flows, the extended thermal conductivity and diffusion equations can be derived in the following form:

$$k \theta_{,ii} - \dot{\theta}_{c,c} - T_0 (\gamma_T \dot{e} + b \dot{c}) + W = 0 \quad (6)$$

where:

k [W/mK], $c_{c,c}$ [J/Km³], γ_T [N/m²K], b [J/kgK] – material constants;

W [W/m³] – capacity of internal heat sources.

$$D_T \theta_{,ii} + D_c e_{,ii} + D_c c_{,ii} - \dot{c} + \tau = 0 \quad (7)$$

where:

D_T [kg/msK], D_c [kg/ms], D_c [m²/s] – material constants;
 τ [kg/m³·s] – capacity of internal mass sources.

These equations are complemented with initial and boundary conditions, which can be expressed in the following form:

- initial conditions:

$$\begin{aligned} u_i(\mathbf{X}, t) &= u_{0i}(\mathbf{X}, t); \\ \dot{u}_i(\mathbf{X}, t) &= \dot{u}_{0i}(\mathbf{X}, t); \\ T(\mathbf{X}, t) &= T_0(\mathbf{X}, t); \\ C(\mathbf{X}, t) &= C_0(\mathbf{X}, t); \\ (\mathbf{X}, t) &\in \mathcal{B}_0 \times \{0\}; \\ &i = 1, 2, 3 \end{aligned} \quad (8)$$

- static-type boundary conditions:

$$\begin{aligned} \hat{p}_i(\mathbf{X}, t) &= \sigma_{ji}(\mathbf{X}, t) n_j; \\ (\mathbf{X}, t) &\in \partial \mathcal{B}_p \times \langle 0, \infty \rangle; \\ &i = 1, 2, 3 \end{aligned} \quad (9)$$

- geometric-type boundary conditions:

$$\begin{aligned} u_i(\mathbf{X}, t) &= \hat{u}_i(\mathbf{X}, t); \\ (\mathbf{X}, t) &\in \partial \mathcal{B}_u \times \langle 0, \infty \rangle; \\ &i = 1, 2, 3 \end{aligned} \quad (10)$$

- thermal-type boundary conditions (i.e. condition of type II):

$$\begin{aligned} q_i(\mathbf{X}, t) &= \hat{q}_i(\mathbf{X}, t); \\ (\mathbf{X}, t) &\in \partial \mathcal{B}_{T_2} \times \langle 0, \infty \rangle; \\ &i = 1, 2, 3 \end{aligned} \quad (11)$$

- diffusion-type boundary conditions (i.e. condition of type II):

$$\begin{aligned} \eta_i(\mathbf{X}, t) &= \hat{\eta}_i(\mathbf{X}, t); \\ (\mathbf{X}, t) &\in \partial \mathcal{B}_{C_2} \times \langle 0, \infty \rangle; \\ &i = 1, 2, 3 \end{aligned} \quad (12)$$

Equations of virtual time-work

Equations (4) ÷ (7) constitute a system of coupled partial differential equations with respect to space and time variables, formulated within the framework of the theory of mechanics of continuous media and thermodynamics of irreversible processes. In order to solve the coupled thermodiffusion problem, using for example the time-space element method, a global formula is necessary covering the whole solid under consideration and the whole time interval. One way to transform the local formula into a global formula is to use the virtual time-work method, which is done by analogy with the virtual work equation [2]. Based on the equilibrium equations and the extended thermal conductivity and diffusion equation, the following integral equations were derived:

$$\int_t^t \int_B \delta u_i (\sigma_{ij,j} + \rho f_i - \rho \ddot{u}_i) dB dt = 0 \quad (13)$$

$$\int_t^t \int_B \delta g (k \theta_{,ii} - \dot{\theta} c_{e,c} - T_0 (\gamma_T \dot{e} + b \dot{c}) + W) dB dt = 0 \quad (14)$$

$$\int_t^t \int_B \delta h (D_c D_T \theta_{,ii} + D_c D_e e_{,ii} + D_c^2 c_{,ii} - D_c \dot{c} + D_c \tau = 0) dB dt = 0 \quad (15)$$

Then, the following substitutions are made in expressions (13), (14), (15):

$$\theta \stackrel{\text{def}}{=} T_0 \dot{g} \quad (16)$$

$$c \stackrel{\text{def}}{=} C_0 h \quad (17)$$

The values δu , δg , δh denote variations of the functions u , g , h . These are functions satisfying kinematic, thermal and diffusion boundary conditions and are appropriately differentiated with respect to spatial variables and time. Using the boundary conditions (9) ÷ (12), equation (4), and making appropriate transformations, the virtual time-work equations are obtained in the following form:

$$\begin{aligned} &\int_t^t \int_B \delta u_i \rho f_i dB dt - \int_B \delta u_i \rho \dot{u}_i dB|_{t_0}^{t_1} + \int_t^t \int_B \delta \dot{u}_i \rho \dot{u}_i dB dt + \\ &+ \int_t^t \int_{\partial \mathcal{B}_p} \delta u_i \hat{p}_i d(\partial \mathcal{B}_p) dt - \int_t^t \int_B \delta \varepsilon_{ij} \sigma_{ij} dB dt = 0 \end{aligned} \quad (18)$$

$$\begin{aligned} &\int_t^t \int_B \delta g W dB dt + \int_t^t \int_B \delta \dot{g} T_0 c_{e,c} \dot{g} dB dt + \int_t^t \int_B \delta \dot{g} T_0 C_0 b h dB dt + \\ &+ \int_t^t \int_B \delta \dot{g} T_0 \gamma_T e dB dt - \int_t^t \int_B \delta g_i k T_0 \dot{g}_{,i} dB dt - \int_t^t \int_{\partial \mathcal{B}_T} \delta g \hat{q}_i n_i d(\partial \mathcal{B}_T) dt \\ &- \int_B \delta g T_0 c_{e,c} \dot{g} dB|_{t_0}^{t_1} - \int_B \delta g T_0 C_0 b h dB|_{t_0}^{t_1} - \int_B \delta g T_0 \gamma_T e dB|_{t_0}^{t_1} = 0 \end{aligned} \quad (19)$$

$$\begin{aligned} &\int_t^t \int_B \delta h D_c \tau dB dt - \int_t^t \int_B \delta h_i D_c D_T T_0 \dot{g}_{,i} dB dt - \int_t^t \int_B \delta h_i D_c D_e e_{,i} dB dt - \int_t^t \int_B \delta h_i D_c^2 C_0 h_{,i} dB dt + \\ &+ \int_t^t \int_B \delta h D_c C_0 h dB dt - \int_t^t \int_{\partial \mathcal{B}_C} \delta h D_c \hat{\eta}_i n_i d(\partial \mathcal{B}_C) dt - \int_B \delta h D_c C_0 h dB|_{t_0}^{t_1} = 0 \end{aligned} \quad (20)$$

The individual integrals of equations (18) ÷ (20) denote the time-work or time-energy expressed in $\text{J} \cdot \text{s} = \text{N} \cdot \text{m} \cdot \text{s}$ [1]. Equations (18) ÷ (20) represent the principle of virtual time-work. The couplings of deformations ε_{ij} , temperature θ (described by function g), and diffusion c (described by function h) can be observed. The definition of the virtual time-work equation can be extended to the issue of coupled thermodiffusion as follows: the generalised forces (originating from external interactions in the form of surface forces, thermal and diffusion influences) distributed on the hypersurface bounding the space-time object and the internal forces (whose sources are mass forces, internal heat, and mass sources) acting in the four-dimensional region, perform on the virtual quantities δu_i , δg , δh time-work equal to the internal time-energy accumulated in the analysed region.

Generalizing Hamilton's principle

The following designations are introduced:

- to the equation (15):

$$\mathcal{T}_u = \frac{1}{2} \int_B \dot{u}_i \rho \dot{u}_i dB \quad (21)$$

$$\mathcal{V}_u = \frac{1}{2} \int_B \varepsilon_{ij} \sigma_{ij} dB \quad (22)$$

$$\mathcal{W}_u = \int_B u_i \rho f_i dB + \int_{\partial \mathcal{B}_p} u_i \hat{p}_i d(\partial \mathcal{B}_p) \quad (23)$$

■ to the equation (16):

$$\mathcal{J}_T = \frac{1}{2} \int_B \dot{g} T_0 c_{\varepsilon,c} \dot{g} dB \quad (24)$$

$$\mathcal{V}_T = \frac{1}{2} \int_B (g_i k T_0 \dot{g}_i - \dot{g} T_0 \gamma_T e - \dot{g} T_0 C_0 b h) dB \quad (25)$$

$$\mathcal{W}_T = \int_B g W dB - \int_{\partial B_T} g \hat{q}_i n_i d(\partial B_T) \quad (26)$$

■ to the equation (17):

$$\mathcal{J}_C = \frac{1}{2} \int_B \dot{h} D_C C_0 h dB \quad (27)$$

$$\mathcal{V}_C = \frac{1}{2} \int_B h_i (T_0 D_C D_T \dot{g}_i + D_C D_\varepsilon e_i + C_0 D_C^2 h_i) dB \quad (28)$$

$$\mathcal{W}_C = \int_B h D_C \tau dB - \int_{\partial B_C} h D_C \hat{\eta}_i n_i d(\partial B_C) \quad (29)$$

The equations of virtual time-work take the form:

$$\delta \chi_u = \int_t \delta (\mathcal{J}_u - \mathcal{V}_u + \frac{1}{2} \mathcal{W}_u) dt - \frac{1}{2} \int_B \delta u_i \rho \dot{u}_i d\mathcal{B} \Big|_{t_0}^{t_1} = 0 \quad (30)$$

$$\delta \chi_T = \int_t \delta (\mathcal{J}_T - \mathcal{V}_T + \frac{1}{2} \mathcal{W}_T) dt - \frac{1}{2} \int_B \delta g (T_0 c_{\varepsilon,c} \dot{g} + T_0 C_0 b h + T_0 \gamma_T e) d\mathcal{B} \Big|_{t_0}^{t_1} = 0 \quad (31)$$

$$\delta \chi_C = \int_t \delta (\mathcal{J}_C - \mathcal{V}_C + \frac{1}{2} \mathcal{W}_C) dt - \frac{1}{2} \int_B \delta h D_C C_0 h dB \Big|_{t_0}^{t_1} = 0 \quad (32)$$

where:

χ – the minimised functional, the so-called Lagrange function.

When external impulses (stress, temperature, diffusion) are conservative (i.e. independent of displacements, temperature, and the diffusion of the medium under consideration), then the time-work equations are as follows:

$$\delta \chi_u = \delta \int_t (\mathcal{J}_u - \mathcal{V}_u + \frac{1}{2} \mathcal{W}_u) dt - \frac{1}{2} \int_B \delta u_i \rho \dot{u}_i d\mathcal{B} \Big|_{t_0}^{t_1} = 0 \quad (33)$$

$$\delta \chi_T = \delta \int_t (\mathcal{J}_T - \mathcal{V}_T + \frac{1}{2} \mathcal{W}_T) dt - \frac{1}{2} \int_B \delta g (T_0 c_{\varepsilon,c} \dot{g} + T_0 C_0 b h + T_0 \gamma_T e) d\mathcal{B} \Big|_{t_0}^{t_1} = 0 \quad (34)$$

$$\delta \chi_C = \delta \int_t (\mathcal{J}_C - \mathcal{V}_C + \frac{1}{2} \mathcal{W}_C) dt - \frac{1}{2} \int_B \delta h D_C C_0 h dB \Big|_{t_0}^{t_1} = 0 \quad (35)$$

Assuming that the variations δu_i , δg , δh vanish at time t_0 (the beginning of observation) and t_1 (the end of observation, analysis), the integral of the Lagrange function can be expressed in the form:

$$\mathcal{L} = \mathcal{J} - \mathcal{V} + 1/2 \mathcal{W} \quad (36)$$

In the time interval t_0, t_1 , this expression reaches an extreme value in the case of a 'real' motion relative to the allowed virtual displacements δu_i , virtual temperature (expressed as function δg) and virtual diffusion (expressed as a function δh), vanishing firstly at times t_0 i t_1 at all points of the solid and secondly at the boundary surface ∂B_u , ∂B_T , ∂B_C , where displacements, temperature (expressed by g) and

diffusion (expressed by h) are given during the entire period $\langle t_0, t_1 \rangle$. This principle means that among all dynamic paths that satisfy the boundary conditions ∂B_u , ∂B_T , ∂B_C at each time instant t , and which start and end with the real conditions at any two times t_0 and t_1 at each solid point, the real dynamic path is distinguished from the others by the fact that the Lagrange function (36) reaches an extremum (minimum).

Conclusion

Using the analogy presented in the monographs by Fung [8], Nowacki [9, 10], Kączkowski [11] and Podhorecki [2], the Hamilton's principle was extended to include components related to diffusion and the coupling of the mechanical, thermal and diffusion fields.

The virtual time-work equations (18) ÷ (20), and thus also the Hamilton's principle (33) ÷ (35), cannot be expressed explicitly as a minimum of a well-defined functional. However, it is known that such formulas allow the use of direct methods, such as the time-space element method or any other method to solve a system of ordinary coupled differential equations. From the variation principle (18) ÷ (20) the coupled thermodiffusion equations in deformable continuous media can be obtained.

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