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MATHEMATICAL PHYSICS

On the phenomenological modelling of physical phenomena

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Abstract. Mathematical modelling of physical phenomena is based on the laws of physics, but for complicated processes, phenomenological models could enhance the descriptive and prescriptive power of the analysis. This paper describes some hybrid models, where in addition to the physics-driven part, some phenomenological variables (based on observations) are added. The internal variables widely used in continuum mechanics for modelling dissipative processes and the phenomenological variables used in modelling neural impulses are described and compared. The appendices describe two models of neural impulses and test problems for two classical cases: the wave equation and the diffusion equation. These test problems demonstrate the usage of phenomenological variables for describing dissipation as well as amplification.

Keywords: science-driven models, internal variables, phenomenological variables, hybrid models, mathematical modelling.

1. INTRODUCTION

Mathematical modelling is an excellent tool for describing phenomena in the real world. The famous saying 'Mathematics is the language in which God has written the Universe' is attributed to Galileo Galilei. Leaving aside the physical history of the universe, the laws of nature are described mathematically and form the cornerstones of mathematical modelling. In the philosophy of science, such models are usually called either science-driven [1] or theoretical [2]. In many cases, however, these models represent highly idealized cases that may even lead to the question of their applicability [3]. It is stressed that one should always know the conditions under which these models are derived (*ceteris paribus* – other things being equal). To better reflect reality, models derived from physical laws (first principles) are usually modified by introducing additional hypotheses and combining several phenomena (cf. Cartwright [3]). For understanding wave motion, for example, the models are derived from the conservation of momentum (Newton's second law), and the wave equation is one of the basic equations of mathematical physics. It is directly applicable to the modelling of dynamical processes in elastic lossless media, but difficulties appear when one has to account for viscoelastic, thermoelastic, plastic, etc. effects or the influence of the microstructure of a material to processes in macroscale. The governing equations are then modified (see, for example, [4]) based on physical mechanisms. This is a developing field of modelling due to practical implications.

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It is not always possible to understand the essence of physical mechanisms, especially when several of them are coupled. Nevertheless, observations (experiments) help to understand many aspects of processes under investigation, which permit to describe empirical relationships between the phenomena. In this case, a model is based on phenomenology rather than on physical theory. Portides [1] explains that such a model compensates for the lack of knowledge 'of how exactly and to what extent each part of a system contributes to the latter's investigated behaviour'. In other words, most of the system is too complex for a straightforward application of fundamental laws, which are typically composed for an idealized model system, and phenomenological models are used to describe the relationships between the variables of the model within the measured values.

In the philosophy of science, phenomenological ideas are based on the studies of Edmund Husserl (1859–1938). Leaving aside his criticism towards science as an objective theory, his idea of focusing attention on phenomena rather than explanations has helped us to understand the world [5]. However, as we demonstrate in Section 3, the description of the physical basis of the phenomenology under study helps the choice of phenomenological variables and their dynamical models.

In what follows, we shall explain some phenomenological models combining the knowledge from two fields: continuum mechanics and neuroscience. Although the terminology is different (internal variables and phenomenological variables, respectively), the ideology of modelling is similar. Our analysis supports the ideas of Morrison [2] that the most effective models 'have a rather hybrid nature' – neither purely theoretical (science-driven) nor phenomenological. The main criterion for such a model is its applicability, i.e. how the derived model meets the world. Suárez [6] prefers to use the concept of 'mediating models'. He says: 'Mediating models always stand between theory and the physical world.' History is actually full of discussions on modelling [7]. The variations of models are certainly larger than mentioned above, and the reader is referred to the overview by Frigg and Hartmann [8] for an expanded list of models. Our analysis is based on our studies of physical and hybrid models [4,9]. In Section 2, the concept of internal variables in continuum mechanics is described. Further, Sections 3 and 4 are devoted to the modelling of processes in nerves. Section 3 describes the ideas of Hodgkin and Huxley [10] on modelling the propagation of an action potential (AP) in a single axon. In Section 4, the idea of using internal variables for modelling temperature changes accompanying the propagation of an AP is analysed. The discussion and conclusions are presented in Section 5. Solutions to a model problem presented in the appendices helps to understand the role of phenomenological models describing processes in dissipative and active media.

2. INTERNAL VARIABLES IN CONTINUUM MECHANICS

The concept of internal variables has turned out to be extremely useful in describing the complex behaviour of many physical phenomena in the framework of irreversible thermodynamics. The idea of using internal (sometimes called hidden) variables is traced back to the studies of P. Duhem, P. Bridgman, and J. Kestin, as well as to an early paper of Coleman and Gurtin [11]. The contemporary description of internal variables was advocated by Gérard Maugin [12,13]. The crucial point is to distinguish between observable (e.g. strain and temperature) and internal (hidden) variables. Maugin [13] says that internal variables 'are supposed to account in a more or less crude way for the complex internal microscopic processes that occur in the material and manifest themselves at a macroscopic scale in the form of dissipation'. According to Duhem (see [13]), internal variables in this framework have no inertia and are governed by evolution equations of the first order in time. In a simple case, following Maugin and Muschik [14,15], the general scheme of modelling a stress state includes observable variables χ and internal variables α. Then the law of (mechanical) state for stress σ can be written as

$$\sigma = \sigma(\chi, \alpha) \tag{1}$$

and the internal variable α is governed by an evolution law

$$\dot{\alpha} = f(\chi, \alpha) + g(\chi, \alpha)\dot{\chi}, \tag{2}$$

where $f(\chi,\alpha)$ and $g(\chi,\alpha)$ are certain functions, and the dot denotes time derivative.

Several questions arise when applying the notion of internal variables. The first question is related to the nature and choice of internal variables, which may be scalars, vectors or tensors. As mentioned by Maugin [12], it ‘is a matter of decision at the outset from the scientist’. Indeed, there are many possibilities depending on the phenomena under investigation [13]. The second and extremely important question is related to the construction of the evolution law (2). It is proposed to use the Clausius–Duhem dissipation potential $\mathscr{D}$ and derive then (2) from the dissipation inequality [12]. This means that the basis for modelling is related to thermodynamics ‘being of a pure dissipative nature’ [13]. In other words, the second law of thermodynamics is used that guarantees the thermodynamic compatibility. It is, however, demonstrated that, by including inertial effects in the dissipation inequality, it is possible to distinguish between dissipative and inertial effects [12]. This is dependent on the scales of the process, most often on the time scales related to observable and internal variables.

The theory of internal variables has been effectively used for the analysis of viscosity, viscoplasticity, damage, semi-conduction, superconductivity, ferrofluidicity, nematic liquid crystals, etc. [14,15]. Although the basic theory of internal variables in continuum mechanics is well elaborated, there are many mathematical-physical problems that require further attention. For example, in dynamics, the conservation of momentum is the basis for deriving mathematical models [4,16]. The governing equations for observable variables are then wave equations (of the hyperbolic type), but internal variables are governed by the parabolic type of evolution laws. Such mixed hyperbolic-parabolic systems need special attention to be solved.

In philosophical terms, the internal variables are phenomenological. A good example is damage mechanics [14,15], where a scalar internal variable α is introduced. The case $\alpha = 0$ corresponds to the initial state (no microcracks), and the case $\alpha = 1$ means fracture. The evolution law for α in the case of ductile damage is related to the dynamics of plasticity parameters.

In principle, the number of internal variables depends on the process. Berezovski et al. [17] have proposed a concept of dual internal variables for describing the behaviour of microstructured materials. In their model, the variations of deformation and temperature due to the microstructure are taken as internal variables, which influence the process at the macroscale. Such processes are analysed in detail by Berezovski and Ván [18] (see also [4]). An example of deriving an evolution equation for the internal variable, starting from the second law of thermodynamics, is presented in Appendix A.

To sum up, in continuum mechanics internal variables are widely used. The corresponding models include the fundamental laws (first principles) together with the evolution laws for internal variables. In other words, a science-driven model is combined with additional assumptions or observations to form a hybrid model to better capture observable reality.

3. PROPAGATION OF AN ACTION POTENTIAL

In electrophysiology, the celebrated Hodgkin–Huxley (HH) model describes the propagation of an action potential in a single axon [10]. This is an excellent example of using phenomenological variables, and we describe the modelling idea in more detail than the usage of internal variables in continuum mechanics (Section 2).

An axon can be modelled as a tube in a certain environment (extracellular fluid). The wall of the tube is composed of amphiphilic phospholipids (a biomembrane), and inside the tube is the axoplasmic fluid, shortly axoplasm. Since the concentrations of ions (mostly Na^+ and K^+) in the extracellular fluid and axoplasm are different, there is a net voltage difference between the inside and outside of a cell. Equilibrium potentials for each type of ion are calculated from the Nernst equation (see Appendix B). The axon wall contains ion channels through which several types of ions can pass from the inside to the environment and vice versa. The ion currents, i.e. the flow through these channels, regulate the shape of the propagating AP. Hodgkin and Huxley [10] measured the AP and proposed a mathematical model that describes how the AP is evolving in time in a giant axon of the giant squid.

AP is an electrical signal propagating along the axon and governed by a cable equation, where inductance is neglected but the membrane current I as a driving component has been added. This current has according to the HH model four components: capacitive current I_C, ion currents of potassium I_K and sodium I_{Na}, and a leakage current I_l (consisting mainly of Cl^- ions):

$$I = C_M \frac{\mathrm{d}V}{\mathrm{d}t} + I_{Na} + I_K + I_l, \tag{3}$$

where C_M is the membrane capacity, V is the displacement of the membrane potential from its resting value and t is time. It means that only two ion currents are specified as sodium and potassium ions, and all the other possible currents are denoted as leakage. Following the experiments, Hodgkin and Huxley understood that a fast inward current was carried by Na^+ ions, and a more slowly activated outward current was carried by K^+ ions. The ingenious proposal by Hodgkin and Huxley [10] was to introduce phenomenological variables n, m and h related to I_K and I_{Na}. It is extremely interesting and educational to follow the formation of their idea (see also remarks by Raman and Ferster [19]).

For the potassium conductance g_K, it was proposed:

$$g_K = n^4 \bar{g}_K, \tag{4}$$

$$\frac{\mathrm{d}n}{\mathrm{d}t} = \alpha_n(1-n) - \beta_n n, \tag{5}$$

where $\bar{g}_K$ is a constant and 'n is a dimensionless variable that can vary between 0 and 1' [10].

The explanation of why these assumptions were made is worth repeating here because they demonstrate clearly what such a choice means. Hodgkin and Huxley explain [10]: 'These equations may be given a physical basis if we assume that potassium ions can only cross the membrane when four similar particles occupy a certain region of the membrane. n represents the proportion of the particles in a certain position (for example at the inside of the membrane) and $1-n$ represents the proportion that are somewhere else (for example at the outside of the membrane). α_n determines the rate of transfer from outside to inside, while β_n determines the transfer in the opposite direction.'

The description of sodium conductance needs activation and inactivation to be taken into account. It was proposed:

$$g_{Na} = m^3 h \bar{g}_{Na}, \tag{6}$$

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \alpha_m(1-m) - \beta_m m, \tag{7}$$

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \alpha_h(1-h) - \beta_h h, \tag{8}$$

where $\bar{g}_{Na}$ is a constant and α_m, β_m, α_h, β_h are the rate constants.

Here Hodgkin and Huxley [10] chose two variables m and h because 'it was simpler to apply to the experimental results' (rather than choosing one variable but governed by a second-order equation). Again, an explanation for these assumptions [10] is the following: 'These equations may be given a physical basis if sodium conductance is assumed proportional to the number of sites on the inside of the membrane which are occupied simultaneously by three activating molecules but are not blocked by an inactivating molecule. m then represents the proportion of activating molecules on the inside and $1-m$ the proportion on the outside; h is the proportion of inactivating molecules on the outside and $1-h$ the proportion on the inside.'

The HH model is an excellent example of using observation for phenomenological description. Attention must be paid to the idea that the phenomenological variables are included in a combination (n^4 and m^3h) that is directly related to the assumptions based on the physical phenomena, as the quotations above demonstrate.

The next step in the modelling was to determine the rate constants in Eqs (5), (7) and (8). This was done by a careful fitting of theoretical curves to the experiments [10]. Note that the expressions for rate constants correspond to the experiment of a giant axon of a squid at a fixed temperature (in the HH experiment, 6.3° C). The full HH model is presented in Appendix B.

Every phenomenological model raises questions about its applicability. The ionic hypothesis (referred to as conductance-based modelling) proposed by Hodgkin and Huxley [10] has turned out to be widely applicable. Although clearly justified and based on observations, the number of parameters in the HH model is high. It is quite natural that one might think about reducing the number of parameters. In this context, a simplified model known as the FitzHugh–Nagumo (FHN) model must be mentioned [20], which includes only one abstracted ionic (recovery) current. In the original notation, it reads:

$$h\frac{\partial^2 u}{\partial s^2} = \frac{1}{c}\frac{\partial u}{\partial t} - w - \left(u - \frac{u^3}{3}\right), \tag{9}$$

$$c\frac{\partial w}{\partial t} + bw = a - u, \tag{10}$$

where s is the distance along the axon, u is the voltage, and w is the recovery current. Constants h, c, b, a are positive. Compared with the HH model, variable w corresponds to h and n, while m is embedded in the nonlinearities of Eq. (9). Although the coefficients are not specified for the concrete nerve, the FHN model can describe the characteristics of the AP, such as the existence of a threshold, the asymmetric shape of the AP, the overshoot and the existence of the refraction length.

Contemporary experiments have revealed many structural complexities and the molecular specifics of ion channels [21]. It is a real challenge to include more details in the modelling to enhance the predictive power of modelling, while keeping the models simple enough to be practical.

Connor and Stevens [22] have proposed a model similar to the HH model, but specifying different inward I_I and outward I_K, I_A ion currents. In their study, all currents were described by two phenomenological variables, which may include activation and inactivation terms. Morris and Lecar [23] have included Ca^{2+} ions in their model and proposed the corresponding rate equations. Deng [24] has proposed a model where n^4 and m^3h of the HH model were replaced simply by the influence of n, m and h. Actually, all these studies demonstrate the special character of phenomenological modelling: the choice of phenomenological variables depends on the researcher. Hodgkin and Huxley [10] noted: ‘ ... our equations are anything more than an empirical description of the time-course of the changes in permeability to sodium and potassium. An equally satisfactory description of the voltage clamp data could no doubt have been achieved with equations of very different form...’. The freedom of choice by a researcher was also stressed by Maugin [12] in the case of internal variables used in continuum mechanics.

4. HEAT PRODUCTION IN AXONS

It has been demonstrated in several experiments that the propagation of an AP in an axon is accompanied by the generation and absorption of heat and temperature changes [25–27]. These processes are complicated and need attention not only because of the temperature changes (which are small) but mostly to understand the general energy balance in nerves. The possible mechanisms of heat production can be explained by Joule heating (energy transfer from the electrical current to thermal effects) and also by energy transfer from mechanical waves in the biomembrane and axoplasm into the temperature increase. In addition, Abbott et al. [25] proposed that ‘... the positive heat is due to exothermic chemical reactions ... and the negative heat to endothermic reactions’. It is clear that a combination of these mechanisms is possible. While the interaction of electric-thermal and mechanical-thermal effects is understood, the chemical-thermal interaction in nerves, in the context of nerve pulse propagation, has been more or less a hypothesis by Abbott et al. [25]. Recently, a phenomenological model of this phenomenon has been proposed by Tamm et al. [28] by using the concept of internal variables.

The temperature change in an axon is governed by the Fourier law, and the basic heat equation can be used with a driving force:

$$\Theta_T = \alpha\Theta_{XX} + F(Z, J, P, U), \tag{11}$$

where Θ is the temperature, α is the thermal diffusivity, F is a driving force, Z is the potential (AP), J is the combined ion current, P is the pressure in the axoplasm and U is the longitudinal density change in the biomembrane, while X and T are dimensionless space and time, respectively. Indices X and T denote differentiation.

It was proposed that the part of the driving force F_{chem} that is related to chemical reactions has a simple form

$$F_{\text{chem}} = -\tau\Omega, \tag{12}$$

where τ is a physical coefficient and Ω is the internal variable. The internal variable Ω is governed by an evolution equation (cf. Eq. (2))

$$\Omega_T + \varepsilon\Omega = \zeta J, \tag{13}$$

where ε, ζ are coefficients and J is the ionic current from the AP model.

The fitting of the coefficients against experimentally measured temperature profiles [25] gave satisfactory results in the dimensionless form [28,29]. It was possible to distinguish slower and faster relaxation to the equilibrium state and to compare the influence of various mechanisms of heat production. In principle, it is possible to separate endo- and exothermic processes by introducing two internal variables Ω_{en} and Ω_{ex}, but then fitting the parameters to experimental results will be more difficult. However, such an analysis may help to better understand the physics behind the phenomenon.

This mechanism is part of a coupled model, which describes the propagation of a wave ensemble in a single axon [9]. The full model, including all the electric, mechanical and thermal effects, is presented in Appendix C.

5. DISCUSSION AND CONCLUSIONS

Above, we have elaborated some problems of phenomenological modelling, which were raised in Introduction. The usage of internal variables in continuum mechanics and phenomenological parameters in electrophysiology were briefly analysed. Both concepts, despite the used terminology, are related to the phenomenological modelling of physical phenomena, and the terminology is different due to the various scientific communities.

Both concepts stress the role of a researcher in choosing the variables for the phenomenological description (see Hodgkin and Huxley [10] and Maugin [12]). Such a choice is described in detail by Raman and Ferster [19] in their comments to the basic papers of Hodgkin and Huxley. Although the choice by Hodgkin and Huxley [10] turned out to work well, there was still a question 'whether there are any unexplained observations which have been neglected in an attempt to make experiments fit into a tidy pattern' [10].

The distinction between observable and internal variables is very clearly stressed by Maugin [12,13], and this is a clear sign that, in practice, the best results are obtained by using hybrid models. As analysed by Morrison [2], hybrid models include science-driven (theoretical) and descriptive (phenomenological) parts. This is evident from our examples (see Appendix B and Appendix C). An interesting question is to find a proper balance between the observable and phenomenological variables. In modelling the processes in nerves, it is clear that physics shapes the signals in nerves [30,33], and phenomenology is used to describe the processes (ion currents, heat production) where the present knowledge is not sufficient to elaborate physics-based models.

A difference between these two concepts is in constraints, which, in some sense, are based on initial studies. In continuum mechanics, Maugin [12,13] has characterized internal variables as an important concept for describing dissipative processes. Based on the earlier studies of Duhem and Gibbs, Maugin [13] stresses the role of thermodynamics in the processes with internal variables and presents the thermodynamic framework for the analysis. In electrophysiology, Hodgkin and Huxley [10] have used phenomenological variables for describing the activation and inactivation of an AP. This means that phenomenological modelling can be used for energy influx as well as for energy outflux. Although the HH model gives excellent results proven by many experiments, the contemporary understanding about the role of various ion channels (see, for example, Gonzáles et al. [21]) calls for modifications to this celebrated model. Regardless of the modifications, the principle of activation and inactivation must be followed.

The phenomenological models are certainly descriptive, but, as said by Morrison [2], they 'are able to mediate between theory and the world and intervene in both domains'. To model observation is not an easy problem – a researcher must have a sharp eye and understand the issue. In Appendix D, it is demonstrated that physical modelling and phenomenological modelling give similar results when properly calibrated.

One thing is clear: the more we understand the physics and chemistry of various fields, the more we understand the observations that happen in continuum mechanics or electrophysiology, with phenomenological modelling being one tool for better understanding. However, when using phenomenological variables, special attention must be paid to the calibration and interpretation of rate constants, like Hodgkin and Huxley [10] did for the modelling of ion currents. This means that the application of a derived model is restricted to a concrete case.

Basically, the idea of using internal variables is to describe a process that is either unknown, too complicated for an easy description or hidden from direct observations but has an observable effect on the processes that can be measured or modelled. It should be stressed that if the internal or phenomenological variables are introduced in a given model, it is important to clearly state the underlying assumptions made when introducing them.

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APPENDIX A

AN EXAMPLE FROM CONTINUUM MECHANICS

As an example, it is demonstrated how thermodynamical considerations permit us to derive governing equations for the internal variable within the framework of continuum mechanics. The example models heat conduction in a microstructured material, where the internal variable α describes the influence of changes in temperature due to microstructure. The model is described in detail in [31,32], here the main idea is presented.

The second law of thermodynamics can be written as

$$S_t + \nabla \cdot \mathbf{S} \geq 0, \quad \mathbf{S} = \frac{\mathbf{Q}}{T} + \mathbf{K}, \tag{14}$$

where S is the entropy density per unit volume, $\mathbf{S}$ is the entropy flux, $\mathbf{Q}$ is the heat flux, T is the absolute temperature and $\mathbf{K}$ is the extra entropy flux (that vanishes in most cases). Index t means differentiation with respect to time t. The dissipation inequality follows from Eq. (14):

$$ST_t + \mathbf{S} \cdot \nabla T \leq h_{\text{int}} + \nabla \cdot (T\mathbf{K}), \tag{15}$$

where $h_{\text{int}} = -W_t$, and W is the Helmholtz free energy. The free energy is proposed to include temperature T and the internal variable α:

$$W = W(T, \alpha, \nabla\alpha). \tag{16}$$

Leaving the details aside (see [32]) for the quadratic free energy (16) and linear thermodynamic fluxes, the evolution equation governing the behaviour of the internal variable α is derived from the dissipation inequality (15):

$$\alpha_t = M_{11}T(C\nabla^2\alpha - B\alpha) - M_{12}\nabla T, \tag{17}$$

where B and C are material parameters, and M_{11}, M_{12} are constants characterizing thermodynamic forces. It is obvious that the changes in α are driven by the temperature gradient. The heat conduction equation now takes the form

$$\rho c_p T_t - M_{22}\nabla^2 T = -M_{21}\nabla \cdot [T_0(c\nabla^2\alpha - B\alpha)], \tag{18}$$

where ρ is the density and c_p is the heat capacity. The constants M_{22} and M_{21} characterize thermodynamic forces. Equation (18) has a clear structure: the LHS models the classical heat conduction, while the RHS models the influence of the microstructure. If $\alpha = 0$, then the result is a standard heat conduction equation.

APPENDIX B

THE HODGKIN–HUXLEY MODEL

In the following, the full Hodgkin–Huxley (HH) model [10,19] is presented. The total current I across the membrane is given by

$$I = C_M \frac{\mathrm{d}V}{\mathrm{d}t} + \bar{g}_K n^4 (V - V_K) + \bar{g}_{Na} m^3 h (V - V_{Na}) + \bar{g}_l (V - V_l), \tag{19}$$

where V is the displacement of the membrane potential from its resting value, C_M is the membrane capacity per unit area and V_K, V_{Na}, V_l denote equilibrium potentials of the potassium, sodium and leakage (chloride and other) ions. Ionic permeability of the membrane is expressed in terms of ionic conductances (g_K, g_{Na} and g_l).

The equilibrium potentials V_{ion} for each type of ion satisfy the Nernst equation:

$$V_{\text{ion}} = \frac{k_B T}{q} \ln\left(\frac{[\text{outside}]_{\text{ion}}}{[\text{inside}]_{\text{ion}}}\right), \tag{20}$$

where q is the charge of the ion, k_B is the Boltzmann constant, T is absolute temperature, and $[\text{outside}]_{\text{ion}}$, $[\text{inside}]_{\text{ion}}$ denote extra- and intracellular concentrations of a given ion.

Opening and closing of the ion channels is modelled by phenomenological parameters n (K ‘turning on’), m and h (Na ‘turning on’ and ‘turning off’, respectively). These dimensionless parameters are in the interval from zero to one and are determined from the following kinematic equations:

$$\frac{\mathrm{d}n}{\mathrm{d}t} = \alpha_n(1-n) - \beta_n n, \tag{21}$$

$$\frac{\mathrm{d}m}{\mathrm{d}t} = \alpha_m(1-m) - \beta_m m, \tag{22}$$

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \alpha_h(1-h) - \beta_h h. \tag{23}$$

The expressions for the parameters α_i and β_i have been calibrated experimentally [10]:

$$\alpha_n = \frac{0.01(V+10)}{\exp\left(\frac{V+10}{10}\right)-1}, \tag{24}$$

$$\beta_n = 0.125\exp\left(\frac{V}{80}\right), \tag{25}$$

$$\alpha_m = \frac{0.1(V+25)}{\exp\left(\frac{V+25}{10}\right)-1}, \tag{26}$$

$$\beta_m = 4\exp\left(\frac{V}{18}\right), \tag{27}$$

$$\alpha_h = 0.07\exp\left(\frac{V}{20}\right), \tag{28}$$

$$\beta_h = \frac{1}{\exp\left(\frac{V+30}{10}\right)+1}. \tag{29}$$

The expressions for α_i and β_i are appropriate to the temperature of 6.3° C in the giant squid axon. For other temperatures, the right side of Eqs (15) and (16) must be scaled by a factor

$$\phi = Q_{10}^{(T-T_{\text{base}})/10}. \tag{30}$$

Here Q_{10} is the ratio of the rates for an increase in temperature of 10° C. For the squid axon $T_{\text{base}} = 6.3°$ C and $Q_{10} = 3$.

From cable theory, it is known that the membrane current per unit length i is given by

$$i = \frac{1}{r_1+r_2}\frac{\partial^2 V}{\partial x^2}, \tag{31}$$

where r_1 and r_2 are the external and internal resistances per unit length, and x is the distance along the fibre. Since for a large volume of conducting fluid, r_1 is negligible compared to r_2, (31) can be rewritten as

$$I = \frac{a}{2R_2}\frac{\partial^2 V}{\partial x^2}, \tag{32}$$

where a is the radius of the fibre, and R_2 is the specific resistance of the axoplasm. Combining Eq. (32) with Eq. (19), a second-order partial differential equation describing an evolution of AP is derived:

$$\frac{a}{2R_2}\frac{\partial^2 V}{\partial x^2} = C_M\frac{\mathrm{d}V}{\mathrm{d}t} + \bar{g}_K n^4 (V-V_K) + \bar{g}_{Na} m^3 h (V-V_{Na}) + \bar{g}_l (V-V_l). \tag{33}$$

This is a hybrid model based on fundamental principles and phenomenology (variables n, m, h). Nelson [34] calls the HH model 'as one of the most beautiful and fruitful examples of what can happen when we apply the tools and ideas of physics to a biological problem'.

APPENDIX C

THE COUPLED MODEL

In Section 3, an overview of modelling of the AP is given. In Section 4, it is described how to use the concept of internal variables for modelling heat production in axons. Engelbrecht et al. [9] have proposed a coupled model for describing the propagation of an AP and its accompanying mechanical and thermal effects. Here, we briefly present the mathematical details of the model in a dimensionless form [9].

The AP is governed by the FitzHugh–Nagumo (FHN) model [20]:

$$\begin{aligned} Z_T &= DZ_{XX} - J + Z\left(Z - C_1 - Z^2 + C_1 Z\right), \\ J_T &= \varepsilon_1\left(C_2 Z - J\right). \end{aligned} \tag{34}$$

Here, Z is the AP, J is the ion current, D is a coefficient, ε is the time-scale difference parameter and $C_i = a_i + b_i$, where a_i is the 'electrical' activation coefficient and $b_i = -\beta_i U$ is the 'mechanical' activation constant; β_i are coupling coefficients. Here and further, indices T and X denote partial derivates against dimensionless time and space, respectively. Note that here the ion current J also plays a role in the evolution of an internal variable (cf. Eq. (2)).

The pressure wave (PW) is governed by a modified wave equation (the wave equation with viscous and coupling terms):

$$P_{TT} = c_2^2 P_{XX} - \mu_2 P_T + F_2(Z,J), \tag{35}$$

where P is the pressure, c^2 is the characteristic velocity in fluid, μ_2 is the viscous coefficient and F_2 models the influence from the AP.

The longitudinal wave (LW) in the biomembrane is governed by the improved Heimburg–Jackson (iHJ) model [35,36]:

$$\begin{aligned} U_{TT} = {} & c_3^2 U_{XX} + NUU_{XX} + MU^2 U_{XX} + NU_X^2 + 2MUU_X^2 \\ & - H_1 U_{XXXX} + H_2 U_{XXTT} - \mu_3 U_T + F_3(Z,J,P), \end{aligned} \tag{36}$$

where $U = \Delta\rho$ is the longitudinal density change, c_3 is the velocity of sound in an unperturbed state, N, M are nonlinear coefficients and H_i are dispersion coefficients, μ_3 is a viscosity/friction coefficient, and F_3 models the influence from the AP and PW.

The transverse displacement (TD) of the biomembrane is calculated from the LW as $W \propto U_X$ (drawing inspiration from the theory of rods) [37,38]:

$$W = KU_X, \tag{37}$$

where K is a coefficient.

The temperature Θ is governed by the classical heat equation with a coupling term:

$$\Theta_T = k\Theta_{XX} + F_4(Z,J,U,P), \tag{38}$$

where Θ is the temperature, k is the thermal conductivity coefficient, and F_4 models the influence from the AP, LW and PW.

Coupling forces based on the ideas presented in [39,40] are the following:

$$F_2 = \eta_1 Z_X + \eta_2 J_T + \eta_3 Z_T, \tag{39}$$

$$F_3 = \gamma_1 P_T + \gamma_2 J_T - \gamma_3 Z_T, \tag{40}$$

$$F_4 = \tau_{11} Z^2 + \tau_2\left(P_T + \varphi_2(P)\right) + \tau_3\left(U_T + \varphi_3(U)\right) - \tau_4 \Omega, \tag{41}$$

where η_i, γ_i and τ_i are coefficients. Following the formalism of internal variables, Ω is determined either from

$$\Omega_T + \varepsilon_4 \Omega = \zeta J \tag{42}$$

or

$$\Omega_T = \varphi_4(J) - \frac{\Omega - \Omega_0}{\tau_\Omega}, \quad \Omega_0 = 0, \quad \tau_\Omega = \frac{1}{\varepsilon_4}, \tag{43}$$

where

$$\varphi_2(P) = \lambda_2 \int P_T \, \mathrm{d}T, \quad \varphi_3(U) = \lambda_3 \int U_T \, \mathrm{d}T, \quad \varphi_4(J) = \zeta \int J \, \mathrm{d}T \tag{44}$$

and ε_4, τ_Ω, λ_i and ζ are coefficients.

Temperature effects are governed by a hybrid model, partly describing the physics, partly the chemical reactions using phenomenology (internal variable Ω). Numerical simulations [9,28] have demonstrated qualitatively a good correspondence to the experimental results.

APPENDIX D

TEST PROBLEMS

Here we present simple dimensionless model problems to demonstrate the use of internal variables for modelling some basic phenomena. We start by demonstrating how phenomenological modelling could be used for modelling dissipative wave propagation. It is well known that dissipation can be modelled by introducing dissipative terms in the stress-strain relation [4]. Then the one-dimensional dimensionless equation of motion is

$$u_{tt} - c^2 u_{xx} = -k_1 u_t + k_2 u_{txx}, \tag{45}$$

where c is the wave speed and $k_1, k_2 > 0$ are coefficients. Here and further, the indices denote differentiation with respect to coordinate x and time t, respectively. With an additional fourth-order dispersive term, Eq. (45) can be used for modelling transverse wave propagation in a piano string [41]. With $k_2 = 0$, Eq. (45) models a string on a viscous subgrade [42], and with $k_1 = 0$, viscoelastic effects in solids [38].

The initial value problem with a $\mathrm{sech}^2(x)$-type initial pulse is posed for Eq. (45) and solved numerically using the NDSolve function in Wolfram Mathematica with the following initial conditions at $t = t_0$: $u(x,t_0) = \mathrm{sech}^2(x)$, $\frac{\partial}{\partial t} u(x,t_0) = 0$ and $\Omega(x,t_0) = 0$. The effect of both dissipative terms is demonstrated in Fig. 1.

The same process can be modelled by using the concept of internal variables. To this end, a dimensionless wave equation with forcing can be used:

$$u_{tt} - c^2 u_{xx} = f(x,t), \tag{46}$$

where $f(x,t)$ is an external forcing and the forcing itself depends on the internal variable Ω:

$$f(x,t) = \pm \tau \Omega, \tag{47}$$

where τ is a coefficient. In the following example, the internal variable is governed by the equation

$$\Omega_t = u_{xx} - \Omega. \tag{48}$$

The solution to the system (46)–(48) with the initial conditions $u(x,t_0) = \mathrm{sech}^2(x)$, $\frac{\partial}{\partial t} u(x,t_0) = 0$, $\Omega(x,t_0) = 0$ is shown in Fig. 2. It can be seen that the concept of internal variables can be used for modelling dissipation (with $f(x,t) = -\tau\Omega$) and amplification (with $f(x,t) = \tau\Omega$). In mathematical terms, amplification may lead to stability loss. So, special attention must be devoted to the constraints of the process through stability analysis.

For a second example, we demonstrate how the concept of internal variables can be used for modelling heat propagation in the presence of an additional process. A dimensionless heat equation with additional forcing is used:

$$u_t - \alpha u_{xx} = f(x,t), \tag{49}$$

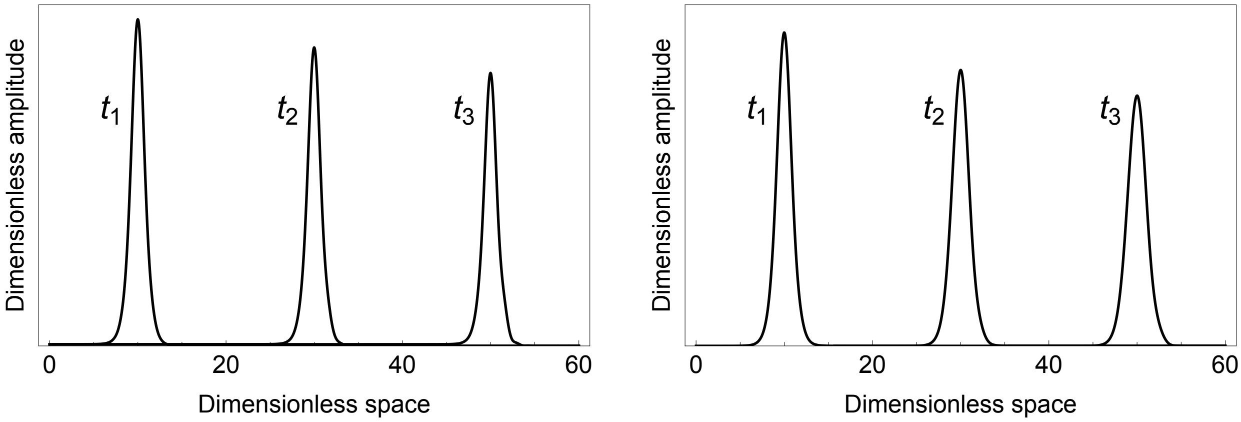

Fig. 1. Solutions to the dissipative wave equation (45). The effect of the term u_t ($k_1 = 0.01$, $k_2 = 0$) is demonstrated in the left panel; the effect of the term u_{txx} ($k_1 = 0$, $k_2 = 0.01$) is demonstrated in the right panel. The pulses propagate to the right, profiles at dimensionless times $t_1 = 10$, $t_2 = 30$, $t_3 = 50$ are shown, and $c = 1$ for both cases.

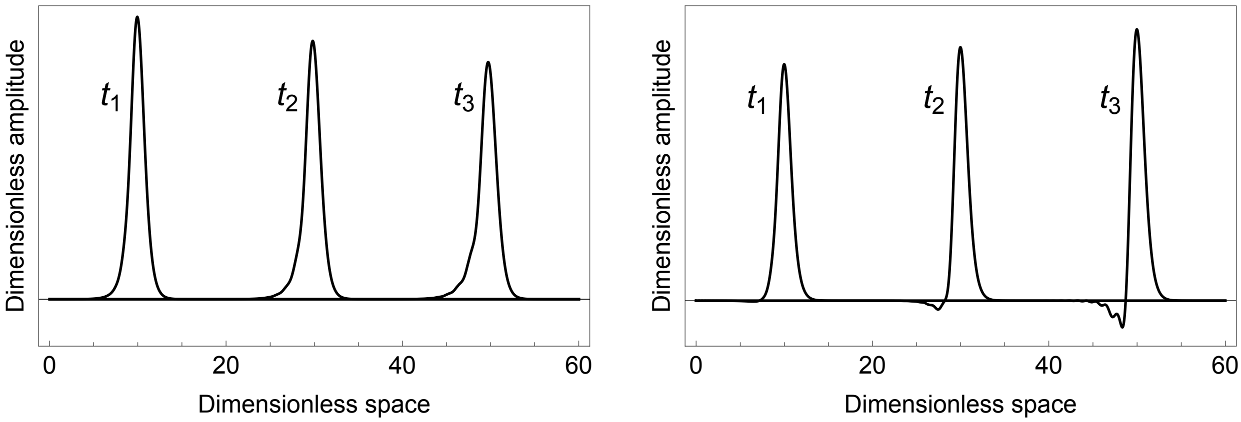

Fig. 2. Solutions to the system (46)–(48) in the case of $f(x,t) = -\tau\Omega$ (left panel) and $f(x,t) = \tau\Omega$ (right panel). The pulses propagate to the right, and profiles at dimensionless times $t_1 = 10$, $t_2 = 30$, $t_3 = 50$ are shown. $c = 1$ and $\tau = 0.02$ for both cases.

where α is a coefficient and $f(x,t) = \pm\tau\Omega$ is the external influence. This term can be interpreted as a source term that models a process either adding or removing energy from the system. In this example, the internal variable Ω is governed by

$$\Omega_T + \varepsilon\Omega = 0, \tag{50}$$

where ε is a coefficient. Note that Eq. (49) is taken similar to Eq. (42) in the coupled model (Appendix C). The difference is that in the case of the coupled model, evolution of the internal variable Ω is influenced by the AP through the ionic current J. In the test problem, we use a sech^2-type initial condition for Ω.

The system (49)–(50) is solved numerically with the initial conditions $u(x,t_0) = \mathrm{sech}^2(x)$, $\Omega(x,t_0) = \mathrm{sech}^2(x)$ for three values of τ: $\tau = 0$ corresponds to the case of classical heat equation (reference case), $\tau < 0$ and $\tau > 0$. The solutions to the system (49)–(50) are depicted in Fig. 3, where it can be seen that with different values of parameter τ, the process governed by Eq. (49) can be made slower or faster. This is also demonstrated in Fig. 4, where amplitude changes at $x = 0$ are shown in time. Such a possibility stems exactly from the structure of the governing equation (50) of the internal variable (cf. also the kinematic equations (21)–(23)). For the heat production in nerves (Section 4), such a model permits distinguishing slower (exothermic external influence) and faster (endothermic external influence) relaxation compared to the classical heat equation ($\tau = 0$).

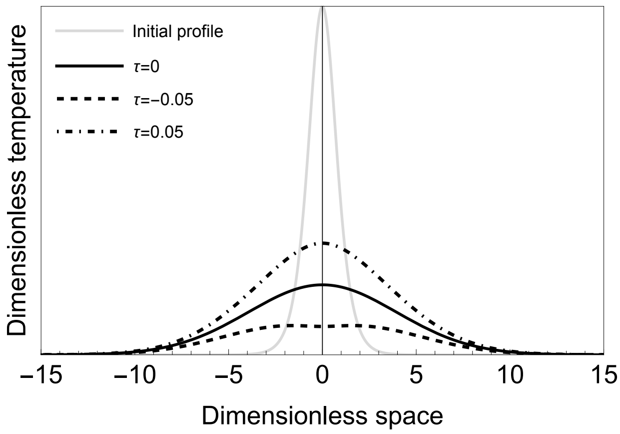

Fig. 3. Solutions to the system (46)–(48) in the case of $f(x,t) = 0$ (solid line), $f(x,t) = -\tau\Omega$ (dashed line) and $f(x,t) = \tau\Omega$ (dot-dashed line). For all cases $\alpha = 0.25$, $\varepsilon = 0.1$ and $\tau = 0.05$. Initial profile is depicted in light grey and solutions are shown at dimensionless time $t = 30$.

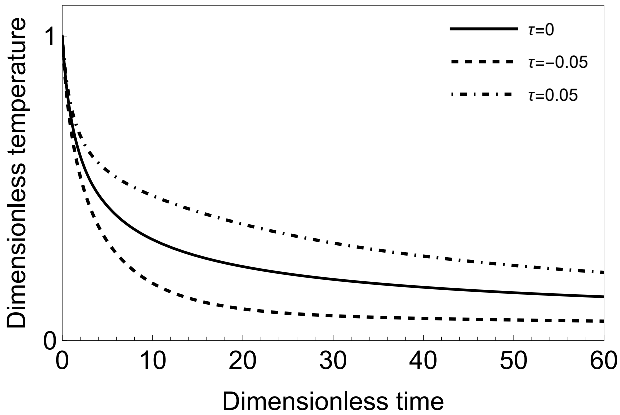

Fig. 4. Amplitude changes in time for the test problem (49)–(50) depicted in Fig. 3 at $x = 0$.

These test problems of the classical wave equation and diffusion equation demonstrate clearly that by adding phenomenological (internal) variables, several modified processes can be described.

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Füüsikaliste nähtuste fenomenoloogilisest modelleerimisest

Jüri Engelbrecht, Kert Tamm ja Tanel Peets

Füüsikaliste nähtuste modelleerimisel ei piisa teinekord füüsikaseadustest ja tuleb kasutada vaatlustel põhinevaid kirjeldusi. Pideva keskkonna mehaanikas kasutatakse sisemuutujate mõistet, neuroteaduses närviimpulsside levi modelleerimisel aga fenomenoloogilisi muutujaid. Artiklis analüüsitakse nende mudelite sarnasusi ja erinevusi. Kui pideva keskkonna mehaanikas on tähelepanu dissipatiivsetel protsessidel, siis närviimpulsside modelleerimisel tuleb arvestada aktsioonipotentsiaali võimendusega ja tekkiva temperatuuri relaksatsiooniga. Mõlemal juhul on võimalik kasutada fenomenoloogilisi muutujaid. Analüüsist järeldub, et tihti on otstarbekas kasutada hübriidmudeleid, kus füüsikalistele seaduspärasustele on lisatud mõne protsessi fenomenoloogiline, vaatlustel põhinev kirjeldus. Artikli lisades on kirjeldatud konkreetseid närviimpulsside mudeleid ning testprobleeme hüperboolsete (laine tüüpi) ja paraboolsete (difusioonitüüpi) võrrandite analüüsimisel, kui lisatud on fenomenoloogiline muutuja. Need probleemid demonstreerivad ilmekalt fenomenoloogiliste muutujate paindlikkust nii dissipatsiooni kui ka võimenduse modelleerimisel.