

Comments on the thermodynamical background to the growth and remodelling theory applied to a model of muscle fibre contraction

J. Rosenberg^{a,*}, M. Svobodová^a

^aFaculty of Applied Sciences, University of West Bohemia, Univerzitní 22, 306 14 Plzeň, Czech Republic

Received 21 September 2009; received in revised form 7 July 2010

Abstract

Muscle fibre contraction is a complex thermomechanical process. The change in muscle fibre length (isotonic contraction) and tension (isometric contraction) may be regarded as muscle fibre growth (change in length) and remodelling (change in stiffness).

In this study a general mathematical model based on the growth and remodelling theory and the theory of irreversible thermodynamics is proposed. The isometric contraction of muscle fibre is treated as an isothermal process. The relevance of chemical agents diffusion is also discussed.

© 2010 University of West Bohemia. All rights reserved.

Keywords: growth, remodelling, thermodynamics, muscle contraction

1. Introduction

A lot of papers dealing with the theory of body growth and remodelling (GRT) have been published. This study follows the approach discussed in [2]. The goal of this paper is to add physical meaning to certain variables appearing in [2], especially in the case in which the theory is applied to the modelling of muscle contraction.

The theory of irreversible thermodynamics is applied in this study, see [3, 5, 6], because growth and remodelling imply processes that are dissipative and far from equilibrium. First, three well-known thermodynamical theories, including the theory of thermodynamics of chemical reactions, are summarised. Then the GRT is formulated according to the thermodynamics of internal variables. Finally, this general formulation is specialized to a simple one-dimensional (1D) model of muscle fibre contraction, see also [9].

2. Irreversible thermodynamics – an overview

As mentioned above, attention is paid to three different theories of irreversible thermodynamics – **classical irreversible thermodynamics (CIT)**, **the theory with internal variables (IVT)**, **the extended irreversible thermodynamics (EIT)**.

*Corresponding author. Tel.: +420 377 632 325, e-mail: rosen@kme.zcu.cz.

2.1. Classical irreversible thermodynamics (CIT)

The theory is based on the local equilibrium hypothesis [3]: “*The local and instantaneous relations between thermodynamic quantities in a system out of equilibrium are the same as for a uniform system in equilibrium.*” This means that each material point is assumed as a thermodynamical system in equilibrium with state variables changing in the course of time. Exchange of mass and energy between these material points is allowed.

The validation of this hypothesis is given by *Deborah number* $De = \tau_m/\tau_M$, where τ_m is the equilibration time inside the system corresponding to the material point and according to [3] is approximately $10^{-12}s$ (namely, the time elapse between two collisions between particles at normal pressure and temperature); τ_M is the macroscopic time. If $De \ll 1$ then the local equilibrium hypothesis is appropriate.

Let the space of state variables $\mathbf{a} = [a_i(\mathbf{x}, t)]$ consist of extensive variables appearing in Gibbs’ equation, i.e., thermodynamical variables such as specific internal energy $u(\mathbf{x}, t)$, specific volume $v(\mathbf{x}, t)$, mass fraction $c_k(\mathbf{x}, t)$ of the k th component, plus the velocity field $\mathbf{v}(\mathbf{x}, t)$. \mathbf{x} is the position vector of the material point. The evolution equations have generally the form of balance equations. The superposed dot denotes time derivation.

$$\rho \dot{\mathbf{a}} = -\nabla \cdot \mathbf{J}^{\mathbf{a}} + \sigma^{\mathbf{a}}, \tag{1}$$

where $\mathbf{J}^{\mathbf{a}}$ is the flux term of the extensive variables and $\sigma^{\mathbf{a}}$ is the source term.

To obtain entropy production the right-hand side (RHS) of equation (2) is substituted by (1)

$$\dot{s} = \Gamma_i \dot{a}_i, \tag{2}$$

where $\Gamma_i(\mathbf{x}, t)$ is the conjugate intensive state variable to the extensive state variable $a_i(\mathbf{x}, t)$, s is the specific entropy, and after steps described in [5] the following relation is obtained

$$\sigma^s = J_{\alpha} X_{\alpha}, \tag{3}$$

where X_{α} are the thermodynamical forces related to the gradient of intensive variables.

The simplest relation between fluxes and forces is the linear one

$$J_{\alpha} = L_{\alpha\beta} X_{\beta}. \tag{4}$$

The number of the phenomenological coefficients $L_{\alpha\beta}$, which depend on intensive variables, can be reduced by enforcing the Curie’s law and Onsager-Casimir’s reciprocal relation, see [3].

2.2. Internal variables theory (IVT)

The theory is based on the accompanying state axiom [3]: “*To each non-equilibrium state corresponds an accompanying equilibrium state and to every irreversible process is associated an accompanying ‘reversible’ process.*”

A comprehensive introduction to IVT can be found in [3].

Let the set of the above mentioned state variables consist of specific internal energy u and other local equilibrium variables \mathbf{a} . Let it be enlarged by the set of so-called internal variables ξ “*measurable but not controllable*” corresponding to inner microprocesses for which $De > 1$.

It is assumed that the volume element n far from equilibrium is suddenly surrounded by an adiabatic rigid enclosure which forbids heat and momentum flux. Consequently, the values of u , \mathbf{a} and ξ remain unmodified, but the temperature T and the entropy s relax to the different

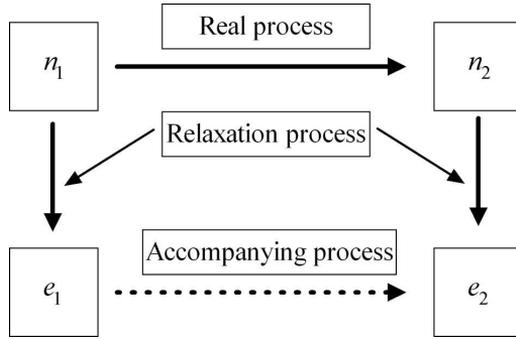


Fig. 1. Correspondence between the accompanying reversible processes and the real irreversible processes

values $T_e \neq T_n, s_e \neq s_n$, where the index e corresponds to the accompanying equilibrium state. The correspondence between processes is explained in the fig. 1.

Gibbs' equation for the accompanying entropy $s[\text{J kg}^{-1}\text{K}^{-1}]$ is used in the less general form as follows, in connection with the accompanying equilibrium state,

$$\dot{s} = T^{-1}\dot{u} - T^{-1}\rho^{-1}\mathbf{F}_e \cdot \dot{\mathbf{a}} + T^{-1}\mathcal{A} \cdot \dot{\boldsymbol{\xi}}, \quad (5)$$

where $\rho[\text{kg m}^{-3}]$ is the mass density, \mathbf{F}_e is the force conjugate to the observable \mathbf{a} and \mathcal{A} is the affinity (or configurational or Eshelby force) conjugate to $\boldsymbol{\xi}$.

The balance law (1) for the specific internal energy $u[\text{J kg}^{-1}]$ can be written in the following form

$$\rho\dot{u} = -\nabla \cdot \mathbf{q} + \mathbf{F} \cdot \dot{\mathbf{a}}, \quad (6)$$

where \mathbf{F} is the force producing work in the real space and is generally different from \mathbf{F}_e acting on the fictitious accompanying process. $\mathbf{q}[\text{Wm}^{-2}]$ is the heat flux (according to the first law of thermodynamics). The second term on the RHS is the source term including the inner production via, e.g., chemical processes and thermodynamic couplings. The additional power term - the last one - in (5) represents an internal power which in case of real irreversible evolution is dissipated inside the system. Consequently, this additional power does not appear in (6).

Substituting (6) into (5) one obtains

$$\rho\dot{s} = -\nabla \cdot (\mathbf{q}T^{-1}) + \mathbf{q} \cdot \nabla T^{-1} + T^{-1}(\mathbf{F} - \mathbf{F}_e) \cdot \dot{\mathbf{a}} + \rho T^{-1}\mathcal{A} \cdot \dot{\boldsymbol{\xi}}. \quad (7)$$

Comparing (7) to the general form (1) the second law of thermodynamics can be written as follows

$$\sigma^s = \rho\dot{s} + \nabla \cdot (T^{-1}\mathbf{q}) = \mathbf{q} \cdot \nabla T^{-1} + T^{-1}(\mathbf{F} - \mathbf{F}_e) \cdot \dot{\mathbf{a}} + \rho T^{-1}\mathcal{A} \cdot \dot{\boldsymbol{\xi}} \geq 0, \quad (8)$$

or more generally according to (3)

$$\sigma^s = J_\alpha X_\alpha + T^{-1}\rho\mathcal{A} \cdot \dot{\boldsymbol{\xi}} \geq 0. \quad (9)$$

It should be pointed out that linear expressions for fluxes (4) are not mandatory. If Helmholtz's free energy $f[\text{J kg}^{-1}]$ (10) is introduced

$$f = u - Ts, \quad (10)$$

one obtains

$$\dot{f} = -\dot{T}s + \frac{1}{\rho} \mathbf{F}_e \cdot \dot{\mathbf{a}} - \mathcal{A} \cdot \dot{\boldsymbol{\xi}}. \quad (11)$$

Then, by substituting (11) into (8), the Clausius-Duhem inequality is obtained

$$-\rho(\dot{f} + s\dot{T}) + \mathbf{F} \cdot \dot{\mathbf{a}} + T^{-1} \mathbf{q} \cdot \nabla T \geq 0 \Rightarrow \rho \dot{f} \leq -\rho s \dot{T} + \mathbf{F} \cdot \dot{\mathbf{a}} + T^{-1} \mathbf{q} \cdot \nabla T. \quad (12)$$

2.3. Extended irreversible thermodynamics

According to [4], CIT and IVT are limited to the states non far from equilibrium due to the assumption of the either local or accompanying equilibrium state existence. CIT can not be applied in situations in which the characteristic relaxation time of the involved irreversible dissipation process (e.g. chemical, mechanical, thermal or electric) is of the same order of dynamic characteristic time of interest, i.e., the *Deborah number* is close to 1. To bridge this gap, EIT introduces the notion of local nonequilibrium state. Thermodynamic fluxes are introduced in the set of state variables. These fluxes describe the interaction of a material point with its neighborhood. The entropy depends not only on the heat flux but also on these fluxes, which are regarded as controllable.

In the following, the attention is paid to IVT only for the reason of its generality and relative simplicity. Although the majority of microprocesses in muscle tissue are much quicker than mechanical deformation of tissue – *Deborah number* is much smaller than 1 – and CIT could be applied, there are certain processes (e.g. within muscle fibre contraction) for which the description in terms of IVT is useful (e.g. the description of the muscle fibre stiffness change within isometric contraction).

3. Thermodynamics of chemical reactions

This chapter shows briefly the possible application of IVT to chemical reactions systems (see e.g. [3] or [5] – a little bit more general approach according to [7] will be shown later). The other thermo-mechanical processes and the internal variables are omitted and only a single chemical reaction is taken into account.

The first law of thermodynamics has the form (compare with (6))

$$\rho \dot{u} = -\nabla \cdot \mathbf{q}. \quad (13)$$

Gibbs' equation is then (compare (5))

$$\dot{s} = T^{-1} \dot{u} - \sum_{k=1}^n \bar{\mu}_k T^{-1} \dot{c}_k, \quad (14)$$

where $c_k = m_k/m$ is the concentration (mass fraction), m_k the mass of k th component, m the total mass and $\bar{\mu}_k [\text{J kg}^{-1}]$ the chemical potential of the k th component measured per unit mass – μ_k is then per unit mol ($M_k \bar{\mu}_k = \mu_k$ where M_k is the molar mass). Because of [3]

$$\rho \dot{c}_k = \nu_k M_k \dot{Y}, \quad (15)$$

where ν_k is the stoichiometric coefficient of the k th component and $\dot{Y} [\text{mol m}^{-3} \text{s}^{-1}]$ the velocity of reaction per unit volume. Relation (14) can be rewritten in the form

$$\rho \dot{s} = T^{-1} \rho \dot{u} - \sum_{k=1}^n T^{-1} \nu_k \mu_k \dot{Y}. \quad (16)$$

Introducing the affinity of reaction \mathcal{A} [J mol⁻¹] as

$$\mathcal{A} = - \sum_{k=1}^n \nu_k \mu_k, \quad (17)$$

and using (13) the following equation is obtained for isothermal process

$$\rho \dot{s} = -\nabla \cdot (\mathbf{q}T^{-1}) + \mathcal{A}T^{-1}\dot{Y}. \quad (18)$$

This, compared with the general relation (1), gives

$$\mathbf{J}^s = \mathbf{q}T^{-1} \quad (19)$$

for the entropy flux and

$$\sigma^s = \mathcal{A}T^{-1}w > 0, \quad (20)$$

where $w = \dot{Y}$, for its production.

For coupled chemical reactions, relation (15) generalizes to

$$\rho \dot{c}_k = \sum_{j=1}^r \nu_{kj} M_k \dot{Y}_j; \quad k = 1, 2, \dots, n, \quad (21)$$

where ν_{kj} is the stoichiometric coefficient of the component k in the reaction j . Entropy production is then expressed (due to the generalization of (20)) as

$$\sigma^s = \sum_{j=1}^r \mathcal{A}_j T^{-1} w_j > 0, \quad (22)$$

where \mathcal{A}_j is the affinity of the reaction j .

Chemical reactions are often accompanied by mass transport. In this case, (22) takes the form (in an isothermal process, neglecting mechanical processes and internal variables)

$$\sigma^s = \sum_{j=1}^r \mathcal{A}_j T^{-1} w_j - \sum_{\alpha=1}^{n-1} T^{-1} \mathbf{J}_\alpha \cdot \nabla (\Delta \bar{\mu}_\alpha) \geq 0, \quad (23)$$

where $\Delta \bar{\mu}_\alpha = \bar{\mu}_\alpha - \bar{\mu}_n$, the index r represents the number of reactions, n the number of components and \mathbf{J}_α is the flux of the α th component.

If thermo-mechanical processes and internal variables are included, the main relations (5), (6), (7), (8), (11), (12) can be finally written in the following form (see e.g. [7]), by combining (23) with (5) and adding the term corresponding to mass flow,

$$\begin{aligned} T\dot{s} &= \dot{u} - \rho^{-1} \mathbf{F}_e \cdot \dot{\mathbf{a}} + \mathcal{A} \cdot \dot{\boldsymbol{\xi}} - \rho^{-1} \Delta \bar{\mu}_\alpha (-\nabla \cdot \mathbf{J}_\alpha + M_\alpha \nu_{\alpha r} \dot{Y}_r) = \\ &= \dot{u} - \rho^{-1} \mathbf{F}_e \cdot \dot{\mathbf{a}} + \mathcal{A} \cdot \dot{\boldsymbol{\xi}} + \rho^{-1} \mathcal{A}_r \dot{Y}_r + \rho^{-1} \Delta \bar{\mu}_\alpha \nabla \cdot \mathbf{J}_\alpha. \end{aligned} \quad (24)$$

The term in brackets represents the mass fraction rate of the α th constituent given by the classical diffusion equation

$$\rho \dot{c}_\alpha = -\nabla \cdot \mathbf{J}_\alpha + M_\alpha \nu_{\alpha r} \dot{Y}_r. \quad (25)$$

The Lavoisier principle $M_\alpha \nu_{\alpha r} = 0$ has been used.

Moreover, taking (6) into account, one has that

$$\rho \dot{u} = -\nabla \cdot \mathbf{q} + \mathbf{F} \cdot \dot{\mathbf{a}} + \rho r, \quad (26)$$

where r is consistent with the inner source of heat

$$\begin{aligned} \rho \dot{s} = & -\nabla \cdot (\mathbf{q}T^{-1}) + \mathbf{q} \cdot \nabla T^{-1} + T^{-1}(\mathbf{F} - \mathbf{F}_e) \cdot \dot{\mathbf{a}} + \rho T^{-1} \mathcal{A} \cdot \dot{\boldsymbol{\xi}} + \\ & + T^{-1} \mathcal{A}_r \dot{Y}_r + T^{-1} \Delta \bar{\mu} \nabla \cdot \mathbf{J} + T^{-1} \rho r \end{aligned} \quad (27)$$

and

$$\dot{f} = -\dot{T}s + \rho^{-1} \mathbf{F}_e \cdot \dot{\mathbf{a}} - \mathcal{A} \cdot \dot{\boldsymbol{\xi}} - \rho^{-1} \mathcal{A}_r \dot{Y}_r - \rho^{-1} \Delta \bar{\mu}_\alpha \nabla \cdot \mathbf{J}_\alpha. \quad (28)$$

The second law of thermodynamics (8) takes the form

$$\begin{aligned} \sigma^s = & \rho \dot{s} + \nabla \cdot (T^{-1} \mathbf{q}) - \nabla \cdot (T^{-1} \Delta \bar{\mu} \mathbf{J}) - T^{-1} \rho r = \\ = & \mathbf{q} \cdot \nabla T^{-1} + T^{-1}(\mathbf{F} - \mathbf{F}_e) \cdot \dot{\mathbf{a}} + \rho T^{-1} \mathcal{A} \cdot \dot{\boldsymbol{\xi}} + \\ & T^{-1} \mathcal{A}_{chem} \cdot \mathbf{w} - \mathbf{J} \cdot \nabla (T^{-1} \Delta \bar{\mu}) \geq 0, \end{aligned} \quad (29)$$

where $\mathcal{A}_{chem} = [\mathcal{A}_r]$; $\mathbf{w} = \dot{\mathbf{Y}} = [w_r = \dot{Y}_r]$; $\mathbf{J} = [\mathbf{J}_\alpha]$; $\bar{\mu} = [\bar{\mu}_\alpha]$, or using (10) and (26)

$$\begin{aligned} & -\rho(\dot{f} + s\dot{T}) + \mathbf{F} \cdot \dot{\mathbf{a}} - T^{-1} \nabla T \cdot \mathbf{q} + T^{-1} \nabla T \cdot (\Delta \bar{\mu} \mathbf{J}) - \nabla \cdot (\Delta \bar{\mu} \mathbf{J}) \geq 0 \Rightarrow \\ \Rightarrow & \rho \dot{f} \leq -\rho s \dot{T} + \mathbf{F} \cdot \dot{\mathbf{a}} - T^{-1} \nabla T \cdot \mathbf{q} + T^{-1} \nabla T \cdot (\Delta \bar{\mu} \mathbf{J}) - \nabla \cdot (\Delta \bar{\mu} \mathbf{J}). \end{aligned} \quad (30)$$

4. Growth and remodelling theory and thermodynamics

The starting point is an initial configuration \mathcal{B}_0 that *grows* and *remodels*, i.e. changes its volume (*growth*), form and anisotropy (*geometrical remodelling*) or material parameters (*material remodelling*). This process is represented in [2] by the tensor \mathbf{P} (*growth tensor* in the following), that relating the initial to the relaxed configuration \mathcal{B}_{rx} , is characterized by a null stress. This configuration is related to the actual configuration \mathcal{B}_t by the deformation tensor \mathbf{F} , where a nonnull stress as induced by growth, geometrical remodelling and external loading exists.

In the following, small deformations only are taken into account, without distinguishing between Lagrangian and Eulerian approach. The deformation gradient between configurations \mathcal{B}_0 and \mathcal{B}_t can be written as

$$\nabla \mathbf{p} = \mathbf{F} \mathbf{P}. \quad (31)$$

The generalized principle of virtual power has been applied in [2] to formulate basic relations. Let the velocity of continuum $\nabla \dot{\mathbf{p}}$ (\mathbf{p} is the placement – the mapping between initial and current configurations) and the velocity of growth $\dot{\mathbf{P}} \mathbf{P}^{-1}$ be considered. The set of test velocities is (\mathbf{v}, \mathbf{V}) . Limiting to small deformations, the generalized virtual power can be expressed as

$$\int_{\mathcal{B}_0} (-\boldsymbol{\tau} \cdot \nabla \mathbf{v} + \mathbf{b} \cdot \mathbf{v} + \mathbf{z} \cdot \mathbf{v} + \mathbf{C} \cdot \mathbf{V} + \mathbf{B} \cdot \mathbf{V}) dV + \int_{\partial \mathcal{B}_0} \hat{\boldsymbol{\tau}} \mathbf{n} \cdot \mathbf{v} dS = 0, \quad \forall (\mathbf{v}, \mathbf{V}), \quad (32)$$

where $\boldsymbol{\tau}$ is the Piola stress tensor, \mathbf{b} the volume force, \mathbf{z} the vector of inner effects, \mathbf{B} the inner remodelling generalized force and \mathbf{C} is the generalized external remodelling force, $\hat{\boldsymbol{\tau}} \mathbf{n}$ is stress specified on boundary and \mathbf{n} is the vector of outer normal. Based on the principle of objectivity, $\mathbf{z} = \mathbf{0}$, see [2]. Applying Green's theorem and rearranging, the following equations are obtained

$$\text{Div } \boldsymbol{\tau} + \mathbf{b} = 0 \quad \text{on } \mathcal{B}_0, \quad \mathbf{B} + \mathbf{C} = \mathbf{0} \quad \text{on } \mathcal{B}_0, \quad \hat{\boldsymbol{\tau}} \mathbf{n} = \boldsymbol{\tau} \mathbf{n} \quad \text{on } \partial \mathcal{B}_0. \quad (33)$$

Further in this study the isothermal hypothesis is kept, but allow for chemical reactions and the mass flux, adopting the IVT approach. In order to compare this approach with the previous one, the state and internal variables are renamed $\mathbf{a} = [\mathbf{F}, \mathbf{P}]$, $\boldsymbol{\xi} \approx \mathbf{K}$. The first law of thermodynamics has the form (28). The term depending on $\nabla \cdot \mathbf{J}$ is omitted.

$$\dot{f} = \boldsymbol{\tau}_e \cdot \nabla \mathbf{v} + \mathbf{C}_e \cdot \mathbf{V} - \mathbf{A} \cdot \dot{\mathbf{K}} - \rho^{-1} \mathcal{A}_{chem} \cdot \dot{\mathbf{Y}}. \quad (34)$$

It is supposed that the free energy related to the relaxed configuration f_{rx} depends only on $\mathbf{F}, \mathbf{K}, \mathbf{Y}$. In the initial configuration is then

$$f(\mathbf{F}, \mathbf{P}, \mathbf{K}, \mathbf{Y}) = J f_{rx}(\mathbf{F}, \mathbf{K}, \mathbf{Y}), \quad (35)$$

where $J = \det \mathbf{P}$. For the material derivative of the LHS of (34) the following expression can be derived, where $\mathbf{V} = \dot{\mathbf{P}} \mathbf{P}^{-1}$,

$$\dot{f} = J \left(\frac{\partial f_{rx}}{\partial \mathbf{F}} \cdot \dot{\mathbf{F}} + \frac{\partial f_{rx}}{\partial \mathbf{K}} \cdot \dot{\mathbf{K}} + \frac{\partial f_{rx}}{\partial \mathbf{Y}} \cdot \dot{\mathbf{Y}} + f_{rx} \mathbf{I} \cdot \mathbf{V} \right). \quad (36)$$

Inserting from (36) into (34), considering the velocity term $\nabla \mathbf{v} = (\dot{\mathbf{F}} + \mathbf{FV})\mathbf{P}$, see e.g. [2], and comparing the coefficients in the corresponding terms *the first set of constitutive equations* is obtained

$$\boldsymbol{\sigma}_e = J \frac{\partial f_{rx}}{\partial \mathbf{F}}; \quad \mathbf{A} = -J \frac{\partial f_{rx}}{\partial \mathbf{K}}; \quad \mathcal{A}_{chem} = -J \rho \frac{\partial f_{rx}}{\partial \mathbf{Y}}; \quad J f_{rx} \mathbf{I} = \boldsymbol{\sigma}_e \mathbf{F} + \mathbf{C}_e, \quad (37)$$

where $\boldsymbol{\sigma}_e = \boldsymbol{\tau}_e \mathbf{P}^T$ is the elastic Piola stress tensor.

The second law of thermodynamics takes the form (to be compared with (30) - the term depending on $\nabla \cdot \mathbf{J}$ is omitted)

$$\dot{f} \leq \boldsymbol{\tau} \cdot \nabla \mathbf{v} + \mathbf{C} \cdot \mathbf{V} - \rho^{-1} \mathbf{J} \cdot \nabla (\Delta \bar{\mu}), \quad (38)$$

where \mathbf{J} represents the mass flux and $\Delta \bar{\mu}$ is the difference of the chemical potentials defined above. Inserting from (36), considering $\nabla \mathbf{v} = (\dot{\mathbf{F}} + \mathbf{FV})\mathbf{P}$ the following relation is obtained

$$J \left(\frac{\partial f_{rx}}{\partial \mathbf{F}} \cdot \dot{\mathbf{F}} + \frac{\partial f_{rx}}{\partial \mathbf{K}} \cdot \dot{\mathbf{K}} + \frac{\partial f_{rx}}{\partial \mathbf{Y}} \cdot \dot{\mathbf{Y}} + f_{rx} \mathbf{I} \cdot \mathbf{V} \right) \leq \boldsymbol{\sigma} \cdot \dot{\mathbf{F}} + (\boldsymbol{\sigma} \mathbf{F} + \mathbf{C}) \cdot \mathbf{V} - \rho^{-1} \mathbf{J} \cdot \nabla (\Delta \bar{\mu}). \quad (39)$$

Using (37), then

$$(\boldsymbol{\sigma} - \boldsymbol{\sigma}_e) \cdot \dot{\mathbf{F}} + (\mathbf{C} - J f_{rx} \mathbf{I} + \boldsymbol{\sigma} \mathbf{F}) \cdot \mathbf{V} + \rho^{-1} \mathcal{A}_{chem} \cdot \dot{\mathbf{Y}} + \mathbf{A} \cdot \dot{\mathbf{K}} - \rho^{-1} \mathbf{J} \cdot \nabla (\Delta \bar{\mu}) \geq 0. \quad (40)$$

The term in brackets can be written in the form

$$(\mathbf{C} - J f_{rx} \mathbf{I} + \boldsymbol{\sigma} \mathbf{F}) = \mathbf{C} - \mathbf{E} \quad \text{where} \quad \mathbf{E} = J f_{rx} \mathbf{I} - \boldsymbol{\sigma} \mathbf{F} \quad (41)$$

and $(\boldsymbol{\sigma} - \boldsymbol{\sigma}_e) = \boldsymbol{\sigma}_{dis}$ represents the dissipative component of the stress tensor.

The second set of constitutive equations – the evolution equations, see e.g. [5], – can be obtained from (40) according to the linear phenomenological relations using the Onsager's coefficients $L_{\alpha\beta}$ (4) which should satisfy the corresponding inequalities,

$$\begin{aligned} \boldsymbol{\sigma}_{dis} &= L_{\sigma F} \dot{\mathbf{F}} + L_{\sigma E} (\mathbf{C} - \mathbf{E}) + L_{\sigma A} \mathcal{A}_{chem} + L_{\sigma A} \mathbf{A} - L_{\sigma \mu} \nabla (\Delta \bar{\mu}), \\ \mathbf{V} &= L_{VF} \dot{\mathbf{F}} + L_{VE} (\mathbf{C} - \mathbf{E}) + L_{VA} \mathcal{A}_{chem} + L_{VA} \mathbf{A} - L_{V\mu} \nabla (\Delta \bar{\mu}), \\ \dot{\mathbf{Y}} &= L_{YF} \dot{\mathbf{F}} + L_{YE} (\mathbf{C} - \mathbf{E}) + L_{YA} \mathcal{A}_{chem} + L_{YA} \mathbf{A} - L_{Y\mu} \nabla (\Delta \bar{\mu}), \\ \dot{\mathbf{K}} &= L_{KF} \dot{\mathbf{F}} + L_{KE} (\mathbf{C} - \mathbf{E}) + L_{KA} \mathcal{A}_{chem} + L_{KA} \mathbf{A} - L_{K\mu} \nabla (\Delta \bar{\mu}), \\ \mathbf{J} &= L_{JF} \dot{\mathbf{F}} + L_{JE} (\mathbf{C} - \mathbf{E}) + L_{JA} \mathcal{A}_{chem} + L_{JA} \mathbf{A} - L_{J\mu} \nabla (\Delta \bar{\mu}). \end{aligned} \quad (42)$$

In matrix form

$$\begin{bmatrix} \sigma_{dis} \\ \mathbf{V} \\ \dot{\mathbf{Y}} \\ \dot{\mathbf{K}} \\ \mathbf{J} \end{bmatrix} = \mathbf{L} \begin{bmatrix} \dot{\mathbf{F}} \\ (\mathbf{C} - \mathbf{E}) \\ \mathcal{A}_{chem} \\ \mathbf{A} \\ -\nabla(\Delta\bar{\mu}) \end{bmatrix}. \quad (43)$$

Clearly, not all coefficients are non-zero in the certain case. They need to satisfy the following conditions

$$L_{ii} \geq 0; \quad L_{ii}L_{jj} \geq \frac{1}{4}(L_{ij} + L_{ji})^2; \quad i, j = 1, 2, \dots, 5. \quad (44)$$

They can have different tensor character and should satisfy Curie's conditions and Onsager's reciprocal relations. For example, Fick's law, which obtains when $L_{JF} = L_{JE} = L_{JA} = L_{JA} = 0$.

In general, if the matrix \mathbf{L} is diagonal, then the system is fully uncoupled. In that case the first row represents the usual relation for the dissipative tensor, the second one corresponds to the stress controlled growth according to [2], the third one allows to satisfy (20), the relation in the fourth row was used e.g. in [9] and finally the fifth row is the mentioned Fick's law.

5. Growth and remodelling theory applied to muscle fibre excitation

During muscle fibre stimulation, its inner structure and consequently either its force (in *isometric stimulation*) or its length (in *isotonic stimulation*) changes. Muscle contraction can be considered as a sort of growth or/and remodelling process. Let be assumed that the whole process is isothermal and isometric and not fully coupled. While these assumptions are not necessarily warranted, they are used to make the model as simplest as possible. However, the discussed approach could allow for more complex models.

As a result of (37), f_{rx} has to contain the term $\mathcal{A}_{chem}Y$. The source of energy for the muscle fibre contraction is the hydrolysis of adenosin triphosphate (*ATP*). In this process, *ATP* transforms into adenosin diphosphate (*ADP*) and diphosphate groups P_i . For a detailed description of this complex process, see, e.g., [3]. Here *ATP* hydrolysis only is taken into account. According to [1], the chemical potential (the change in partial free energy per mole) is given by

$$\mathcal{A}_{chem} = -30558 + RT \ln \frac{[ADP][P_i]}{[ATP]}, \quad (45)$$

where $[..]$ means the concentration of the corresponding chemical component. R represents the gas constant and T is the absolute temperature.

5.1. 1D model of muscle fibre without coupling

Firstly, the couplings is not taken into account – in the matrix \mathbf{L} (42) diagonal terms only are non-zero and positive. The diffusion is also neglected – $L_{J\mu} = 0$.

Let the muscle fibre be modelled as a 1D continuum of the initial length l_0 . Its actual length after growth, remodelling and loading let be l , where for the isometric process $\dot{l} = 0$. The relaxed length - after growth and remodelling – is then l_{rx} . For the corresponding deformation gradients $\mathbf{P} = \gamma \mathbf{e} \otimes \mathbf{e}$, $\mathbf{F} = \varphi \mathbf{e} \otimes \mathbf{e}$, $\nabla p = \varepsilon \mathbf{e} \otimes \mathbf{e}$, where \mathbf{e} is the unit vector in the muscle fibre direction, the following relations can be written

$$\gamma = \frac{l_{rx}}{l_0}, \quad \varphi = \frac{l}{l_{rx}}, \quad \varepsilon = \frac{l}{l_0}. \quad (46)$$

For small deformations ($J = 1$), free energy has the simple form

$$f = f_{rx} = \frac{1}{2}k(\varphi - 1)^2 + \rho^{-1}\mathcal{A}_{chem}Y. \quad (47)$$

Another form of the free energy for living tissues is following

$$f = \frac{k}{\lambda} \left(e^{\frac{\lambda}{2}(\varphi-1)^2} - 1 \right) + \rho^{-1}\mathcal{A}_{chem}Y, \quad (48)$$

where for $\lambda \rightarrow 0$ the same result as in (47) is obtained. The equations (37), (42) have then the form

$$\sigma_e = \frac{\partial f}{\partial \varphi}, \quad (49)$$

$$\sigma_{dis} = h\dot{\varphi}, \quad (50)$$

$$C - E = g\dot{\gamma}\gamma^{-1}, \quad E = f - \varphi\sigma, \quad (51)$$

$$\dot{Y} = L\mathcal{A}_{chem}, \quad (52)$$

$$\dot{k} = -\frac{1}{m} \frac{\partial f}{\partial k}, \quad (53)$$

further in this study the new simpler notation of the Onsager's coefficients is introduced as follows $h \equiv L_{\sigma F}$, $g \equiv L_{VE}^{-1}$, $L \equiv L_{YA}$, $m \equiv L_{KA}^{-1}$ and $k \sim \mathbf{K}$ represents the stiffness as an internal variable. Equations (51), (52), (53) have the form

$$\dot{l}_{rx} = l_{rx}^3 \frac{(C - \rho^{-1}\mathcal{A}_{chem}Y) + \frac{k}{\lambda} e^{\frac{\lambda}{2}(\frac{l}{l_{rx}}-1)^2} [\lambda \frac{l}{l_{rx}} (\frac{l}{l_{rx}} - 1) - 1] + \frac{k}{\lambda}}{gl_{rx}^2 + hl^2}, \quad (54)$$

$$\dot{k} = -\frac{1}{m} \left[\frac{1}{\lambda} \left(e^{\frac{\lambda}{2}(\frac{l}{l_{rx}}-1)^2} - 1 \right) \right], \quad (55)$$

$$\dot{Y} = L\mathcal{A}_{chem}. \quad (56)$$

If the dimensionless variables are introduced

$$y = k\sqrt{\frac{|m|}{g}}; \quad x \equiv \varphi = \frac{l}{l_{rx}}; \quad \tilde{t} = \frac{t}{\sqrt{g|m|}}, \quad \tilde{C} = (C - \rho^{-1}\mathcal{A}_{chem}Y)\sqrt{\frac{|m|}{g}}, \quad (57)$$

then for $h = 0$ the following system of equations defining the nonlinear dynamical system is obtained

$$\frac{dx}{d\tilde{t}} = x' = -x \left\{ \tilde{C} + \frac{y}{\lambda} e^{\frac{\lambda}{2}(x-1)^2} [\lambda x(x-1) - 1] + \frac{y}{\lambda} \right\}, \quad (58)$$

$$\frac{dy}{d\tilde{t}} = y' = \text{sgn}(m) \left[-\frac{1}{\lambda} (e^{\frac{\lambda}{2}(x-1)^2} - 1) \right]. \quad (59)$$

Equation (56) is omitted. It is assumed that $\tilde{C}(\tilde{t})$ is a general function of the dimensionless time. In [8] it is shown that the system (58), (59) is unstable even if $h \neq 0$. Therefore it is needed to admit some sort of coupling.

5.2. 1D model of muscle fibre with coupling

Relations (42) offer a lot of possibilities even if Onsager's and Curie's constraints are respected. One of the simpler possibilities is to assume that the diffusion processes affect the change of k . After introducing the notations

$$-L_{K\mu} \nabla(\Delta \bar{\mu}) = r_\mu, \tilde{r}_\mu = r_\mu m, \quad (60)$$

the second equation defining the discussed dynamical system is obtained in the form

$$y' = \text{sgn}(m) \left[\tilde{r}_\mu - \frac{1}{\lambda} (e^{\frac{\lambda}{2}(x-1)^2} - 1) \right]. \quad (61)$$

This system is stable, as proved in [8], and exhibits interesting properties. It can also be tuned so as to simulate successfully the behaviour of muscle fibres during isometric stimulation.

6. Conclusion

This study shows how different processes running in muscle tissue can be included in the theory of growth and remodelling [2]. The equations (42) allow to take into account chemical processes, mass transport and changes of internal variables, which correspond to the processes on the micro scale.

It was shown that

- * the outer remodelling force C may represent running chemical processes in the case of muscle contraction. In other applications, it can have different meaning, which can be clarified using the mentioned approach.
- * the quantity r_μ used in [9] and shown to be necessary for the stability of the system, can result from diffusion processes running within the tissue.
- * taking into account more couplings (42), very complex models allowing to describe more precisely the behaviour of materials can be obtained.

The approach of this study is general enough to be applied to other types of continua, e.g., to different smart materials. This represents a challenge for future research, together with the analysis of the properties of the corresponding dynamical systems, such as their stability, attractors, bifurcations et cetera.

List of symbols

u	internal energy [J kg^{-1}]
$\boldsymbol{\xi}, \mathbf{K}, \rightarrow k$	internal variables
$\mathbf{a} = [a_i(\mathbf{x}, t)]$	space of state variables
s	entropy [$\text{J kg}^{-1}\text{K}^{-1}$]
T	absolute temperature [K]
ρ	density [kg m^{-3}]
\mathbf{q}	heat flux [W m^{-2}]
\mathbf{F}, \mathbf{F}_e	forces conjugated to \mathbf{a}
$\mathbf{F}, \rightarrow \varphi$	deformation gradient in GRT [2]
$\mathcal{A}, \rightarrow \mathbf{A}$	affinity conjugate to $\boldsymbol{\xi}$ (in GRT to \mathbf{K})
\mathbf{J}, J_k	mass flux [$\text{kg m}^{-2}\text{s}^{-1}$]
$\mathbf{w} = \dot{\mathbf{Y}}, w_r$	velocity of the r th reaction [$\text{mol m}^{-3}\text{s}^{-1}$]
f, f_{rx}	Helmholtz's free energy [J kg^{-1}]
σ^s	rate of the internal entropy [$\text{J K}^{-1}\text{s}^{-1}\text{m}^{-3}$]
$\bar{\mu}_k, \mu_k$	chemical potential of the k th component [J kg^{-1}], [J mol^{-1}]
M_k	molar mass [kg mol^{-1}]
ν_k, ν_{kr}	stoichiometric coefficients [3]
c_k	concentration [3]
$\mathcal{A}, \mathcal{A}_r$	affinity of the r th reaction [J mol^{-1}]
$\mathcal{A}_{chem} = [\mathcal{A}_r]$	
$\mathbf{E}, \rightarrow E$	Eshelby type tensor [J kg^{-1}]
$\mathbf{p}, \nabla \mathbf{p}, \rightarrow \varepsilon$	placement
\mathbf{v}, \mathbf{V}	continuum velocity, growth and remodelling velocity resp.
$\mathbf{P}, \rightarrow \gamma$	growth and remodelling tensor
$\boldsymbol{\sigma}, \boldsymbol{\sigma}_e, \boldsymbol{\sigma}_{dis}$	Piola stress tensor [J kg^{-1}]
$\mathbf{C}, \rightarrow \mathbf{C}$	outer remodelling couple
r	inner source of heat [$\text{J kg}^{-1}\text{s}^{-1}$]

Acknowledgements

The work has been supported by the research project MSM 4977751303.

The authors would like to thank the reviewers for their challenging suggestions related to the paper subject.

References

- [1] Crofts, A., Biological energy conversion, Course held on University of Illinois at Urbana-Champaign, 1996.
- [2] DiCarlo, A., Quiligotti, S., Growth and balance, *Mechanics Research Communications* 29 (2002) 449–456.
- [3] Lebon, G., Jou, J., Vazquez-Casas, J., Understanding non-equilibrium thermodynamics, Springer-Verlag Berlin Heidelberg, 2008.
- [4] Lu, X., Hanagud, S. V., A nonequilibrium irreversible thermodynamics model for material damping, *International Journal of Solids and Structures* 44 (10) (2007) 3 278–3 303.
- [5] Maršík, F., Dvořák, I., *Biothermodynamika*, Academia, Praha, 1998.

- [6] Maugin, G. A., The thermodynamics of nonlinear irreversible behaviors – An introduction, World Scientific Publishing, Singapore, 1999.
- [7] Rambert, G., Jugla, G., Grandidier, J., Cangemi, L., A modelling of the direct couplings between heat transfer, mass transport, chemical reactions and mechanical behaviour. *Composites Part A: Applied Science and Manufacturing*, 37 (4) (2006) 571–584.
- [8] Rosenberg, J., Hynčák, L., Growing and remodelling material as a dynamical system, *Applied and Computational Mechanics* 1 (2007) 621–630.
- [9] Rosenberg, J., Hynčák, L., Modelling of the influence of the stiffness evolution on the behaviour of the muscle fibre, In: *Human Biomechanics 2008, International Conference, Praha, Czech Republic*, 2008.