BIOTHERMOHYDROMECHANICS: THEORY AND APPLICATIONS

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Biosystems are open thermodynamic systems, which are in a non-equilibrium state continuously exchanging mass and energy with environment. Mass, charge, momentum, heat and entropy fluxes are produced in numerous biochemical reactions and physical interactions. The biological tissues possess viscoelastic and thermoelastic properties, exhibit active and passive movements and deformations. Mechanical and thermal properties, moisture diffusion and electric currents are strongly cross-coupled producing different phenomena in living bodies [1–3]. The biotissues and artificial composite materials manufactured for implants, prosthesis and tissue substitutes are hygroscopic and their rheological parameters are temperature and moisture dependent. Dealing with such materials the practical problems need more theoretical basis, so one has to consider the thermo-hygro-mechanical properties and processes in their cross-coupling, as well as with superposition of external mechanical and electromagnetic loads.

The total energy produced by an organism per unit mass is the metabolic rate W, which is an important indicator of thermodynamic state of the body. The metabolic rate in mammals depends on the body mass M as

$$W = 3.41M^{0.734}\ (J/s) \qquad (1)$$

where $M \sim 10^{-2} - 10^{3}$ [4] in spite of different size, shape, physiology and living conditions of the bodies and structure of their regulatory systems [5]. For birds the scaling law differs from (1) only by factor, not by power: $W = 6M^{0.734}$ J/s for Passeriformes and $W = 3.64M^{0.733}$ J/s for other birds [6]. The scaling power ~ 0.75 is found for the intracellular structures, unicellular organisms, tissues and multicellular organisms [7]. For endothermic animals the relation (1) is determined by necessity to keep a relative constant core body temperature, which provides an optimal metabolism. The animals can increase/decrease the heat production according to the corresponding decrease/increase in the environmental temperature due to their complex thermoregulatory system, which includes low and high temperature sensors, intracellular mechanisms, vascular branching systems as effective heat exchangers, morphological and behavioral mechanisms of body heating/cooling [8].

Different organisms are similar in their biochemistry; therefore, principles of energy production, transfer and exchange are common and the living bodies obey thermodynamic laws independently of their complexity, size and evolutionary age [5,7]. The core body temperature T_b is relatively constant for mammals of different body mass and bigger for the birds which also possess higher metabolic rate, and mean temperature $T_b = 40,5\ ^\circ C$ for Passeriformes and $T_b = 39,5\ ^\circ C$ for other birds [6].

Short-distance heat and mass exchange is provided by radiation, heat conduction, diffusion and active molecular and membrane transport (molecular motors). Long-distance transport in high plants and multicellular organisms is provided by special conducting systems (blood vessels and respiratory pathways in animals, xylem and phloem conducting systems in plants, trophic fluids transport systems in molluscs and others). Heat transfer and thermoregulation in living organisms is coupled with mass transfer and flow of biological liquids and gases. As open thermodynamic systems the organisms can keep the total entropy S at some constant level ($S=S_0$=const) and even decrease it ($dS<0$) during the functioning, growth and morphological development by increasing the order and producing highly structured inhomogeneities via special active energy-depended mechanisms.

Biosystems could work in a steady state condition ($dS=0$) and some approaches consider life as permanent transitions between different steady states ($S_1 \to S_2 \to S_1, S_1 \to S_3 \to S_1, S_1 \to S_4 \to S_5 \to S_1$), e.g. muscle and heart contraction as a transition from the relaxed to the contracted states and vice versa; transmission of nerve impulses as transitions between the relaxed and excited states characterized by different transmembrane electric potentials. Both relaxed and excited states are considered as steady states with different balanced entropy production S_i and exchange with environment $S_e = -S_i$. Some biological processes like tumour growth and development or apoptosis (programmed cell death) are characterized by irreversible increase in entropy and step-by-step transitions far from the steady state.

Heat and mass production in bioelectrochemical reactions, heat transmission, radiation and transfer, cell divisions, tissue growth and development are tightly connected with acquisition of the new substances (nutrition), liquid-solid and sol-gel phase transitions, delivery and distribution of the new matter via the long-distance transport systems and local tissue and cellular mechanisms (pumping, diffusion, osmosis, active membrane transport, molecular motors) [9]. In that way heat production, transfer and thermoregulation must be considered in connection with biothermohydromechanic (BTHM) processes and some important examples are observed in the paper.

Biothermodynamics (BTD) is study of energy and entropy production and transformations in living organisms. Often BTD is reduced to biochemical

thermodynamics as a study of the thermodynamic parameters of specific molecular protein–protein, protein–DNA, drug–receptor, and other interactions at molecular level. Actually BTD also includes cellular, tissue, organ levels, systems of organs (e.g. circulatory, respiratory, digestive systems), whole living bodies, collectives of organisms and ecosystems [10].

Biofluids mostly possess complex composition (multicomponent solutions, viscoelastic fluids, cellular suspensions) and undergo stress, chemical and temperature dependent phase transitions. The interconnection of concentration, temperature, electrical, magnetic, chemical effects are proper to biofluids. In that way BTHM is an interdisciplinary study enveloping physical, chemical and specific physiological processes grounding on NET. Investigation of thermomechanical and hydromechanical processes in biological systems leads to better understanding of life and elaboration novel approaches in medical diagnostics and treatment, disease prevention and rehabilitation, ergonomics and sports, biomedical engineering and advanced technologies (nanotechnologies, biomimicking, and nature–inspired solutions). In its turn, unusual properties, structure organization and function of living organisms stimulate development of new mathematical models and effective numerical methods stimulating theoretical sciences.

1. BTHM of biomolecules and molecular structures. Coupling of thermo- and hydromechanics at molecular level. The biological molecules like proteins, lipoproteins, vitamins, enzymes, RNA and DNA, phospholipids of the cell membranes, receptor molecules are large, and their conformation is important for the biochemical, electrical, adhesive and aggregation properties and abilities. Folding of the large molecules and their equilibrium shapes are described by the minimal Gibbs energy $dG=0$, $d^2G>>0$ at given constant temperature and pressure. Unfolding of the large polymer molecules by the fluid flow is important for many vital biological processes like fibrin polymerization and blood clot formation. Folding and unfolding accompanied by the conformation and entropy changes induce variations in chemical and physical properties of the molecules. Thermal stress above or below the physiological body temperatures leads to unfolding of the proteins towards the thermally unstable or denature structures [11]. Computer-assisted 3D visualization of molecular structures (Fig.4) is based on minimization of the potential energy

$$U(r_{ij}) = \sum_{\substack{\text{all nonbond} \\ \text{pairs } (ij)}} \frac{q_i q_j}{r_{ij}} + \frac{a_{ij}}{r_{ij}^{12}} - \frac{b_{ij}}{r_{ij}^{6}}$$

where $r_{ij} = r_i - r_j$, r_i, r_j are the position vectors and q_i, q_j are electric charges of the particles i and j, a_{ij}, b_{ij} are constants.

For the bound pairs the term presenting the Van der Waals forces in $U(r_{ij})$ is taken into account. The corresponding mathematical algorithms are based on iterations of the position vectors of all the atoms in the protein computed on

Newton equation with temperature-dependent term (Nosé–Hoover algorithm) [12,13]

$$m_i \frac{\partial^2 r_i}{\partial t^2} = -\frac{\partial}{\partial r_i} \sum_j U(r_{ij}) - \zeta m_i \frac{\partial r_i}{\partial t}$$

where $\frac{d\zeta}{dt} = \frac{1}{\lambda \tau}\left(T - T_0\right)$, τ and λ are relaxation time and dimension parameter.

Determination of the Van der Waals, contact and solvent accessible surfaces, position of the active centers and hydrophobic core of the structure are important for different biomedical and biotechnological applications including computer modeling of drugs, fiber and structure formation, genetic modification technologies and tissue engineering. Hydration of the surface also leads to conformational changes and variations in mechanical and electrical properties of the biomolecules. In that way in the living systems hygro- and thermal processes are coupled starting at the molecular level.

2. BTHM of molecular motors. Molecular motors like dynein, kinesin, myosin, actin, DNA and RNA polymerase, bacterial cilia and flagella consume energy, for instance, the chemical free energy released by the ATP hydrolysis, and converts it into mechanical work. They operate at the conditions when the fluctuations due to thermal noise are not insignificant [14].

Motion of amoebas is determined by the gel–sol phase transitions, contraction of the cytoskeleton and the motion of the liquid contents of the cell in certain direction forming a pseudopodium. Motion of the flagellates is supported by active deformation of the flagellum/flagella, wave propagation along each flagellum accompanied in some samples by rotation of the flagellum and body in the opposite directions. Biomolecular motors are more efficient than the man-made ones. The ratio of the wave propagation along the flagellum (U) and the cell velocity (V) for the unicellular is approximately U/V~0.2. The flagellum-type motion is very efficient and it is also used by the multicellular organisms like threadlike worms (U/V~0.4), annelid worms, leech and water snakes (U/V~0.3) and is reproduced in fishes.

Molecular motors are mechanochemical systems transforming chemical energy into mechanical work. The cyclic motion of actin and myosin bundles, sliding fibres in cilia and flagella, contraction of the cytoskeleton are examples of transformation of the chemical energy accumulated in ATP molecules into macroscopic motion and deformation. When the length L of a polymeric fibre depends on concentration of some chemicals and enzymes, pH of the solution or external electric field producing the tensile force f, the mechanical work is connected with variation of the internal energy U of the system

$$dU = TdS - pdV + fdL + \psi\, dE + \sum_j \mu_j dn_j$$

where T, S, p, V are the temperature, entropy, pressure and volume of the system, μ_j is the chemical potential of the j-th substance with concentration n_j, ψdE is electrical work.

When the work is produced by a single reactive component forming a fibre with varying length at p,T=const, the mechanochemical cycle can be described in both $\mu(n)$ and $f(L)$ variables and the efficiency of the work is

$$\theta = -\oint f dL / \oint \mu dn$$

and is quite high for the muscles, ~50% [15].

Then the Gibbs energy variation is

$$(dG)_{p,T} = fdL - Ad\xi$$

where A and ξ are affinity and extent of reaction, which gives that affinity depends on the length of the contracting fibre

$$\left(\frac{\partial f}{\partial \xi}\right)_L = -\left(\frac{\partial A}{\partial L}\right)_\xi$$

When electric field is important for the mechanochemical system, the electrochemical potential must be taken instead of μ. In experiments with contracting muscles and muscle cells the dependencies $f(L)$ and $f(v)$, where $v = dL/dt$ are preferable for measurements. The isotonic force–velocity relationship of the contracting muscle was founded by A.V. Hill

$$(P + a)(v + b) = const = (P_{max} + a)b\ ,\quad P_{max} = P\big|_{v=0}$$

where P and P_{max} are external load and maximal isometric tension. The mechanical power produced by the muscle may be obtained from in the form

$$\dot{W} = Pv = \frac{P_{max} - P}{P + a} Pb$$

The heat produced by the contracting muscle consists of the activation heat Q_a connected with Ca -dependent activation of the actomyosin system, heat of contraction Q_c: $\Delta E = W + Q_a + Q_c$. When a muscle becomes shorter, the produced energy is bigger, than for the isometric contraction (Fenn effect) [16]. Then the efficiency is determined as $\theta = W/(W + Q)$. For the contraction phase $\theta \sim 45\%$ in frogs and $\theta \sim 75\%$ in tortoises, exhibiting significant importance of the molecular mechanics of muscle contraction on thermodynamics.

Carbon and some protein nanotubes are considered as components of molecular motors of live cells and artificial devices for biomedical applications. Double layer carbon nanotubes composed by a long single-walled inner nanotube and a short outer tube demonstrated a directional motion with the temperature variation in the thermal bath [17]. A tail of carbon atoms put relaxing inside a carbon nanotube shows flagella-type motion under the variation of initial

temperature [18]. Carbon nanotubes working as guns and molecular motors exhibit the entropy production decreasing with temperature stress [19].

3. Subcellular and cellular level. The intracellular transport of the molecules, vesicles and organelles is provided by active transfer along the tubulin tubes, actin filaments and other types of fibres. It is high-order well-controlled energy-dependent transport, which thermodynamics is not fully known yet. The dynamical instability of the tubes which are in permanent assembling-disassembling state, a strong influence of the intracellular electric field and biochemical regulation are provided by interconnection of the mass, charge, heat and energy fluxes [20] The effect of temperature on cell mechanics can be elucidated by using atomic force microscopy. The complex shear modulus *G* of human alveolar epithelial cells has been measured at different temperatures (13–37 °C) and a wide frequency range (0.1–25.6 Hz). It was shown that with increasing temperature, cells become stiffer and more solid-like. Cell prestress also increases with temperature. Inhibiting actomyosin contraction attenuated the temperature dependence of *G* and prestress, which means that the dependence of cell mechanics on temperature is dominated by the contractile activity of molecular motors. Each cell contains ~10^4 chemicals and their concentrations are in periodical variations with different time periods and amplitudes. The oscillation periods serve as biological clock determining the order in the intracellular processes.

The living cells are far from an equilibrium state. The entropy production dS_i due to the irreversible processes inside the cell and the entropy exchange dS_e through the cell membrane possess time variations and fluctuations resulting in permanent variation of the total entropy production $dS=dS_i–dS_e$. Transformation of a normal cell to a tumor cell is usually accompanied by large variations in dS.

Some collective phenomena like directed motion of the cells towards some center/centers, aggregation and formation of the multicellular formations (like plasmodium) are interesting for BTHM and NET [2,9,21]. In suspensions of the moving and aggregating cells the concentric and spiral waves similar the ones in the “chemical clock” of the Belousov–Zabotinsky reaction can be observed. The unicellular algae can move towards the sunlight and form a hexagonal network on the water surface. The network covers the maximal sun-radiated surface at a given cellular mass. The light reception, energy transfer into the mechanical work, directed motion, aggregation and the network formation are interconnected via BTHM phenomena.

The motion of the cells in a water solution can be described as active diffusion in the concentration field $b(t,\vec{r})$ of the attractant. The simplest model of the concentration field C of the cells is [22]

$$\begin{aligned} \frac{\partial C}{\partial t} &= \nabla \cdot D_b \nabla b + \alpha C \\ \frac{\partial b}{\partial t} &= \nabla \cdot (D_C \nabla C - \delta \cdot b \nabla f(b)) + \beta - \gamma C b \end{aligned} \qquad (2)$$

where α is the cell birth rate, β is the source of the attractant, γ is adsorption of the attractant by the bacteria; δ is the chemotaxis rate, $\xi = \chi E_{chem}$ is kinetic energy of the bacteria movement due to accumulation of the chemical energy E_{chem}, and according to experimental studies $f(b) = b/(b_0 + b)$, $\alpha = \alpha_0 b/(b_0 + b)$. The diffusion coefficient D_b for the attractant is a temperature-dependent constant value, while cell diffusion coefficient D_C is determined by the abovementioned system parameters, fluid density ρ and viscosity μ and can be computed using the dimension analysis method in the form:

$$D_C = D_C(\gamma, b, \rho, R, \mu, \xi(T)) = \frac{\xi\gamma b}{\rho R} \cdot F\left(\frac{\xi\gamma b}{6\pi\mu\rho R}\right)$$

The equations (2) may be completed by the nonlinear terms of the cell birth and nutrition leading to the limiting cycle and stochastic solutions. Besides, some experimentally observed phenomena like cell concentration in the regions with high ∇b can be driven from (1) [22].

3. Tissue level. Biological tissues consist of the cells and extracellular matter synthesized by the cells. For instance, the bones consist of the collagen produced by the bone cells and crystals of Ca salts. The polymerized collagen fibers are organized in the 5-level extracellular structures reinforced by the calcium crystals resulting in the compact and sponge bone tissue. The cellular contents are approx 4% of the dry bone matter [22]. The extracellular matrix is organized according to the directions of maximal extension and compression of the loaded bone exhibiting the optimal mechanical properties, i.e. maximal strength and durability at total lightweight design. The principles of reinforcement in plants and animals are similar: the rigid cell walls of the plant cells, the extracellular fibers in rigid and soft tissues, the blood vessel walls and airways are reinforced according to the principals of the stress tensor. Dynamical load conditions proper to all the tissues and organs demand remodeling of the inner structures according to the varying load. The remodeling in the bones and other collagen tissues is connected with piesoelasticity of collagen and interconnection of mechanical (stress and deformation), electrical (dependence of the cell activity on the produced electric potential) and hydromechanical (mass transfer to the reconstructing tissues), providing a strong coupling of the mass, heat, charge and entropy fluxes in living biological tissues.

The tissues are usually considered within the framework of thermodynamics of multicomponent and multiphase continua [22]. The continual models of cancellous and sponge bone gave rise to the models of adaptive materials (smart materials), which properties can be controlled and changed by external stimuli (stress, electric field, temperature, moisture contents, pH and others).

The balance equations for the rigid and soft biomaterials are based on the thermodynamic laws and theory of viscoelasticity:

$$\rho\frac{\partial^2\vec{u}}{\partial t^2}=\mathrm{div}\cdot\hat{P}+\vec{f}\,,\quad \mathrm{div}\cdot\vec{u}=0\,,\quad \rho c_V\frac{\partial T}{\partial t}=-\nabla\vec{q}+\dot{Q}$$

$$\rho\frac{\partial C_{\alpha\beta}}{\partial t}=Q_{\alpha\beta}+Q^{e}_{\alpha\beta}+M_\beta\sum_\gamma I^\gamma_\alpha\nu_{\beta\gamma} \tag{3}$$

where indexes α and β relate to the number of phase and component, $\vec{u}$ is displacement vector, $\hat{P}$ is the stress tensor, $\vec{f}$ is an external force, ρ is density, C_V is the heat capacity, $\vec{q}$ is the heat flux, $\dot{Q}$ is the heat production, $C_{\alpha\beta}$ is the mass concentration, $Q_{\alpha\beta}$ and $Q^{e}_{\alpha\beta}$ are mass exchange between the phases and with environment, M_β is molecular mass, I^γ_α is velocity of the $\gamma-$th chemical reaction, $\nu_{\beta\gamma}$ is a stoichiometric coefficient.

For the contracting muscle as an active biological media two phases give a simple and effective model with an active phase $\alpha=1$ (actin and myosin fibers) and a passive one $\alpha=2$ (cell membranes, intracellular and extracellular structures, fascia, arteries and veins) [23]. The relationship between the thermodynamic fluxes and forces determines the rheological model and the coupling between the fluxes:

$$P_{ik}=-pg_{ik}+\sigma_{ik}\,,\quad q_i=-\lambda_{ik}\nabla_k T\,,$$

$$A_{iklm}\frac{\partial\sigma_{lm}}{\partial t}+\sigma_{ik}=E_{iklm}\left(\varepsilon_{lm}+B_{lmjn}\frac{\partial\sigma_{jn}}{\partial t}\right),$$

$$\dot{Q}_T=\dot{Q}_0+\dot{Q}^1_{klmn}\frac{\partial\Delta_{lm}}{\partial t}+\dot{Q}^2\mathrm{Tr}\left\{\frac{\partial\Delta_{ik}}{\partial t}\eta_{jklm}\frac{\partial\Delta_{lm}}{\partial t}\right\}, \tag{4}$$

$$Q_{1\beta}=\sum_p n^{p\beta}(\mu^{2p}-\mu^{1p})+\sum_\gamma S_{\gamma\beta}A_\gamma\,,$$

$$I_\gamma=\Lambda^\gamma_{iklm}\frac{\partial\Delta_{lm}}{\partial t}+\sum_p S_{p\beta}(\mu^{2p}-\mu^{1p})+\sum_\gamma k_{\gamma\beta}A_\gamma$$

where p is the pressure, g_{ik} is the metric, A, B_{iklm} are tensors of relaxation, E_{iklm} is elasticity tensor, σ_{ik} and ε_{lm} are stress and small strain tensors, $\Delta_{ik}=K_{iklm}\varepsilon_{lm}-M_{iklm}\sigma_{lm}$ are irreversible deformations of the active phase, M_{iklm} is compliance tensor for the active phase, η_{jklm} is the viscosity tensor.

At some simplifications the model (3)–(4) gives Hill's heat production in the contracting muscle (fourth equation in (4)). The cross-coupled phenomena in (4) describes the dependence of the mechano-chemical reactions on the irreversible strain rate $\partial\Delta_{ik}/\partial t$ and the gradient of interphase chemical potentials $\mu^{2p}-\mu^{1p}$, which is known for the muscles as dependence of the activity of the actomyosin system on the muscle contraction rate and the

concentrations of Na^+-K^+ATPase. In that way the continual macroscopic model describes the experimental data and empirical scalar dependences.

4. Organ and system levels. Different tissues form organs which functions are based on the long-distance fluid flow, mass and heat exchange which are strongly coupled. Heat transfer is mainly provided by the fluid flow systems (blood and airflows). The 2d and 3d systems designed as distributed heat and mass exchangers. The branching bronchial tree divides up to the smallest airways covered by a "carpet" of alveoli. The area of that 2d surface is ~100m2 in humans. It's an excellent example of a large exchange surfaces packed into a relatively small volume of chest. The blood circulation systems are also presented by the sets of tubes with optimal BTHM properties [24]. The structure principles of the conducting systems of animals can be used as a nature inspired engineering solutions in technical heat and mass exchangers [25].

Interconnection of the heat, mass and electric charge fluxes $\vec{J}_h, \vec{J}_m, \vec{J}_e$ at both long distance and local tissue levels are described by the thermodynamic relationships

$$\vec{J}_j = L_{jh}\vec{X}_h + L_{jm}\vec{X}_m + L_{je}\vec{X}_e$$

where $j = h, m, e$, $\vec{X}_{h,m,e}$ are the thermal, chemical and electric forces, $X_h = \nabla(T)^{-1}$, $X_m = -(T)^{-1}\nabla\mu$, $X_e = -(T)^{-1}\nabla\psi$. For the active biosystems additional forces and fluxes related to the active component can be added.

Pennes bioheat equation [26] is used for thermal stress analysis in biosystems:

$$\rho(\vec{r})c(\vec{r})\frac{\partial T(t,\vec{r})}{\partial t} = \nabla(k(\vec{r})\nabla T(\vec{r})) + \rho_B c_B W_B(t,\vec{r})(T_B(t,\vec{r}) - T(t,\vec{r})) + q(t,\vec{r})$$

where ρ and ρ_B are the tissue and blood mass density, c and c_B are the specific heat of tissue and blood, W_B is the blood perfusion rate, T_B is the supplying arterial blood temperature, k is the thermal conductivity of the tissue, q is the distribution of metabolic heat production in the tissue.

5. Collective motion. Contrary to the kinematic model (2) the dynamical models of the crowds of human beings, schools of fish, herds and flock at different external conditions are considered in NET. Mixture models are very successful for describing a collective motion of interacting individuals considered as particles with different properties (mean velocity, mass-inertia properties, activity, attraction/distraction laws). Different populations of particles can be described as continua with different temperatures and other thermodynamic properties. As a result a hydrodynamic-type system of equations have been obtained by both Boltzmann kinetic theory, momentum theory and mixture

models. Here the model is presented for one type of particles and it can be generalized by substituting the corresponding indices [21,22]:

$$\frac{\partial n}{\partial t} + \mathrm{div}(n\vec{u}) = \sigma_n$$

$$n\frac{d\vec{u}}{dt} = -\nabla(nT) - \mathrm{div}\hat{p} + n\left\langle \dot{\vec{v}} \right\rangle + \int \sigma_T(\vec{v} - \vec{u})d\vec{v}d\vec{z} \qquad (5)$$

$$n\frac{dT}{dt} = -\nabla(n\vec{\Gamma}) - 2nT\mathrm{div}\vec{u} - 2p : \nabla\vec{u} + 2n\left\langle (\vec{v} - \vec{u})\dot{\vec{v}} \right\rangle + \int \sigma_T((\vec{v} - \vec{u})^2 - T)d\vec{v}d\vec{z}$$

where n is numerical concentration, $\vec{u}$ is velocity, $\vec{v} = \langle \vec{u} \rangle$ is the mean value, σ_n is the source term, $\hat{p}$ is the stress tensor $p_{ij} = nT\delta_{ij} + n\int (v_j - u_j)(v_i - u_i)d\vec{v}d\vec{z}$

The model describes the crowd motion in a confined geometry: in the buildings, stadiums, squares, and shopping centres. The motion of crowds looks like a fluid flow around the obstacles with certain stream lines, flow separation and secondary flows.

6. Conclusions. NET approaches work very well at different scales of biological systems exhibiting deep interconnection of the BTHM processes.

7. Acknowledgements. The work is partially supported by international research grant № M423/11.

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