Summary of Professional Accomplishments - Habilitation

1. **First name and surname:** Lucjan Sapa
2. **Diplomas and scientific degrees:**
   (a) PhD in mathematics in the field of mathematical sciences, Jagiellonian University in Cracow, Faculty of Mathematics and Physics;

   dissertation: *Difference method for a parabolic-elliptic system*
   supervisor: prof. dr. hab. Marian Malec
   reviewers: prof. dr. hab. Tadeusz Dłotko
   prof. dr. hab. Zdzisław Kamont
   prof. dr. hab. Stanisław Sędziwy

   (b) master's degree in mathematics, Jagiellonian University in Cracow, Faculty of Mathematics and Physics;

   master thesis: *Newton's method of solving of equations*
   supervisor: prof. dr. hab. Bolesław Szafirski

   (c) master's degree in informatics, Jagiellonian University in Cracow, Faculty of Mathematics and Physics;

   master thesis: *Finite difference method for a parabolic-elliptic system*
   supervisor: prof. dr. hab. Marian Malec
3. **Employment in research units:**
   (a) assistant at Faculty of Applied Mathematics of AGH University of Science and Technology in Cracow;
   (b) lecturer at Faculty of Applied Mathematics of AGH University of Science and Technology in Cracow;
   (c) senior lecturer at Faculty of Applied Mathematics of AGH University of Science and Technology in Cracow;
   (d) assistant professor at Faculty of Applied Mathematics of AGH University of Science and Technology in Cracow.
4. **Scientific achievements set out in art. 219 para 1 point 2 of the Act of 20 July 2018 Law on Higher Education and Science (Journal of Laws of 2020, item 85, as amended):**
   (a) series of publications under the title: **Analitycal and numerical methods for partial differential equations and systems in diffusion and transport models**;
   (b) publications included in the series:

   [A1] L. Sapa, *A finite difference method for quasi-linear and nonlinear differential functional parabolic equations with Dirichlet's condition*, Annales Polonici Mathematici 93 (2008), 113-133.

   [A2] L. Sapa, *Existence, uniqueness and estimates of classical solutions to some evolutionary system*, Opuscula Mathematica 35 (2015), 935–956.

[A3] L. Sapa, *Global existence and uniqueness of a classical solution to some differential evolutionary system*, Rocky Mountain Journal of Mathematics 47 (2017), 2351–2380.

[A4] R. Filipek, P. Kalita, L. Sapa, K. Szyszkiewicz, *On local weak solutions to Nernst–Planck–Poisson system*, Applicable Analysis 96 (2017), 2316–2332.

I enclose the statements of the co-authors.

[A5] L. Sapa, *Difference methods for parabolic equations with Robin condition*, Applied Mathematics and Computation 321 (2018), 794–811.

[A6] L. Sapa, B. Bożek, M. Danielewski, *Existence, uniqueness and properties of global weak solutions to interdiffusion with Vegard rule*, Topological Methods in Nonlinear Analysis 52 (2018), 423–448.

I enclose the statements of the co-authors.

[A7] B. Bożek, L. Sapa, M. Danielewski, *Difference methods to one and multidimensional interdiffusion models with Vegard rule*, Mathematical Modelling and Analysis 24 (2019), 276–296.

I enclose the statements of the co-authors.

[A8] L. Sapa, B. Bożek, K. Tkacz-Śmiech, M. Zajusz, M. Danielewski, *Interdiffusion in many dimensions: mathematical models, numerical simulations and experiment*, Mathematics and Mechanics of Solids 25 (2020), 2178–2198.

I enclose the statements of the co-authors.

[A9] L. Sapa, *Parabolic-elliptic system modeling biological ion channels*, Journal of Differential Equations 291 (2021), 1–26, doi.org/10.1016/j.jde.2021.04.030.

The articles [A3] - [A9] are published in journals included in the Journal Citation Reports (JCR). The journal in which the article [A1] is published has been in this database since 2009 (in the year of publication it was on the Philadelphia List), while the journal in which the article [A2] is published has been on the Philadelphia List since 2019 and is not yet available in the JCR database. The sum of the points according to the MNiSzW score for the articles included in the achievement is equal to 391 (calculated according to the year of publication). According to the JCR database, their total impact factor is equal to 10,411 (calculated according to the year of publication). The total number of citations for these articles according to the Web of Science database is equal to 29 (including 15 without self-citations). The average volume of each of the nine works is approximately 22.5 pages. Only me is the author of five articles.

(c) discussion of the scientific goal and the results of the [A1] - [A9] cycle and other scientific research works:

1 Introduction

1.1 Diffusion phenomenon

Diffusion is one of the most common physical phenomena in nature. The name comes from the Latin word "diffusio" that is, spreading. It is a process of spontaneous spreading and permeation of molecules or energy in any medium (e.g. in a gas, liquid, solid, etc.), resulting from the chaotic collisions of molecules of the diffusing substance with each other or with the molecules of the surrounding medium. Contrary to mixing, it does not require additional energy from outside the system. Two basic types of diffusion are considered:

- tracked diffusion - a microscopic process involving a chaotic single motion molecules, e.g. Brownian motion,
- chemical diffusion - a macroscopic process involving macroscopic amounts of matter (or energy), usually described by the continuity equation, also known as the diffusion equation, and leading to the equalization of the concentration (or temperature) of each of the diffusing substances throughout the system.

Diffusion research, already conducted in the 18th century, led to the formulation of elementary linear equations with constant coefficients describing diffusion in solids: the Laplace (1782), Poisson (1813), Fourier (1822) and Fick (1855) equations. With the development of the theory and the progress of experimental research, these equations were generalized by adding new terms, often nonlinear, variation of coefficients, adding new equations, entering areas with a complex structure, so that they more and more accurately model real physical phenomena.

The basic laws describing diffusion are Fick's laws [29]. Fick's first law states that the diffusion flux of the ith component is proportional to the negative gradient concentration of this component, which is given by the formula

$$J_i = -D_i \nabla c_i. \tag{1}$$

A physical parameter D_i is called the diffusion coefficient and is usually determined experimentally. Fick's second law states that the change in the concentration of the ith component over time is minus the divergence of the flux corresponding to this component, i.e.

$$\partial_t c_i = -\mathrm{div} J_i. \tag{2}$$

The relationship (2) is called the continuity equation. This equation is, in fact, a local conservation law. As a result of theoretical considerations and conducted laboratory experiments, it turned out that in order to explain certain phenomena occurring in the systems of diffusing substances, it is necessary to "enrich" the flux by adding the appropriate term [21, 23, 71, 74] or define it with the use of a differential equation [45, 58], generated by additional diffusion-free transport. I will write about it in more detail in further parts of this dissertation.

1.2 The goal of the dissertation

As a scientific achievement to obtain the habilitation degree, I submit a series of nine publications [A1] - [A9]. I consider three specific diffusion models and the general situation:

- diffusive mass transport in solid materials,
- electrodiffusion in ion selective electrodes and biological ion channels,
- ion current flow in neurons,
- other local and nonlocal diffusion models.

These models are described by nonlinear partial differential equations or systems of such equations of parabolic, parabolic-elliptic and hyperbolic types with initial-boundary and initial conditions. I study one- and multidimensional situations, local and nonlocal. The main results focus on the construction of new models or the generalization of existing ones, e.g. by taking into account an additional physical law, proposing more physical boundary conditions or weakening assumptions, and on the proof of theorems about the existence and properties of classical or weak solutions in the suitable Sobolev spaces, as well as on the construction of numerical methods (difference methods, the Galerkin method) and the proof of theorems concerning their properties.

I will discuss the results of this scientific achievement in the next four chapters. I start each chapter with a historical outline, then construct or provide examples of mathematical models, and then discuss specific articles in a purely mathematical context, i.e. briefly present the results, formulate main theorems and briefly present the idea of proofs. In order not to extend the presentation excessively, I do not formulate auxiliary theorems and lemmas, usually non-trivially proven, but only mention them when discussing the articles. Due to the diversity of the subject matter, the notation in individual papers is generally different. As the Reader will certainly want to supplement the summaries below with reading the articles, I will use the original notation as much as possible, which will facilitate a deeper analysis.

Other scientific and research achievements, not included in the series, I will discuss in the last chapter.

2 Interdiffusion in solids, [A6], [A7], [A8]

I will start with the construction of mathematical models. The quantitative description of dissipative mass transport is particularly important in materials science and hydrodynamics. Transport in multicomponent fluids is described by the system of Navier-Stokes equations with the initial condition and different boundary conditions [24]. The process of diffusion in solids cannot be described by the Navier-Stokes system, because in this case there are no technical possibilities to effectively determine the viscosity coefficients, there are many phases, the diffusing layer is very thin and there are no large mass flows, which implies the exclusion of the convective component. By interdiffusion we mean multicomponent transport when all the components diffuse into each other. An attempt to mathematically model interdiffusion in multicomponent solids was initiated by Darken [21] in 1948. This author considered a physically closed binary sample with a known constant concentration

$$c_1 + c_2 = c \tag{3}$$

and assumed that the mass transfer takes place only in one direction. The symbols c_1, c_2 represent the concentrations of the first and second components. He constructed his model based on the continuity equations (2) for fluxes, allowing the movement of the medium,

$$J_i = -D_i \partial_x c_i + c_i v^D, \quad i = 1, 2, \tag{4}$$

where $D_i > 0$ are constant component diffusion coefficients, and v^D is the so-called drift velocity. The drift is the local speed of the sample relative to a reference frame, which may be the boundary. Second velocity is the diffusion velocity of the ith component determined by the formula $v_i^d := -D_i \partial_x (\ln c_i)$. The fluxes J_i are called the Darken fluxes, and the method described is called the bi-velocity method. Let us stress that J_i is a generalization of the Fick flux (1). The introduction of the drift velocity explains the movement of the so-called Kirkendall's plane [77]. It is the boundary surface movement between, in this case, two diffusing media in the sample. The theoretical description of the Kirkendall effect has important implications in applications. One of them is the prevention or suppression of voids at the interface of alloys with metals known as the Kirkendall porosity. Recently, the drift velocity has also been used to describe electrodiffusion in electrochemistry [83].

Darken's one-dimensional method was generalized to a multicomponent case and modified to a system of generalized parabolic differential equations in place of the differential-algebraic system in the nineties of the last century by Danielewski, Bożek, Holly and Filipek [19, 40].

It turns out that such a system is easier to study both analytically and numerically. In [A6] s-component equivalent of the equation (3), I generalized with co-authors allowing the so-called Vegard's rule

$$\sum_{i=1}^{s} \Omega_i c_i = 1, \tag{5}$$

where Ω_i mean mole fractions [82]. Thus, the total concentration $c := \sum_{i=1}^{s} c_i$ can be variable in time and space. In [A7] and [A8], we generalized Darken's method for a multidimensional case by formulating a system of parabolic-elliptic differential equations.

I will now present the construction of the above-mentioned systems of differential equations. Let $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$ be an open bounded set with the smooth boundary $\partial\Omega$. Let moreover $T > 0$ be given. The diffusion coefficients $D_i > 0$ are constant or depend on the concentrations, i.e. $D_i = D_i(c_1, ..., c_s)$. Consider the differential-algebraic system (2), (5) with fluxes of the form (4) specified on the set $[0, T] \times \overline{\Omega}$, and now $i = 1, ..., s$. We set the initial condition

$$c_i(0, x) = c_{0i}(x), \quad x \in \Omega \tag{6}$$

and the boundary conditions for fluxes

$$J_i \cdot \mathbf{n} = j_i(t, x), \quad (t, x) \in [0, T] \times \partial\Omega, \tag{7}$$

where $\mathbf{n}$ is the outside normal vector to the boundary $\partial\Omega$, $i = 1, ..., s$, and "$\cdot$" means the standard scalar product in $\mathbb{R}^n$. Multiplying the equations (2) by Ω_i and adding them by sides, then using Vegard's rule (5), we get the volume continuity equation (volume transport)

$$\operatorname{div}\Big(\sum_{i=1}^{s} \Omega_i J_i(t, x)\Big) = 0, \quad (t, x) \in [0, T] \times \overline{\Omega}. \tag{8}$$

Consider firstly a one-dimensional case, n=1. Let $\Omega = (-\Lambda, \Lambda) \subset \mathbb{R}$. It follows from the equation (8) that

$$\sum_{i=1}^{s} \Omega_i J_i(t, x) = K(t), \quad (t, x) \in [0, T] \times \overline{\Omega}, \tag{9}$$

where $K : [0, T] \to \mathbb{R}$ is an arbitrary function. The relations (7), (9) imply uniqueness of the function K of the form

$$K(t) = \sum_{i=1}^{s} \Omega_i j_i(t, \Lambda) = -\sum_{i=1}^{s} \Omega_i j_i(t, -\Lambda), \quad t \in [0, T]. \tag{10}$$

The second equality in (10) is in fact an assumption on the boundary evolutions j_i. On the other hand, (5) and (7) give

$$\sum_{i=1}^{s} \Omega_i J_i(t, x) = -\sum_{i=1}^{s} \Omega_i D_i \partial_x c_i(t, x) + v^D(t, x), \quad (t, x) \in [0, T] \times \overline{\Omega}. \tag{11}$$

In consequence, we get the drift

$$v^D(t, x) = \sum_{i=1}^{s} \Omega_i D_i \partial_x c_i(t, x) + K(t), \quad (t, x) \in [0, T] \times \overline{\Omega}. \tag{12}$$

Finally, we obtain the strongly coupled nonlinear second order evolution partial differential system

$$\partial_t c_i + \partial_x\Big(-D_i \partial_x c_i + c_i\Big(\sum_{k=1}^{s} \Omega_k D_k \partial_x c_k + K(t)\Big)\Big) = 0, \quad (t, x) \in [0, T] \times \Omega \tag{13}$$

with the nonlinear coupled boundary conditions

$$-D_i \frac{\partial c_i}{\partial \mathbf{n}} + c_i \Big(\sum_{k=1}^{s} \Omega_k D_k \frac{\partial c_k}{\partial \mathbf{n}} + K(t)\mathbf{n} \Big) = j_i(t,x), \quad (t,x) \in [0,T] \times \partial\Omega, \tag{14}$$

$i = 1, ..., s$. In the further part, we will name (13), under a suitable assumption, a generalized parabolic system.

Consider a multidimensional case, $n \geq 2$. The volume continuity equation (8) cannot now be used to calculate the drift because it does not imply the independence of the vector field under divergence from the spatial variable x. Let us stress that now the drift is a vector function $v^D : [0,T] \times \overline{\Omega} \to \mathbb{R}^n$. We postulate that the drift is potential, i.e. there is a scalar potential $F : [0,T] \times \overline{\Omega} \to \mathbb{R}$ such that

$$v^D = -\nabla F. \tag{15}$$

The drift potential assumption is physically justified because even above the Tammann temperature (2/3 of the melting point), the viscosity in solids is so high that $\mathrm{rot} v^D = 0$ can be assumed. This postulate was also confirmed experimentally in the works [A8] and [B16]. Substituting (15) into the continuity equations (2) and the volume continuity equation (8), we obtain a strongly coupled nonlinear parabolic-elliptical system of the form

$$\begin{cases} \partial_t c_i + \mathrm{div}\Big(-D_i \nabla c_i - c_i \nabla F \Big) = 0, & (t,x) \in [0,T] \times \Omega, \\ -\triangle F = \mathrm{div}\Big(\sum_{k=1}^{s} \Omega_k D_k \nabla c_k \Big), & (t,x) \in [0,T] \times \Omega, \\ \int_\Omega F dx = 0, & t \in [0,T], \end{cases} \tag{16}$$

$i = 1, ..., s$. Multiplying the fluxes (4) by Ω_i and $\mathbf{n}$, adding them by sides, then using the Vegard rule (5) and the boundary relation (7), we have

$$\frac{\partial F}{\partial \mathbf{n}} = -\sum_{k=1}^{s} \Omega_k \Big(D_k \frac{\partial c_k}{\partial \mathbf{n}} + j_k(t,x) \Big), \quad (t,x) \in [0,T] \times \partial\Omega. \tag{17}$$

Hence the nonlinear coupled boundary conditions are implied

$$\begin{cases} -D_i \frac{\partial c_i}{\partial \mathbf{n}} - c_i \frac{\partial F}{\partial \mathbf{n}} = j_i(t,x), & (t,x) \in [0,T] \times \partial\Omega, \\ \frac{\partial F}{\partial \mathbf{n}} = -\sum_{k=1}^{s} \Omega_k \Big(D_k \frac{\partial c_k}{\partial \mathbf{n}} + j_k(t,x) \Big), & (t,x) \in [0,T] \times \partial\Omega, \end{cases} \tag{18}$$

$i = 1, ..., s$. The compatibility condition on the boundary evolutions j_i follows from the Gauss theorem,

$$\int_{\partial\Omega} \sum_{i=1}^{s} \Omega_i j_i(t,x)\, dS = 0, \quad t \in [0,T]. \tag{19}$$

Both the boundary condition (14) and the first boundary condition in (18) can be viewed as generalized nonlinear Robin's conditions for the concentrations c_i. In turn, the second boundary condition in (18) is Neumann's condition for the potential F. Let us stress that the parabolic-elliptic initial-boundary problem (16), (6), (18) also makes sense in the one-dimensional case, $n = 1$ - Remark 1 in [A7], and [A8]. In addition, it is equivalent to the problem (13), (6), (14). Due to the strong coupling, i.e. through the second spatial derivatives, the systems (13) and (16) are not studied in such well-known monographs as [12, 14, 17, 22, 24, 28, 54, 75, 90].

[A6] In this article we proved Theorems 4.6, 5.1 about the existence, uniqueness and nonnegativity of global in time weak solutions in appropriate Sobolev spaces, of the one-dimensional nonlinear initial-boundary problem (13), (6), (14). Moreover, in the case of a closed system, when the fluxes on the boundary $\partial\Omega$ are equal to zero, we proved theorem 6.1 about the asymptotic behavior of the solution. This theorem is interpreted in such a way that the physical system in the limit, i.e. if t goes to plus infinity, homogenized itself.

Let $\varrho_i = M_i c_i$, $\Theta_i = D_i$, $j_{i,L} = -j_{(\cdot,-\Lambda)}$, $j_{i,R} = j_{(\cdot,\Lambda)}$ denote, respectively, the densities, the diffusion coefficients of the components and the evolution of the fluxes on the boundary of the interval $\Omega = (-\Lambda, \Lambda) \subset \mathbb{R}$, where $M_i > 0$ are the molar mass of the components. Now the differential problem (13), (6), (14) has the form

$$\partial_t \varrho_i + \partial_x \Big(-\Theta_i \partial_x \varrho_i + \varrho_i \Big(\sum_{j=1}^{s} \frac{\Omega_j \Theta_j}{M_j} \partial_x \varrho_j + K(t) \Big) \Big) = 0, \quad (t,x) \in [0,T] \times \Omega, \tag{20}$$

$$\varrho_i(0,x) = \varrho_{0i}(x), \quad x \in \Omega, \tag{21}$$

$$\left\{ \begin{array}{l} -\Theta_i \partial_x \varrho_i + \varrho_i \left(\sum_{j=1}^{s} \frac{\Omega_j \Theta_j}{M_j} \partial_x \varrho_j + K(t) \right) = j_{i,L}(t), \quad (t,x) \in [0,T] \times \partial\Omega, \\ -\Theta_i \partial_x \varrho_i + \varrho_i \left(\sum_{j=1}^{s} \frac{\Omega_j \Theta_j}{M_j} \partial_x \varrho_j + K(t) \right) = j_{i,R}(t), \quad (t,x) \in [0,T] \times \partial\Omega, \end{array} \right. \tag{22}$$

$i = 1, ..., s$. The total mass of the ith component of the mixture at the fixed moment $t \in [0,T]$ is given by

$$m_i(t) = \int_\Omega \varrho_i(t,x) dx, \quad i = 1, ..., s, \tag{23}$$

while by

$$\overline{m}_i(t) = \frac{1}{2\Lambda} \int_\Omega \Omega_i \frac{\varrho_i(t,x)}{M_i} dx, \quad i = 1, ..., s, \tag{24}$$

the average value of the local volume fraction $\Omega_i \varrho_i / M_i$ is denoted. Integrating (20) over the interval Ω, using (23), and integrating once again over the interval $(0,t)$, we get

$$m_i(t) = \int_\Omega \varrho_{0i}(x) dx + \int_0^t \left(j_{i,L}(\tau) - j_{i,R}(\tau) \right) d\tau \tag{25}$$

for $t \in [0,T]$, $i = 1, ..., s$. Hence $\overline{m}_i$, $i = 1, ..., s$ are known functions also. Let

$$1^\perp = \{ \xi = (\xi_1, ..., \xi_r) \in \mathbb{R}^s : \ \xi_1 + ... + \xi_r = 0 \} \tag{26}$$

stands for the vector space orthogonal to the vector subspace $\{\alpha 1 : \alpha \in \mathbb{R}\}$, where $1 = (1, ..., 1) \in \mathbb{R}^s$. Define the Sobolev spaces

$$H = \left\{ f = (f_1, ..., f_s) \in L^2(\Omega, 1^\perp) : \ \int_\Omega f_i(x) dx = 0, \ i = 1, ..., s \right\}, \tag{27}$$

$$V = \left\{ f \in H^1(\Omega, 1^\perp) : \ f \in H \right\}. \tag{28}$$

The norms in V and H are generated by the scalar products

$$(f,g)_V = \int_\Omega \partial_x f \cdot \partial_x g dx \quad f, g \in V, \tag{29}$$

$$(f,g)_H = \int_\Omega f \cdot g dx, \quad f, g \in H. \tag{30}$$

Then $V \subset H \subset V^*$ constitute the evolutional triple with the embeddings being dense, continuous and compact [2], [90]. Let

$$\mathcal{K} = \{ \kappa = (\kappa_1, ..., \kappa_s) \in \mathbb{R}^s : \ \kappa_1 + ... + \kappa_s = 1, \ k_i \geq 0, \ i = 1, ..., s \}. \tag{31}$$

Define the family of linear operators

$$A_\kappa : 1^\perp \mapsto 1^\perp, \quad A_\kappa \xi = \sum_{i=1}^{s} \Theta_i(\kappa)\xi_i e_i - (\Theta(\kappa)\cdot\xi)\kappa \tag{32}$$

for $\kappa \in \mathcal{K}$, where $\xi \in 1^\perp$, $e_i = (0, ..., 0, 1, 0, ..., 0)$ with 1 in the ith entry, $i = 1, ..., s$. We assume the following conditions.

Assumption H

(H$_0$) $\varrho_0(x) = (\varrho_{01}(x), ..., \varrho_{0s}(x)) \geq 0$ and $\sum_{i=1}^{s} \frac{\Omega_i \varrho_{0i}(x)}{M_i} = 1$ for $x \in \Omega$.

(H$_1$) $\int_\Omega \varrho_{0i}(x)dx + \int_0^t (j_{i,L}(\tau) - j_{i,R}(\tau))\, d\tau \geq 0$ for $t \in [0,T]$, $i = 1, ..., s$.

(H$_2$) $\sum_{i=1}^{s} \frac{\Omega_i j_{i,L}(t)}{M_i} = \sum_{i=1}^{s} \frac{\Omega_i j_{i,R}(t)}{M_i}$ for $t \in [0,T]$.

(H$_3$) $\varrho_0 \in L^2(\Omega)$.

(H$_4$) $j_{i,L}, j_{i,R} \in L^\infty(0,T)$, $i = 1, ..., s$.

(H$_5$) $\Theta_i : \mathbb{R}^s \to \mathbb{R}_+$, $i = 1, ..., s$ fulfill the Lipschitz condition and are bounded.

(H$_6$) The following *generalized parabolicity condition* holds:

$$\int_\Omega (A_g \partial_x f)\cdot \partial_x f dx \geq \mu \|f\|_V^2 - \nu \|f\|_H^2 \tag{33}$$

for some $\mu > 0$, $\nu \geq 0$ and for all $f \in V$, $g = (g_1, ..., g_r) \in H^1(\Omega, \mathbb{R}^r)$, $g_1 + ... + g_s = 1$, $g_i \geq 0$, $i = 1, ..., s$.

The assumptions (H_0) i (H_2) imply the relation

$$\sum_{i=1}^{s} \overline{m}_i(t) = 1, \tag{34}$$

thanks to which it is possible to change variable as follows

$$w_i(t,x) = \frac{\Omega_i \varrho_i(t,x)}{M_i} - \overline{m}_i(t), \quad i = 1, ..., s. \tag{35}$$

Put $w = (w_1, ..., w_s)$ and $\overline{m} = (\overline{m}_1, ..., \overline{m}_s)$. For any fixed $w \in L^2(0,T;V)$ and $t \in (0,T)$, the symbolem $\langle\ ,\ \rangle_{V^*\times V}$ means a linear continuous functional of the form

$$\langle w'(t), v\rangle_{V^*\times V} = \sum_{i=1}^{s} \langle w_i'(t), v_i\rangle, \tag{36}$$

where $\langle\ ,\ \rangle$ is a linear continuous functional acting on $L^2(0,T;H^1(\Omega,\mathbb{R}))$, $v \in V$. Denote the functions

$$\begin{aligned} \Gamma_{i,L}(t) &= K(t)\overline{m}_i(t) - \frac{\Omega_i j_{i,L}}{M_i}, \quad i = 1, ..., s, \\ \Gamma_{i,R}(t) &= K(t)\overline{m}_i(t) - \frac{\Omega_i j_{i,R}}{M_i}, \quad i = 1, ..., s, \\ \Gamma_L &= (\Gamma_{1,L}, ..., \Gamma_{r,L}), \\ \Gamma_R &= (\Gamma_{1,R}, ..., \Gamma_{r,R}), \\ \Gamma &= (\Gamma_L, \Gamma_R), \end{aligned} \tag{37}$$

for $t \in [0, T]$. The original initial-boundary value problem (20)–(22) has the following weak version.

Problem P. Find $w \in L^2(0, T; V)$ such that $w' \in L^2(0, T; V^*)$, for a.e. $t \in (0, T)$ $w(t) + \overline{m}(t) \in \mathcal{K}$,

$$\begin{aligned} \langle w'(t), v\rangle_{V^* \times V} + \int_\Omega \left(A_{w(t)+\overline{m}(t)} \partial_x w(t)\right) \cdot \partial_x v dx - K(t) \int_\Omega w(t) \cdot \partial_x v dx \\ = \Gamma_R(t) \cdot v(\Lambda) - \Gamma_L(t) \cdot v(-\Lambda) \quad \text{for each} \quad v \in V, \end{aligned} \tag{38}$$

and the initial condition holds

$$w(0) = w_0. \tag{39}$$

We proved the following theorems.

Theorem 1 ([A6], Thm. 4.6). *If Assumption H is satisfied, then Problem P has a solution.*

Theorem 2 ([A6], Thm. 5.1). *If Assumption H is satisfied, then Problem P has in $L^4(0, T; V)$ at most one solution.*

Theorem 3 ([A6], Thm. 6.1). *Let $w : [0, \infty) \to H$ be a solution of Problem P on each interval $[0, T]$ for $T \in \mathbb{R}_+$. If Assumption H is satisfied with $j_{i,L}(t) = j_{i,R} \equiv 0$, $t \in [0, \infty)$, $i = 1, ..., s$ and $\nu = 0$ w (33), then $w \in L^2(0, \infty; V) \cap L^\infty(0, \infty; H)$, $w' \in L^2(0, \infty; V^*)$, the function $[0, \infty) \ni t \mapsto \|w(t)\|_H^2$ is nonincreasing and $\lim_{t\to\infty} \|w(t)\|_H^2 = 0$.*

We proved Theorem 1 using the Galerkin method and the properties of the family of automorphisms A_κ, $\kappa \in \mathcal{K}$. These properties are formulated in Remark 4.1 and Lemmas 4.2, 4.3. In addition, we used the Riesz-Fréchet theorem, the Picard theorem, the Banach-Alaoglu theorem, the Gronwall lemma, the Aubin-Lions lemma and the properties of the Sobolev spaces, in particular continuous and dense embeddings. The proof of Theorem 2 is again based on the mentioned properties of the family of automorphisms A_κ, $\kappa \in \mathcal{K}$ using the Gronwall, Hölder and Young inequalities. In the proof of Theorem 3 it is important to use the integral convergence criterion of number series. It is also worth emphasizing that in the case of the constant diffusion coefficients Θ_i, the parabolic condition (33) can be checked using Lemma 3.5. The said family of automorphisms was previously considered in [20].

[A7] In this work, we constructed implicit finite difference methods (FDM) for the nonlinear parabolic-elliptic initial-boundary problem (16), (6), (18) in the one-dimensional case, $n = 1$, and two-dimensional, $n = 2$, assuming that the diffusion coefficients D_i are constant. We also assumed that the physical system is closed, i.e. that $j_i(t, x) \equiv 0$ for $(t, x) \in [0, T] \times \partial\Omega$, but this assumption can be immediately generalized by allowing an open physical system. It is worth yet paying attention to the fact that in the postulate (15) there is a "minus" sign and it is physically justified. However, in this article there is a "plus" sign at this point, which is not physically correct, but does not cause any problems mathematically, and the reasoning will also be true for the minus sign, but in the appropriate formulas the sign will change. The construction of the mentioned difference methods is based on the idea of linearization with spliting on the difference schemes for the elliptic and parabolic parts. Moreover, reducting the differntial problem from s to $(s-1)$ parabolic equations allowed to transfer the Vegard rule for discrete solutions, which is important both from the point of view of mathematics and physics. We proved Theorem 1 about the existence and uniqueness of solutions to the implicit difference schemes and theorems 2, 3 about the equivalence of convergence of the constructed numerical methods for the concentrations c_i and the potential F (see Remarks 4, 6), in the suitable maximum norms. Remarks 5 and 6 imply the analogous equivalence of stability.

In order to illustrate the results, I will describe only the one-dimensional case, because in the two-dimensional case the idea is analogous, but the formulas are much more complex, in particular some matrices become blocky. Let $\Omega = (-\Lambda, \Lambda) \subset \mathbb{R}$. As already mentioned, calculating

$$c_s = \frac{1}{\Omega_s}\Big(1 - \sum_{i=1}^{s-1} \Omega_i c_i\Big) \tag{40}$$

from the Vegard rule (5), the differential problem (16), (6), (18) is reduced to the form

$$\begin{cases} \partial_t c_i = D_i \partial_{xx} c_i - \partial_x c_i \partial_x F - c_i \partial_{xx} F, & (t,x) \in [0,T] \times \Omega, \\ \partial_{xx} F = \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_{xx} c_k, & (t,x) \in [0,T] \times \Omega, \\ \int_\Omega F dx = 0, & t \in [0,T], \end{cases} \tag{41}$$

$$c_i(0,x) = c_{0i}(x), \quad x \in \Omega, \tag{42}$$

$$\begin{cases} -D_i \partial_x c_i + c_i \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_x c_k = 0, & (t,x) \in [0,T] \times \partial\Omega, \\ \partial_x F = \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_x c_k, & (t,x) \in [0,T] \times \partial\Omega, \end{cases} \tag{43}$$

$i = 1, ..., s-1$. We discretize the rectangle $[0,T] \times \overline{\Omega}$ by defining the mesh steps, respectively the space and time, $h = 2\Lambda/(M+1)$, $\tau = T/K$, where $M, K \in \mathbb{N}$ are given. Define nodal poins (t^μ, x_m) as follows: $t^\mu = \mu\tau$, $x_m = -\Lambda + mh$, $\mu = 0, ..., K$, $m = 0, ..., M+1$. For the approximation of the derivatives we use the central, forward and backward difference quotients, and we approximate the integral equation using the trapezoidal method. We define implicit difference schemes for the elliptic part on the potential $F^{\mu+1}$ and for the parabolic part on the concentrations $c_i^{\mu+1}$ of the form

$$\begin{cases} -F_0^{\mu+1} + F_1^{\mu+1} = P_0^\mu(c) := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(-c_{k,0}^\mu + c_{k,1}^\mu\big), \\ F_{m-1}^{\mu+1} - 2F_m^{\mu+1} + F_{m+1}^{\mu+1} = P_m^\mu(c) \\ \quad := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(c_{k,m-1}^\mu - 2c_{k,m}^\mu + c_{k,m+1}^\mu\big), \\ F_M^{\mu+1} - F_{M+1}^{\mu+1} = P_{M+1}^\mu(c) := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(c_{k,M}^\mu - c_{k,M+1}^\mu\big), \\ F_0^{\mu+1} + 2\sum_{m=1}^{M} F_m^{\mu+1} + F_{M+1}^{\mu+1} = 0, \end{cases} \tag{44}$$

$$\begin{cases} q_{i,0}^\mu c_{i,0}^{\mu+1} + q_{i,1}^\mu c_{i,1}^{\mu+1} = Q_{i,0}^\mu := 0, \\ d_{i,m-1}^\mu c_{i,m-1}^{\mu+1} + v_{i,m}^\mu c_{i,m}^{\mu+1} + u_{i,m+1}^\mu c_{i,m+1}^{\mu+1} = Q_{i,m}^\mu := e_{i,m}^\mu c_{i,m}^\mu, \\ q_{i,M}^\mu c_{i,M}^{\mu+1} + q_{i,M+1}^\mu c_{i,M+1}^{\mu+1} = Q_{i,M+1}^\mu := 0, \end{cases} \tag{45}$$

where

$$\begin{aligned} \kappa &= \frac{\tau}{h^2}, \\ v_{i,m}^\mu &= 1 + 2\kappa D_i, \\ d_{i,m-1}^\mu &= -\kappa D_i - \frac{1}{4}\kappa\big(F_{m+1}^{\mu+1} - F_{m-1}^{\mu+1}\big), \\ u_{i,m+1}^\mu &= -\kappa D_i + \frac{1}{4}\kappa\big(F_{m+1}^{\mu+1} - F_{m-1}^{\mu+1}\big), \\ e_{i,m}^\mu &= 1 - \kappa\big(F_{m-1}^{\mu+1} - 2F_m^{\mu+1} + F_{m+1}^{\mu+1}\big), \\ q_{i,0}^\mu &= q_{i,M+1}^\mu = D_i, \\ q_{i,1}^\mu &= -D_i + \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\left(c_{k,1}^\mu - c_{k,0}^\mu\right), \\ q_{i,M}^\mu &= -D_i + \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\left(c_{k,M}^\mu - c_{k,M+1}^\mu\right), \end{aligned}$$

for $m = 1, ..., M$, $i = 1, ..., s-1$, $\mu = 0, ..., K-1$. If $v_{i,m}^{\mu(m)} \neq 0$, then we make a sequence of the Gauss substitutions for the scheme (45),

$$\begin{aligned}
v_{i,k}^{\mu(0)} &= q_{i,k}^{\mu}, \quad k = 0, 1, \\
v_{i,m}^{\mu(m)} &= v_{i,m}^{\mu} - d_{i,m-1}^{\mu}\big(v_{i,m-1}^{\mu(m-1)}\big)^{-1} v_{i,m}^{\mu(m-1)}, \quad v_{i,m-1}^{\mu(m)} = 0, \quad v_{i,m+1}^{\mu(m)} = u_{i,m+1}^{\mu}, \\
v_{i,M+1}^{\mu(M+1)} &= q_{i,M+1}^{\mu} - q_{i,M}^{\mu}\big(v_{i,M}^{\mu(M)}\big)^{-1} v_{i,M+1}^{\mu(M)}, \quad v_{i,M}^{\mu(M+1)} = 0, \\
Q_{i,0}^{\mu(0)} &= Q_{i,0}^{\mu}, \\
Q_{i,m}^{\mu(m)} &= Q_{i,m}^{\mu} - d_{i,m-1}^{\mu}\big(v_{i,m-1}^{\mu(m-1)}\big)^{-1} Q_{i,m-1}^{\mu(m-1)}, \\
Q_{i,M+1}^{\mu(M+1)} &= Q_{i,M+1}^{\mu} - q_{i,M}^{\mu}\big(v_{i,M}^{\mu(M)}\big)^{-1} Q_{i,M}^{\mu(M)},
\end{aligned} \tag{46}$$

$m = 1, ..., M$, $i = 1, ..., s-1$.

Theorem 4 ([A7], Thm. 1).

(i) For all the steps h, τ, the system (44) has exactly one solution $F^{\mu+1}$ for given concentrations $(c_1^{\mu}, ..., c_{s-1}^{\mu})$ of the form

$$F_{M+1}^{\mu+1} = \frac{\sum_{k=1}^{s-1} \Omega_k (D_k - D_s)\big[-c_{k,0}^{\mu} - 2\sum_{l=1}^{M} c_{k,l}^{\mu} + (1+2M) c_{k,M+1}^{\mu}\big]}{2(M+1)}, \tag{47}$$

$$F_{m}^{\mu+1} = F_{m+1}^{\mu+1} - \sum_{k=1}^{s-1} \Omega_k (D_k - D_s)(c_{k,m+1}^{\mu} - c_{k,m}^{\mu}), \quad m = M, ..., 0.$$

(ii) The system (45) has exactly one solution $(c_1^{\mu+1}, ..., c_{s-1}^{\mu+1})$ for given concentrations $(c_1^{\mu}, ..., c_{s-1}^{\mu})$ and a potential $F^{\mu+1}$ if and only if the steps h, τ are such small that $v_{i,m}^{\mu(m)} \neq 0$, $m = 0, ..., M+1$, $i = 1, ..., s-1$. It has the formula

$$\begin{aligned}
c_{i,M+1}^{\mu+1} &= \left(v_{i,M+1}^{\mu(M+1)}\right)^{-1} Q_{i,M+1}^{\mu(M+1)}, \\
c_{i,m}^{\mu+1} &= \left(v_{i,m}^{\mu(m)}\right)^{-1} \left(Q_{i,m}^{\mu(m)} - v_{i,m+1}^{\mu(m)} c_{i,m+1}^{\mu+1}\right), \quad m = M, ..., 0,
\end{aligned} \tag{48}$$

for $i = 1, ..., s-1$.

Let (c, F), $c = (c_1, ..., c_{s-1})$ be the solution of (41)–(43) and let (w, G), $w = (w_1, ..., w_{s-1})$ be the solution of (44), (45). Define the errors of the difference method

$$r = c - w, \quad R = F - G, \tag{49}$$

the maksimum norms

$$\begin{aligned}
\|r\|_0 &= \max\big\{|r_{i,m}^{\mu}| : \ \mu = 0, ..., K, \ i = 1, ..., s-1, \ m = 0, ..., M+1\big\}, \\
\|R\|_0 &= \max\big\{|R_{m}^{\mu}| : \ \mu = 1, ..., K, \ m = 0, ..., M+1\big\},
\end{aligned} \tag{50}$$

and the seminorms

$$\|r\|_{(\mu)} = \max\big\{|r_{i,m}^{\tilde{\mu}}| : \ \tilde{\mu} = 0, ..., \mu, \ i = 1, ..., s-1, \ m = 0, ..., M+1\big\}, \tag{51}$$

where $\mu = 0, \ldots, K$. Define also the difference quotients

$$\delta^+ r^\mu_{i,m} = \frac{r^\mu_{i,m+1} - r^\mu_{i,m}}{h}, \tag{52}$$
$$\delta^- r^\mu_{i,m} = \frac{r^\mu_{i,m} - r^\mu_{i,m-1}}{h},$$
$$\delta r^\mu_{i,m} = \frac{r^\mu_{i,m+1} - r^\mu_{i,m-1}}{2h},$$
$$\delta^{(2)} r^\mu_{i,m} = \frac{r^\mu_{i,m-1} - 2r^\mu_{i,m} + r^\mu_{i,m+1}}{h^2},$$

and analogously δR^μ_m, $\delta^{(2)} R^\mu_m$. We introduce the following seminorms

$$\|\delta r\|_0 = \max\left\{|\delta r^\mu_{i,m}| : \ \mu = 0, ..., K, \ i = 1, ..., s-1, \ m = 1, ..., M\right\}, \tag{53}$$
$$\|\delta^{(2)} r\|_0 = \max\left\{|\delta^{(2)} r^\mu_{i,m}| : \ \mu = 0, ..., K, \ i = 1, ..., s-1, \ m = 1, ..., M\right\},$$
$$\|\delta R\|_0 = \max\left\{|\delta R^\mu_m| : \ \mu = 1, ..., K, \ m = 1, ..., M\right\},$$
$$\|\delta^{(2)} R\|_0 = \max\left\{|\delta^{(2)} R^\mu_m| : \ \mu = 1, \ldots, K, \ m = 1, \ldots, M\right\},$$

and the maksimum norms

$$\|r\|_1 = \|r_0\| + \|\delta r\|_0, \tag{54}$$
$$\|r\|_2 = \|r_0\| + \|\delta r\|_0 + \|\delta^{(2)} r\|_0,$$
$$\|R\|_1 = \|R_0\| + \|\delta R\|_0,$$
$$\|R\|_2 = \|R_0\| + \|\delta R\|_0 + \|\delta^{(2)} R\|_0.$$

Theorem 5 ([A7], Thm. 2). *Assume that $(c, F) \in C^{1,2}([0, T] \times \overline{\Omega}, \mathbb{R}^{s-1})$, $c = (c_1, ..., c_{s-1})$ is the solution of (41)–(43) and (w, G), $w = (w_1, ..., w_{s-1})$ is the solution of (44), (45). Then there exist real valued functions $\alpha_i(\tau, h)$, $i = 0, 1, 2$ such that*

$$\|R\|_0 \le 2 \sum_{k=1}^{s-1} \Omega_k |D_k - D_s| \|r\|_0 + \alpha_0(\tau, h), \tag{55}$$
$$\|\delta R\|_0 \le \sum_{k=1}^{s-1} \Omega_k |D_k - D_s| \|\delta r\|_0 + \alpha_1(\tau, h),$$
$$\|\delta^{(2)} R\|_0 \le \sum_{k=1}^{s-1} \Omega_k |D_k - D_s| \|\delta^{(2)} r\|_0 + \alpha_2(\tau, h),$$

and $\lim\limits_{(\tau,h)\to(0,0)} \alpha_i(\tau, h) = 0$, *$i = 0, 1, 2$.*

Theorem 6 ([A7], Thm. 3) *Assume that $(c, F) \in C^{1,2}([0, T] \times \overline{\Omega}, \mathbb{R}^{s-1})$, $c = (c_1, \ldots, c_{s-1})$ is the solution of (41)–(43) and (w, G), $w = (w_1, \ldots, w_{s-1})$ is the solution of (44), (45). Let moreover*

$$\left|\delta G^\mu_m\right| \le A, \quad \left|\delta^{(2)} G^\mu_m\right| \le B, \quad \left|\delta^+ w^\mu_{i,0}\right|, \quad \left|\delta^- w^\mu_{i,M+1}\right| \le C, \tag{56}$$
$$Ah \le 2D_i, \quad \frac{h}{\tau} \le D, \quad \lim_{(\tau,h)\to(0,0)} \frac{h}{\tau} = 0, \tag{57}$$

$i = 1, ..., s-1$, $m = 1, ..., M$, $\mu = 0, ..., K$, where $A, C, D \ge 0$, $B > 0$. Then there exist a real valued function $\beta(\tau, h)$ and a constant $d \ge 0$ such that

$$\|r\|_0 \le \frac{e^{LT} - 1}{L} \Big[\big(1 + h \frac{C}{D_i} \sum_{k=1}^{s-1} \Omega_k |D_k - D_s|\big) d \ \big(\|\delta R\|_0 + \|\delta^{(2)} R\|_0\big) + \beta(\tau, h) \Big] \tag{58}$$

and $\lim\limits_{(\tau,h)\to(0,0)} \beta(\tau,h)=0$, *where* $L=\frac{CD}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|+\left(1+2\Lambda\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\right)B.$

The proof of Theorem 4 is based on the Gauss elimination method. Theorem 5 is shown using the error formula $R^{\mu+1}$, which is found a bit like the formula for $F^{\mu+1}$ in Theorem 4. Justifying of Theorem 6 requires a more advanced technique, namely the recurrence inequality for the seminorms $\|r\|_{(\mu)}$ i $\|r\|_{(\mu+1)}$ with the initial condition $\|r\|_{(0)}=0$ must be usesd. I took this technique from the works [A1], [A5], the content of which I will discuss later.

[A8] In this article, we have generalized the difference methods developed in [A7] for the case of the diffusion coefficients D_i nonlinearly dependent on the concentrations $c_1,...,c_s$, i.e. $D_i=D_i(N_i)$, where $N_i=c_i/(\sum_{k=1}^{s}c_k)$ is a mole fraction. Here the postulate (15) is already fully physically justified, i.e. with the sign "minus". We proved Theorem 1 on the existence and uniqueness of solutions to implicit difference schemes and Theorem 2 on the consistency and asymptotics of the error (see Remark 4). The last statement is important because the used approximation of the nonlinear coefficients D_i is quite subtle. We also described an experiment conducted in a laboratory with a three-component sample of iron, cobalt and nickel, considering a two-dimensional situation, and compared the results of this experiment with numerical simulations. Using the method from [88], we also determined the diffusion coefficients D_i of the three elements as the exponential functions of the mole fractions. These coefficients are not given in physical tables and depend, among others, on the percentage of the sample and the temperature. The conclusion is that the proposed mathematical model with the parabolic-elliptic system and the difference method describe the physical situation very well. This experiment is described in more detail, in many aspects, in [B16]. It is worth noting that the model and the construction of the difference method can be generalized to the three-dimensional case. However, conducting an appropriate experiment in a laboratory is technically complicated. We are currently working on it together with the researchers from the Faculty of Materials Science and Ceramics of AGH.

For the description of the difference method, I will focus on the one-dimensional situation, because in the two-dimensional case the idea is similar. Let $\Omega=(-\Lambda,\Lambda)\subset\mathbb{R}$. Proceeding analogously to [A7], the differential problem (16), (6), (18) we reduce to the form

$$\begin{cases} \partial_t c_i=\partial_x\big(D_i(N_i)\partial_x c_i\big)+\partial_x c_i\partial_x F+c_i\partial_{xx}F, & (t,x)\in[0,T]\times\Omega,\\ -\partial_{xx}F=\sum_{k=1}^{s-1}\Omega_k\partial_x\big(\big(D_k(N_k)-D_s(N_s)\big)\partial_x c_k\big), & (t,x)\in[0,T]\times\Omega,\\ \int_\Omega F dx=0, & t\in[0,T], \end{cases} \tag{59}$$

$$c_i(0,x)=c_{0i}(x),\quad x\in\Omega, \tag{60}$$

$$\begin{cases} -D_i(N_i)\partial_x c_i+c_i\sum_{k=1}^{s-1}\Omega_k\big(D_k(N_k)-D_s(N_s)\big)\partial_x c_k=0, & (t,x)\in[0,T]\times\partial\Omega,\\ \partial_x F=-\sum_{k=1}^{s-1}\Omega_k\big(D_k(N_k)-D_s(N_s)\big)\partial_x c_k, & (t,x)\in[0,T]\times\partial\Omega, \end{cases} \tag{61}$$

$i=1,...,s-1$, which again allowed the transfer of the Vegard rule to discrete solutions (see Remarks 3, 4). We have applied a modification of the method which, in addition to the grid points defined in [A7], also uses half points $x_{m+\frac12}=-\Lambda+(m+\frac12)h$, $m=1,...,M$ [59]. The terms $\partial_x\big(D_i(N_i)\partial_x c_i\big)$ in (59) we approximate at point (t^μ,x_m) with the difference quotients

$$\frac1h\Big(D^\mu_{i,m+\frac12}\frac1h\big(c^{\mu+1}_{i,m+1}-c^{\mu+1}_{i,m}\big)-D^\mu_{i,m-\frac12}\frac1h\big(c^{\mu+1}_{i,m}-c^{\mu+1}_{i,m-1}\big)\Big),$$

where

$$D^\mu_{i,m-\frac12}=D_i\Big(\frac12\big(N^\mu_{i,m-1}+N^\mu_{i,m}\big)\Big),$$
$$D^\mu_{i,m+\frac12}=D_i\Big(\frac12\big(N^\mu_{i,m}+N^\mu_{i,m+1}\big)\Big),$$

$m = 1, ..., M$. We approximate the terms $\partial_x\big(\big(D_k(N_k) - D_s(N_s)\big)\partial_x c_k\big)$ in a similar way, but the concentrations are taken at points t^μ instead of $t^{\mu+1}$. For the approximation of the remaining derivatives, the central, forward and backward difference quotients are used, and the integral equation is approximated by the trapezoidal method. Moreover, the terms $D_i(N_i)$ in the first $(s-1)$ boundary conditions in (61) we approximate by the numbers

$$D^\mu_{i,m} = D_i\big(N^\mu_{i,m}\big)$$

for $m = 0, M+1$ and similarly $D_k(N_k)$, $D_s(N_s)$. But the terms $D_k(N_k)$, $D_s(N_s)$ in the last boundary condition in (61) we approximate by the numbers $D^\mu_{k,\frac{1}{2}}$, $D^\mu_{s,\frac{1}{2}}$, $D^\mu_{k,M+\frac{1}{2}}$, $D^\mu_{s,M+\frac{1}{2}}$. We define implicit difference schemes for the elliptic part on the potential $F^{\mu+1}$ and for the parabolic part the concentrations $c^{\mu+1}_i$ of the form

$$\begin{cases} F^{\mu+1}_0 - F^{\mu+1}_1 = P^\mu_0 := \sum_{k=1}^{s-1}\Omega_k\big(D^\mu_{k,\frac{1}{2}} - D^\mu_{s,\frac{1}{2}}\big)\big(c^\mu_{k,1} - c^\mu_{k,0}\big), \\ -F^{\mu+1}_{m-1} + 2F^{\mu+1}_m - F^{\mu+1}_{m+1} = P^\mu_m := \sum_{k=1}^{s-1}\Omega_k\Big(\big(D^\mu_{k,m-\frac{1}{2}} - D^\mu_{s,m-\frac{1}{2}}\big)c^\mu_{k,m-1} \\ -\big(D^\mu_{k,m+\frac{1}{2}} - D^\mu_{s,m+\frac{1}{2}} + D^\mu_{k,m-\frac{1}{2}} - D^\mu_{s,m-\frac{1}{2}}\big)c^\mu_{k,m} \\ +\big(D^\mu_{k,m+\frac{1}{2}} - D^\mu_{s,m+\frac{1}{2}}\big)c^\mu_{k,m+1}\Big), \\ -F^{\mu+1}_M + F^{\mu+1}_{M+1} = P^\mu_{M+1} := \sum_{k=1}^{s-1}\Omega_k\big(D^\mu_{k,M+\frac{1}{2}} - D^\mu_{s,M+\frac{1}{2}}\big)\big(c^\mu_{k,M} - c^\mu_{k,M+1}\big), \\ F^{\mu+1}_0 + 2\sum_{m=1}^{M} F^{\mu+1}_m + F^{\mu+1}_{M+1} = 0, \end{cases} \tag{62}$$

$$\begin{cases} q^\mu_{i,0}c^{\mu+1}_{i,0} + q^\mu_{i,1}c^{\mu+1}_{i,1} = Q^\mu_{i,0} := 0, \\ d^\mu_{i,m-1}c^{\mu+1}_{i,m-1} + v^\mu_{i,m}c^{\mu+1}_{i,m} + u^\mu_{i,m+1}c^{\mu+1}_{i,m+1} = Q^\mu_{i,m} := e^\mu_{i,m}c^\mu_{i,m}, \\ q^\mu_{i,M}c^{\mu+1}_{i,M} + q^\mu_{i,M+1}c^{\mu+1}_{i,M+1} = Q^\mu_{i,M+1} := 0, \end{cases} \tag{63}$$

where

$$\begin{aligned} \kappa &= \frac{\tau}{h^2}, \\ v^\mu_{i,m} &= 1 + \kappa\left(D^\mu_{i,m+\frac{1}{2}} + D^\mu_{i,m-\frac{1}{2}}\right), \\ d^\mu_{i,m-1} &= \kappa\left(-D^\mu_{i,m-\frac{1}{2}} + \frac{1}{4}\big(F^{\mu+1}_{m+1} - F^{\mu+1}_{m-1}\big)\right), \\ u^\mu_{i,m+1} &= \kappa\left(-D^\mu_{i,m+\frac{1}{2}} - \frac{1}{4}\big(F^{\mu+1}_{m+1} - F^{\mu+1}_{m-1}\big)\right), \\ e^\mu_{i,m} &= 1 + \kappa\left(F^{\mu+1}_{m+1} - 2F^{\mu+1}_m + F^{\mu+1}_{m-1}\right), \\ q^\mu_{i,1} &= -D^\mu_{i,0} + \sum_{k=1}^{s-1}\Omega_k\big(D^\mu_{k,0} - D^\mu_{s,0}\big)\big(c^\mu_{k,1} - c^\mu_{k,0}\big), \\ q^\mu_{i,M} &= -D^\mu_{i,M+1} + \sum_{k=1}^{s-1}\Omega_k\big(D^\mu_{k,M+1} - D^\mu_{s,M+1}\big)\big(c^\mu_{k,M} - c^\mu_{k,M+1}\big), \\ q^\mu_{i,0} &= D^\mu_{i,0}, \\ q^\mu_{i,M+1} &= D^\mu_{i,M+1}, \end{aligned}$$

for $m = 1, ..., M$, $i = 1, ..., s-1$, $\mu = 0, ..., K-1$. If $v^{\mu(m)}_{i,m} \neq 0$, then we make a sequence of the Gauss substitutions for the scheme (63) using anlogous formulas as in (46).

Theorem 7 ([A8], Thm. 1).

(i) For all the steps h, τ, the system (62) has exactly one solution $F^{\mu+1}$ for given concentrations $(c_1^\mu, ..., c_{s-1}^\mu)$ of the form

$$F_{M+1}^{\mu+1} = \frac{\sum_{k=1}^{s-1} \Omega_k \Big[(D_{k,\frac{1}{2}}^\mu - D_{s,\frac{1}{2}}^\mu) c_{k,0}^\mu + \sum_{l=1}^{M} \Big((2l+1)(D_{k,l+\frac{1}{2}}^\mu - D_{s,l+\frac{1}{2}}^\mu)}{2(M+1)} \tag{64}$$

$$\frac{-(2l-1)(D_{k,l-\frac{1}{2}}^\mu - D_{s,l-\frac{1}{2}}^\mu) \Big) c_{k,l}^\mu - (1+2M)(D_{k,M+\frac{1}{2}}^\mu - D_{s,M+\frac{1}{2}}^\mu) c_{k,M+1}^\mu \Big]}{2(M+1)},$$

$$F_m^{\mu+1} = F_{m+1}^{\mu+1} + \sum_{k=1}^{s-1} \Omega_k (D_{k,m+\frac{1}{2}}^\mu - D_{s,m+\frac{1}{2}}^\mu)(c_{k,m+1}^\mu - c_{k,m}^\mu), \quad m = M, ..., 0.$$

(ii) The system (63) has exactly one solution $(c_1^{\mu+1}, ..., c_{s-1}^{\mu+1})$ for given concentrations $(c_1^\mu, ..., c_{s-1}^\mu)$ and a potential $F^{\mu+1}$ if and only if the steps h, τ are small enough that $v_{i,m}^{\mu(m)} \neq 0$, $m = 0, ..., M+1$, $i = 1, ..., s-1$. It has the formula

$$c_{i,M+1}^{\mu+1} = \left(v_{i,M+1}^{\mu(M+1)} \right)^{-1} Q_{i,M+1}^{\mu(M+1)}, \tag{65}$$

$$c_{i,m}^{\mu+1} = \left(v_{i,m}^{\mu(m)} \right)^{-1} \left(Q_{i,m}^{\mu(m)} - v_{i,m+1}^{\mu(m)} c_{i,m+1}^{\mu+1} \right), \quad m = M, ..., 0,$$

for $i = 1, ..., s-1$.

Theorem 8 ([A8], Thm. 2). *Assume that the initial concentrations c_{0i}, $i = 1, ..., s$ are of such regularity that the solution (c, F) of the differential problem (59)–(61) belongs to $C^3([0,T] \times \overline{\Omega}, \mathbb{R}^s)$, $D_i \in C^2([0,1], \mathbb{R}_+)$, $i = 1, ..., s$ and $\sum_{k=1}^{s} c_k \geq \alpha > 0$ for some α. Then the difference method (62), (63) is consistent and the truncation errors $r, R = O(\tau + h)$.*

The proof of Theorem 7 is based on the Gauss elimination method. Theorem 8 is justified using the Taylor formula with the Lagrange rest.

3 Electrodiffusion, [A4], [A9]

I will start again with the construction of mathematical models. Electrodiffusion is a process that combines two phenomena: mass diffusion transport and electric charge transport. Since the charges are located on ions, it was possible to take into account these two processes by properly defining the mass flux and adding an equation for the distribution of the electric field or electric potential. The first mathematical model to describe electrodiffusion was independently developed by Nernst [71] in 1889 and Planck [74] in 1890. This model was later investigated by Debye and Hückel [23]. In the literature it is referred to as the Nernst-Planck-Poisson model, the Poisson-Nernst-Planck model or sometimes the Debye-Hückel model. Transport and diffusion of electrically charged particles (ions, electrons, holes and colloids) play an important role in many disciplines of science and technology, especially in electrochemistry, electrical and biomedical engineering and medicine. It is described in detail in Sections 1 in [A4], [A9]. It is worth emphasizing that Hodgkin and Huxley received the Nobel Prize in Physiology and Medicine [39] in 1963 for their discoveries of ion mechanisms related to excitation and inhibition in the peripheral and central parts of the nerve cell membrane. For many years, intensive research has been carried out on the mechanism of ions transport of various elements in the so-called ion channels located in the cell membranes of various cells of living organisms. There are several biological theories about this, but none of them is entirely satisfactory. The artificial one-dimensional counterpart of biological ion channels are e.g. ion selective electrodes (ISE).

As in the process of mass interdiffusion in solids, electrodiffusion is described by the continuity equations (2). The fluxes are again a generalization of the Fick ones (1) and have the form

$$J_i = -D_i \nabla c_i + u_i c_i E, \tag{66}$$

where c_i mean the component charge concentrations, $D_i > 0$ are the constant diffusion coefficients of the components, E is the electric field strength generated by the total charge with a density $q = F \sum_{i=1}^{s} z_i c_i$ satisfying the relation

$$\mathrm{div} E = \frac{q}{\varepsilon_0 \varepsilon_r}, \tag{67}$$

F is the Faraday constant, z_i are the charge values of the components, and ε_0, ε_r are the vacuum permittivity and the relative permittivity of the medium, respectively. Moreover, $u_i = D_i z_i F/(RT)$ are ion mobilities, where R is the gas constant and T is the fixed temperature of the medium. The above relationship of diffusion coefficients with mobility is called the Einstein-Smoluchowski relation. The fluxes J_i are called the Nernst-Planck fluxes. In most applications, the electric field is replaced by an electric potential according to the formula

$$E = -\nabla \varphi, \tag{68}$$

which simply states that the electric field is a conservative field (this is true in the absence of magnetic fields). Hence, we get a strogly coupled nonlinear parabolic-elliptic system of the form

$$\begin{cases} \partial_t c_i + \mathrm{div}\Big(-D_i\Big(\nabla c_i + \alpha z_i c_i \nabla \varphi\Big)\Big) = 0, & (t,x) \in [0,T] \times \Omega, \\ -\triangle \varphi = \lambda \sum_{i=1}^{s} z_i c_i, & (t,x) \in [0,T] \times \Omega, \end{cases} \tag{69}$$

where $\lambda = F/(\varepsilon_0 \varepsilon_r)$ is the Debye constant, $\alpha = F/(RT)$, $i = 1, ..., s$. In the literature it is called the classical Nernst-Planck-Poisson system (cNPP) or the classical Poisson-Nernst-Planck system (cPNP) [51, 52, 78, 79, 81]. In the above model, the ions are treated as electron gas and the ionic effects are ignored or partially taken into account, such as the size of the ions [44]. Water is a dielectric. In the electrochemical potential, the so-called ideal component, i.e. the electric potential is only allowed. Thus, the system of equations (69) approximates electrodiffusion well, e.g. in the case of a system with suitably low ion concentrations.

We set the initial condition

$$c_i(0, x) = c_{0i}(x), \quad x \in \Omega. \tag{70}$$

A great theoretical and technical challenge is to set the boundary conditions for the system (69) applicable in the modeling of real processes that would be consistent with the experimental results. In the famous works by Biler, Hilhorst, Hebisch and Nadzieja [5, 6, 7, 8, 9], the existence and uniqueness are proved, and the asymptotic nature of solutions is studied, but only of physically closed systems, i.e. the flux of charges is at the boundary $\partial\Omega$ equal to zero, describing chemotaxis. Moreover, these authors assume a physically hardly feasible homogeneous Dirichlet condition on the potential φ. Also in many of the latest mathematical works devoted to ion channels or related issues by Constantin, Eisenberg, Liu, Li, Wang and others, although some generalizations of the system (69) are introduced taking into account some ionic effects and ion collisions, but a non-homogenous flux at the boundary is not allowed [18, 25, 26, 41, 44, 57, 60, 61, 62, 76, 85]. In my opinion for describing physically open systems, i.e. such that the flux of charges flows across the boundary or its part, the Chang-Jaffé (CJ) boundary conditions, used for the first time just by these authors in 1952 for polarization analysis in electrolytes in the one-dimensional case, $n = 1$, are especially useful [13]. Since then, in many works from the electrochemistry such conditions have been considering [10, 30, 56, 63, 80]. The basic idea in defining these conditions is to assume that the normal component of the charge flux at $\partial\Omega$ is proportional to the weighted difference between the flows inside and outside Ω,

$$J_i \cdot \mathbf{n} = -k_{i1} c_{i,out} + k_{i2} c_i, \quad (t,x) \in [0,T] \times \partial\Omega, \tag{71}$$

where k_{i1}, k_{i2} are the material constants, which describe the permeability of the boundary, and $c_{i,out}$ are the component concentrations outside the medium - it is assumed that they are constant. The boundary conditions (71) are typical for the evolutionary system (69) and turn into the Dirichlet condition on charge concentrations for the limit, i.e. the stationary cNPP system. Again, I know a few mathematical articles in which theorems concerning the existence and properties of solutions are proved, but precisely for stationary problems, i.e. in the natural way not using the CJ conditions [4, 26, 38, 43, 44, 55, 57, 60, 61, 76, 87]. From my knowledge it follows that the article [A4] is the first in which the existence and analytical properties of solutions of the one-dimensional cNPP evolutionary system, $n = 1$, with nonlinear boundary conditions, which may be in the form of CJ, are mathematically investigated. The research technique used here was generalized to the three-dimensional case, $n = 3$, in the article [A9], where I proposed an ion channel model. In this work, the mathematically idealized set Ω is a cylinder on the wall of which the flux has a value of zero, and on the input and output, the CJ conditions are given. The Robin condition is set on the potential. The CJ conditions are more difficult for mathematical studing the existence of local solutions over time, mainly due to problems with finding appropriate estimates, and global solutions over time due to the lack of the law of conservation of mass or charge. The difficulties with local proofs were overcome in [A4], [A9] by considering certain closed, bounded, and convex sets instead of closed balls, in the corresponding Sobolev norms.

[A4] In this article, we proved Theorems 4.2, 5.1, 6.1 about the existence, uniqueness and non-negativity of local in time weak solutions in appropriate Sobolev spaces, to the one-dimensional nonlinear parabolic-elliptic system (69) with the initial condition (70), and non-linear boundary conditions on concentrations and the non-homogenous Dirichlet condition on a potential. The boundary conditions may have especially the form of CJ (71) on the basis of Remark 3.2. For simplicity, we considered two types of ions, $s = 2$, but the results can be naturally generalized to any number of components.

Denote $\Omega = (0,1) \subset \mathbb{R}$ and let $T > 0$ be arbitrary. Let functions $u_0, v_0 : \Omega \to \mathbb{R}$, $f_i, g_i : [0,T] \times \mathbb{R} \to \mathbb{R}$, $h_i : [0,T] \to \mathbb{R}$ and constants $\alpha_i, \beta_i, \lambda > 0$ for $i = 1, 2$ be given. We consider the differential problem

$$\begin{cases} u_t = \alpha_1 u_{xx} - \alpha_2 (u\varphi_x)_x, & (t,x) \in [0,T] \times \Omega, \\ v_t = \beta_1 v_{xx} + \beta_2 (v\varphi_x)_x, & (t,x) \in [0,T] \times \Omega, \\ \varphi_{xx} = \lambda(u - v), & (t,x) \in [0,T] \times \Omega, \end{cases} \tag{72}$$

$$u(0,x) = u_0(x), \quad v(0,x) = v_0(x), \quad x \in \Omega, \tag{73}$$

$$\begin{cases} \alpha_1 u_x(t,0) - \alpha_2 u(t,0)\varphi_x(t,0) = f_1(t, u(t,0)), & t \in [0,T], \\ \alpha_1 u_x(t,1) - \alpha_2 u(t,1)\varphi_x(t,1) = f_2(t, u(t,1)), & t \in [0,T], \\ \beta_1 v_x(t,0) + \beta_2 v(t,0)\varphi_x(t,0) = g_1(t, v(t,0)), & t \in [0,T], \\ \beta_1 v_x(t,1) + \beta_2 v(t,1)\varphi_x(t,1) = g_2(t, v(t,1)), & t \in [0,T], \\ \varphi(t,0) = h_1(t), & t \in [0,T], \\ \varphi(t,1) = h_2(t), & t \in [0,T]. \end{cases} \tag{74}$$

If we put $s = 2$, $z_1 = -z$, $z_2 = z$, $(z \in \mathbb{N})$, $u = c_1$, $v = c_2$, $\alpha_1 = D_1$, $\alpha_2 = -D_1 z_1 \frac{F}{RT}$, $\beta_1 = D_2$, $\beta_2 = D_2 z_2 \frac{F}{RT}$, $\lambda = \frac{F}{\varepsilon_r \varepsilon_0}$, then the system (72) is a special case of (69). In accordance with

Remark 2.1, let us assume that $h_1(t) = h_2(t) \equiv 0$. Define the Sobolev spaces $V = H^1(\Omega)$ and $H = L^2(\Omega)$. Then $V \subset H \subset V^*$ constitute the evolution triple with the embeddings being dense, continuous, and compact. Define the set

$$H_+ = \{u \in H : \ u(x) \geq 0 \quad \text{a.e. in} \quad \Omega\}.$$

Assumption H.

(H_0) $u_0 \in H$ and $v_0 \in H$.

(H_1) f_i, g_i, $i = 1, 2$ satisfy the Carathéodory conditions: $f_i(\cdot, u)$ and $g_i(\cdot, u)$ are mesaurable in the Lebesgue sens, and $f_i(t, \cdot)$ and $g_i(t, \cdot)$ are continuous.

(H_2) The following growth conditions hold

$$|f_i(t, u)| \leq a_{1i} + a_{2i}|u|, \quad |g_i(t, u)| \leq b_{1i} + b_{2i}|u|,$$

for a.e. $t \in (0, T)$ and all $u \in \mathbb{R}$, with the constants $a_{1i}, a_{2i}, b_{1i}, b_{2i} \geq 0$, $i = 1, 2$.

(H_3) The following one sided Lipschitz conditions hold

$$\begin{aligned} f_1(t, u_1) - f_1(t, u_2) &\geq -L_{f_1}(u_1 - u_2), \\ g_1(t, u_1) - g_1(t, u_2) &\geq -L_{g_1}(u_1 - u_2), \\ f_2(t, u_1) - f_2(t, u_2) &\leq L_{f_2}(u_1 - u_2), \\ g_2(t, u_1) - g_2(t, u_2) &\leq L_{g_2}(u_1 - u_2), \end{aligned}$$

for a.e. $t \in (0, T)$ and all $u_1, u_2 \in \mathbb{R}$, $u_1 \geq u_2$, with the constants $L_{f_i}, L_{g_i} \geq 0$, $i = 1, 2$.

Assumption H^+.

(H_0^+) $u_0 \in H_+$ and $v_0 \in H_+$.

(H_1^+) For all $u < 0$ and a.e. $t \in (0, T)$

$$f_1(t, u) \leq 0, \quad g_1(t, u) \leq 0,$$

$$f_2(t, u) \geq 0, \quad g_2(t, u) \geq 0.$$

The original initial-boundary value problem (72)–(74) has the following weak version.

Problem PE. Find $u, v \in L^2(0, T; V)$ and $\varphi \in L^2(0, T; H^3(\Omega) \cap H_0^1(\Omega))$ such that $u_t, v_t \in L^2(0, T; V^*)$ and for a.e. $t \in (0, T)$

$$\begin{aligned} &\langle u_t, \eta \rangle_{V^* \times V} + \int_\Omega (\alpha_1 u_x - \alpha_2 u \varphi_x) \eta_x dx && (75) \\ &\quad = f_2(t, u(t, 1))\eta(1) - f_1(t, u(t, 0))\eta(0) \quad \text{for each} \quad \eta \in V, \\ &\langle v_t, \zeta \rangle_{V^* \times V} + \int_\Omega (\beta_1 v_x + \beta_2 v \varphi_x) \zeta_x dx && (76) \\ &\quad = g_2(t, v(t, 1))\zeta(1) - g_1(t, v(t, 0))\zeta(0) \quad \text{for each} \quad \zeta \in V, \\ &\int_\Omega \varphi_x \xi_x dx + \lambda \int_\Omega (u - v)\xi dx = 0 \quad \text{for each} \quad \xi \in H_0^1(\Omega), && (77) \end{aligned}$$

and the initial condition (73) holds.

We proved the following theorems.

Theorem 9 ([A4], Thm. 4.2). *If assumptions* (H_0), (H_1), (H_2) *are satisfied, then there is* $T > 0$ *such that Problem PE has a solution.*

Theorem 10 ([A4], Thm. 5.1). *If Assumption H is satisfied, then Problem PE has at most one solution on* $[0, T]$ *for any* $T > 0$.

Theorem 11 ([A4], Thm. 6.1). *Let Assumptions H, H*$^+$ *hold. Then if a solution to Problem PE exists on* $[0, T]$ *for some* $T > 0$, *we have* $u(t) \in H_+$ *and* $v(t) \in H_+$ *for all* $t \in [0, T]$.

In order to prove Theorem 9, we split Problem PE into two auxiliary problems, the elliptic and parabolic problem. This technique was initiated by Gajewski [33], and then it was used among others by Biler, Hebisch and Nadzieja [5, 6]. In lemmas 4.1 and 4.2 we show that these problems have the unique solution, which allows to define a certain operator Λ_T defined on the set $B = B(T, Q_0, Q_1, Q_2, R_0, R_1, R_2)$ parameterized by the time $T > 0$ and constants $Q_0, Q_1, Q_2, R_0, R_1, R_2 > 0$,

$$\begin{aligned} B = \Big\{ (w, z) \in X_T \, : \, & \|w\|^2_{L^2(0,T;H)} \le Q_0, \ \|w_x\|^2_{L^2(0,T;H)} \le Q_1, \\ & \|z\|^2_{L^2(0,T;H)} \le R_0, \ \|z_x\|^2_{L^2(0,T;H)} \le R_1, \\ & \|w_t\|^2_{L^2(0,T;V^*)} \le Q_2, \ \|z_t\|^2_{L^2(0,T;V^*)} \le R_2 \Big\}, \end{aligned} \tag{78}$$

where

$$X_T = \{(u, v) \in L^2(0, T; V) \times L^2(0, T; V) \, : \, u_t, v_t \in L^2(0, T; V^*)\} \tag{79}$$

with the norm

$$\|(u, v)\|_{X_T} = \|u\|_{L^2(0,T;V)} + \|v\|_{L^2(0,T;V)} + \|u_t\|_{L^2(0,T;V^*)} + \|v_t\|_{L^2(0,T;V^*)},$$

$$\|u\|^2_{L^2(0,T;V)} = \int_0^T \|u(t)\|^2_V \, dt, \quad \|u_t\|^2_{L^2(0,T;V^*)} = \int_0^T \|u_t(t)\|^2_{V^*} \, dt$$

is a Sobolev space. Note that the set B is closed, bounded, convex and nonempty. Then we use Lemmas 4.3, 4.4 and a version of the Schauder–Tychonoff fixed point theorem, which is a consequence of Theorem 1 in [3].

Theorem 12 ([A4], Thm. 4.1). *Let* X *be a reflexive Banach space and let* $C \subset X$ *be a closed, bounded, convex and nonempty set. If the function* $\Lambda : C \to C$ *is sequentially weakly continuous, then it has at least one fixed point.*

Let us stress that B is not a closed ball, as for example in [5, 6], but it is the closed subset of a closed ball. It is this form of the set B that allowed for the selection of parameters and guaranteed the existence of $T > 0$ such that the operator Λ_T was internal, i.e. $\Lambda_T(B) \subset B$. Such difficulties in finding suitable estimates are due to the non-homogenous and nonlinear form of the boundary conditions (74). It is also interesting the auxiliary using of fractional Sobolev spaces $H^s(\Omega)$, $s \in (\frac{1}{2}, 1)$. This made it possible to make the proof of the existence of solutions independent of the size of the constants present in the equations, in particular of the diffusion coefficients D_i, which is important in physical applications. We proved Theorem 10 using the Gronwall, Hölder, Young inequalities and the Ehrling lemma. To prove Theorem 11, we again used Theorem 12 and the barrier method.

[A9] In this article, I studed the model of ion transport and diffusion in biological channels. It is described by the three-dimensional nonlinear parabolic-elliptic system (69) with the initial condition (70), and nonlinear boundary conditions on concentrations and the Robin condition on a potential. An important novelty is considering the Chang–Jaffé boundary conditions for fluxes, on the input and output of the channels (71), and the Robin on a potential, as well as allowing any number of different types of ions with different charges and mobilities. I proved Theorems 4.2, 5.1, 6.1 about the existence, uniqueness and non-negativity of local in time weak solutions in appropriate Sobolev spaces and Lemmas 4.1, 4.2, 4.3, 4.4. I used a similar proof technique as in [A4], but due to the dimension $n = 3$, I constructed a different, more subtle set B, different differential-integral and trace inequalities, and moreover I had to approximate the Sobolev space $L^2(0, T, H^1(\Omega))$ by its dense subspace $L^2(0, T, H^2(\Omega))$. I also proved two auxiliary theorems 3.1, 3.2 about the estimate and regularization of solutions to an elliptic equation with the Robin boundary condition.

We define a simplified cylindrical membrane channel $\Omega \subset \mathbb{R}^3$ with the boundary $\partial\Omega$ belonging to class C^∞ of the form

$$\Omega = \Big\{(x_1, x_2, x_3) \in \mathbb{R}^3 : \ 0 < x_1 < 1, \ x_2^2 + x_3^2 < g^2(x_1)\Big\},$$

where $g \in C^\infty([0, 1], \mathbb{R})$. The boundary $\partial\Omega$ we split into three portions as follows

$$\partial_1\Omega = \Big\{(x_1, x_2, x_3) \in \partial\Omega : \ x_1 = 0\Big\},$$

$$\partial_2\Omega = \Big\{(x_1, x_2, x_3) \in \partial\Omega : \ x_1 = 1\Big\},$$

$$\partial_3\Omega = \Big\{(x_1, x_2, x_3) \in \partial\Omega : \ 0 < x_1 < 1, \ x_2^2 + x_3^2 = g^2(x_1)\Big\}.$$

Thus, $\partial_1\Omega$ and $\partial_2\Omega$ are viewed as the input and output of the channel, respectively and $\partial_3\Omega$ - the wall of the channel. Let functions $c_{0i} : \Omega \to \mathbb{R}$, $a, b, h : [0, T] \times \partial\Omega \to \mathbb{R}$ and constants $D_i, \alpha, \lambda > 0$, $a_{ji}, b_{ji} \geq 0$, $z_i \in \mathbb{R}$, $i = 1, ..., s$, $j = 1, 2$ be given, where $T > 0$ is arbitrary. We consider the differential problem

$$\begin{cases} \partial_t c_i + \operatorname{div}\big(-D_i\big(\nabla c_i + \alpha z_i c_i \nabla\varphi\big)\big) = 0, & (t, x) \in [0, T] \times \Omega, \\ -\triangle\varphi = \lambda \sum_{j=1}^{s} z_j c_j, & (t, x) \in [0, T] \times \Omega, \end{cases} \tag{80}$$

$$c_i(0, x) = c_{0i}(x), \quad x \in \Omega, \tag{81}$$

$$\begin{cases} -D_i\left(\frac{\partial c_i}{\partial n} + \alpha z_i c_i \frac{\partial\varphi}{\partial n}\right) = -a_{1i} + b_{1i} c_i, & (t, x) \in [0, T] \times \partial_1\Omega, \\ -D_i\left(\frac{\partial c_i}{\partial n} + \alpha z_i c_i \frac{\partial\varphi}{\partial n}\right) = -a_{2i} + b_{2i} c_i, & (t, x) \in [0, T] \times \partial_2\Omega, \\ -D_i\left(\frac{\partial c_i}{\partial n} + \alpha z_i c_i \frac{\partial\varphi}{\partial n}\right) = 0, & (t, x) \in [0, T] \times \partial_3\Omega, \\ a(t, x)\frac{\partial\varphi}{\partial n} + b(t, x)\varphi = h(t, x), & (t, x) \in [0, T] \times \partial\Omega, \end{cases} \tag{82}$$

for $i = 1, ..., s$. Define the Sobolev spaces $V = H^1(\Omega)$ and $H = L^2(\Omega)$. Then $V \subset H \subset V^*$ constitute the evolution triple with the embeddings being dense, continuous and compact. Define the set

$$H_+ = \{u \in H : \ u(x) \geq 0 \quad \text{a.e. in} \quad \Omega\}.$$

Assumption H.

(H_0) $c_{0i} \in H$, $i = 1, ..., s$.

(H_1) $\frac{b}{a} \in L^\infty(0, T; C^\infty(\partial\Omega))$, $\frac{h}{a} \in L^\infty(0, T; H^{\frac{1}{2}}(\partial\Omega))$.

(H_2) $\frac{b}{a}(t, x) \geq p_0 > 0$ for a.e. $t \in (0, T)$ and all $x \in \partial\Omega$, $p_0 = \text{const}$.

The original initial-boundary value problem (80)–(82) has the following weak version.

Problem PE. Find $c_i \in L^2(0,T;V)$ and $\varphi \in L^2(0,T;H^2(\Omega))$ such that $\partial_t c_i \in L^2(0,T;V^*)$ and for a.e.. $t \in (0,T)$

$$\langle \partial_t c_i, \eta_i \rangle_{V^* \times V} + \int_\Omega D_i(\nabla c_i + \alpha z_i c_i \nabla \varphi) \circ \nabla \eta_i \, dx \tag{83}$$
$$= \int_{\partial_1 \Omega} (a_{1i} - b_{1i} c_i)\, \eta_i \, d\sigma + \int_{\partial_2 \Omega} (a_{2i} - b_{2i} c_i)\, \eta_i \, d\sigma \quad \text{for each} \quad \eta_i \in V,$$

$$\int_\Omega \nabla \varphi \circ \nabla \xi \, dx + \int_{\partial \Omega} \frac{b}{a} \varphi \, \xi \, d\sigma = \lambda \sum_{j=1}^{s} \int_\Omega z_j c_j \xi \, dx + \int_{\partial \Omega} \frac{h}{a} \xi \, d\sigma \quad \text{for each} \quad \xi \in V, \tag{84}$$

and the initial condition (81) holds.

We proved the following theorems.

Theorem 13 ([A9], Thm. 4.2). *If Assumption H holds, then there exists $T > 0$ such that Problem PE has a solution.*

Theorem 14 ([A9], Thm. 5.1). *If Assumption H holds, then Problem PE has at most one solution on $[0,T]$ for an arbitrary $T > 0$.*

Theorem 15 ([A9], Thm. 6.1). *Let Assumption H be true and $c_{0i} \in H_+$, $i = 1, ..., s$. Then if a solution to Problem PE exists on $[0,T]$ for some $T > 0$, we have $u(t) \in H_+$ and $v(t) \in H_+$ for all $t \in [0,T]$.*

The idea of the proofs of the above theorems is similar to that in [A4], but the set $B = B(T, Q_0, Q_1, Q_2, Q_3)$ now has the form

$$B = \big\{ w \in X_T \, : \, \|w_i\|^2_{L^2(0,T;H)} \le Q_0, \ \|\nabla w_i\|^2_{L^2(0,T;H)} \le Q_1, \ \|\partial_t w_i\|^2_{L^2(0,T;V^*)} \le Q_2, \\ \|w_i\|^4_{L^4(0,T;H)} \le Q_3 \big\}. \tag{85}$$

The difference with (78) is adding of the condition: $\|w_i\|^4_{L^4(0,T;H)} \le Q_3$. The next comments are analogous to the ones following the formulation of Theorem 12.

4 Diffusion and transport of impulses in neurons, [A2], [A3]

The phenomenon of the generation and propagation of nerve impulses in neurons began to be intensively studied in the second half of the 20th century. The neuron, or nerve cell, is the basic element of the nervous system. One of the best known models is the Hodgkin-Huxley one-dimensional reaction-diffusion-kinetic system from 1952,

$$\begin{cases} u_t - u_{xx} = f(u,v), \\ v_t = g(u,v), \end{cases} \tag{86}$$

where f and g have the appropriate form and are given [39]. The function $u \in \mathbb{R}$ is the electric field potential in the neuron, and $v \in \mathbb{R}^3$ describes the conductivity of three types of ions. This model is mathematically complex and has been simplified by Nagumo [70] and FitzHugh [31], [32] to the form

$$\begin{cases} u_t - u_{xx} = -f(u) - v, \\ v_t = bu, \end{cases} \tag{87}$$

where $f(u) = u(a-u)(1-u)$, $a, b > 0$ are constant and $v \in \mathbb{R}$. Mainly due to difficulties in the construction of solutions of a particular form, e.g. of the soliton traveling wave type, caused by the nonlinearity of f, McKean [68] modified this system as follows

$$\begin{cases} u_t - u_{xx} = H(u-a) - u - v, \\ v_t = bu - dv, \end{cases} \tag{88}$$

where H is the Heaviside function and $a, b > 0$, $d \geq$ are constant. More general systems of this type, including both the Hodgkin-Huxley neurobiological model and the Field-Noyes model of the Belousov-Zhabotinsky chemical reaction, with $v \in \mathbb{R}^n$ were investigated in [27], [53]. Hyperbolic generalization of the system (88) in the form

$$\begin{cases} \tau u_{tt} + u_t - u_{xx} = H(u-a) - u - v, \\ v_t = bu - dv, \end{cases} \tag{89}$$

where $\tau \geq 0$ is the relaxation time, was proposed in 2015 in the paper by Likus and Vladimirov [58]. These authors constructed the soliton and proved its stability. The first equation in (89) can be formally derived by replacing the Fick flux in the continuity equation

$$\gamma u_t + \mathrm{div} J = 0 \tag{90}$$

with a flux which satisfies the Cattaneo equation,

$$\tau J_t + J = -k \nabla u \tag{91}$$

taking into account the effects of memory related to the internal structure of the medium, and assuming mathematical simplification $k = \gamma = 1$ [45], [67]. Here u denotes the propagating ion wave. In [34, 35] an even more general model than that in [58] is considered. The results of numerical simulations of the model from [34] are presented in [35], which show that the dynamics of the evolution of the soliton-like solution in the relaxation model is different from what is observed without inclusion this effect.

[A2] In this article I proved Theorem 4.1 about the existence, uniqueness and estimate of local in time, bounded with the first derivatives, with locally Hölder continuous or globally Lipschitz continuous the first derivatives, according to the regularity of initial conditions, solutions of some one-dimensional weakly coupled nonlinear hyperbolic initial differential problem. I also proved Lemma 3.1 about the equivalence of this differential problem to an integral system in the appropriate class of functions. I did not find any results in the literature regarding the existence of solutions to such an initial problem.

Let functions $f : [0,T] \times \mathbb{R}^{2+k} \to \mathbb{R}$, $g = (g_1, ..., g_k) : [0,T] \times \mathbb{R}^{2+k} \to \mathbb{R}^k$ of unknowns $(t, x, p, r) \in [0,T] \times \mathbb{R}^{2+k}$, $u_0, u_1 : \mathbb{R} \to \mathbb{R}$, $v_0 = (v_{01}, ..., v_{0k}) : \mathbb{R} \to \mathbb{R}^k$ and a constant $c \in \mathbb{R}$ be given, where $T > 0$ is fixed. Consider the initial differential problem

$$\begin{cases} u_{tt} - u_{xx} + cu_t = f(t, x, u, v), & (t,x) \in [0,T] \times \mathbb{R}, \\ v_t = g(t, x, u, v), & (t,x) \in [0,T] \times \mathbb{R}, \end{cases} \tag{92}$$

$$\begin{cases} u(0,x) = u_0(x), & x \in \mathbb{R}, \\ v(0,x) = v_0(x), & x \in \mathbb{R}, \\ u_t(0,x) = u_1(x), & x \in \mathbb{R}, \end{cases} \tag{93}$$

where $v = (v_1, ..., v_k)$. If $c > 0$, then the first hiperbolic wave equation in (92) is called the telegraph equation. The rest of k equations of the first order in (92) may be treated as equations with the space parameter x. By the symbol $\| \cdot \|$ we denote the maximum norm in $\mathbb{R}^d$, $d \in \mathbb{N}$

$$\|y\| = \max_{i=1,...,d} |y_i|, \quad y = (y_1, ..., y_d) \in \mathbb{R}^d. \tag{94}$$

In the space of continuous and bounded functions $C_b\left(\Omega,\mathbb{R}^d\right)$ we define the supremum norm

$$\|z\|_0=\sup\left\{\|z\left(\omega\right)\|:\ \omega\in\Omega\right\},\quad z\in C_b\left(\Omega,\mathbb{R}^d\right),\tag{95}$$

where $\Omega=\mathbb{R}$ or $\Omega\subset\mathbb{R}^2$. The space of continuous and bounded functions together with their first derivatives we denote by $C_b^1\left(\Omega,\mathbb{R}^d\right)$. The norm in this space we define by the formula

$$\|z\|_1=\|z\|_0+\|z_t\|_0+\|z_x\|_0,\quad z\in C_b^1\left(\Omega,\mathbb{R}^d\right).\tag{96}$$

The spaces $\left(C_b\left(\Omega,\mathbb{R}^d\right),\|\cdot\|_0\right)$ i $\left(C_b^1\left(\Omega,\mathbb{R}^d\right),\|\cdot\|_1\right)$ are the Banach ones. Let $\alpha\in(0,1]$ be fixed. For any $z\in C_b\left(\Omega,\mathbb{R}^d\right)$ we define a number

$$[z]_{H,\alpha}=\sup\left\{\|z\left(t,x\right)-z\left(\bar{t},\bar{x}\right)\|\left[|t-\bar{t}|+|x-\bar{x}|\right]^{-\alpha}:\ \left(t,x\right),\left(\bar{t},\bar{x}\right)\in\Omega\right\}.\tag{97}$$

If $[z]_{H,\alpha}<\infty$, then it is the smallest Hölder constant for the function z and the exponent α, and it is usually called the Hölder coefficient. If $\alpha=1$, then it is the Lipschitz coefficient. We define the Hölder spaces $C^{0+\alpha}\left(\Omega,\mathbb{R}^d\right)\subset C_b\left(\Omega,\mathbb{R}^d\right)$, $C^{1+\alpha}\left(\Omega,\mathbb{R}^d\right)\subset C_b^1\left(\Omega,\mathbb{R}^d\right)$ with the finite norms, respectively

$$\begin{aligned}\|z\|_{0+\alpha}&=\|z\|_0+[z]_{H,\alpha},\\ \|z\|_{1+\alpha}&=\|z\|_1+[z_t]_{H,\alpha}+[z_x]_{H,\alpha}.\end{aligned}\tag{98}$$

Obviously if $\Omega=\mathbb{R}$, then t and z_t in the above definitions do not appear. Let $\Delta(x,\tau)\subset\mathbb{R}\times[0,\tau]$, $x\in\mathbb{R}$ be any isosceles triangle with the vertices $(x-\tau,0)$, (x,τ), $(x+\tau,0)$. We define the Hölder space $C_{loc}^{1+\alpha}\big([0,\tau]\times\mathbb{R},\mathbb{R}^d\big)\subset C_b^1\left([0,\tau]\times\mathbb{R},\mathbb{R}^d\right)$ of functions $z\in C^{1+\alpha}\big(\Delta(x,\tau),\mathbb{R}^d\big)$ for each $\Delta(x,\tau)$, with the constants

$$\begin{aligned}[z_t]_{H,\alpha,\Delta(x,\tau)}&=\sup\left\{\|z_t\left(t,x\right)-z_t\left(\bar{t},\bar{x}\right)\|\left[|t-\bar{t}|+|x-\bar{x}|\right]^{-\alpha}:\ \left(t,x\right),\left(\bar{t},\bar{x}\right)\in\Delta(x,\tau)\right\},\\ [z_x]_{H,\alpha,\Delta(x,\tau)}&=\sup\left\{\|z_x\left(t,x\right)-z_x\left(\bar{t},\bar{x}\right)\|\left[|t-\bar{t}|+|x-\bar{x}|\right]^{-\alpha}:\ \left(t,x\right),\left(\bar{t},\bar{x}\right)\in\Delta(x,\tau)\right\},\end{aligned}\tag{99}$$

independent of $\Delta(x,\tau)$. We say that z_t, z_x are uniformly Hölder continuous in $[0,\tau]\times\mathbb{R}$. It is clear that if $\alpha=1$, then $C_{loc}^{1+\alpha}\left([0,\tau]\times\mathbb{R},\mathbb{R}^d\right)=C^{1+\alpha}\big([0,\tau]\times\mathbb{R},\mathbb{R}^d\big)$.

Assumption $\mathrm{H}_1[u_0,v_0,u_1]$. The functions $u_0\in C^{1+\alpha}\left(\mathbb{R},\mathbb{R}\right)\cap C^2\left(\mathbb{R},\mathbb{R}\right)$, $v_0\in C^{1+\alpha}\left(\mathbb{R},\mathbb{R}^k\right)$, $u_1\in C^{0+\alpha}\left(\mathbb{R},\mathbb{R}\right)\cap C^1\left(\mathbb{R},\mathbb{R}\right)$ are such that

$$\|u_0\|_0\le\Lambda_1,\quad\|u_1\|_0\le\Lambda_1^{(1)},\quad\|(u_0)_x\|_0\le\Lambda_1^{(1)},$$

$$[u_1]_{H,\alpha}\le\Lambda_1^{(2)},\quad[(u_0)_x]_{H,\alpha}\le\Lambda_1^{(2)},$$

$$\|v_0\|_0\le\Lambda_2,\quad\|g\left(0,\cdot,u_0\left(\cdot\right),v_0\left(\cdot\right)\right)\|_0\le\Lambda_2^{(1)},\quad\|(v_0)_x\|_0\le\Lambda_2^{(1)},$$

$$[g\left(0,\cdot,u_0\left(\cdot\right),v_0\left(\cdot\right)\right)]_{H,\alpha}\le\Lambda_2^{(2)},\quad[(v_0)_x]_{H,\alpha}\le\Lambda_2^{(2)},$$

where the constants Λ_i, $\Lambda_i^{(j)}\ge0$, $i,j=1,2$ are arbitrarily given.

Assumption $\mathrm{H}_2[f,g]$. The functions f, g and the derivatives f_x, f_p, f_{r_i}, g_x, g_p, g_{r_i}, $i=1,...,k$ are continuous. Moreover, there exist nondecreasing functions M_i, $M_i^{(1)}$, H_2, $H_2^{(1)}:\mathbb{R}_+^2\to\mathbb{R}_+$, $i=1,2$ such that for all $t,\bar{t}\in[0,T]$, $x,\bar{x}\in\mathbb{R}$, $(q_1,q_2)\in\mathbb{R}_+^2$, $|p|,|\bar{p}|\le q_1$, $\|r\|,\|\bar{r}\|\le q_2$ we have

$$\begin{aligned}|f\left(t,x,p,r\right)|&\le M_1\left(q_1,q_2\right),\\ |f_x\left(t,x,p,r\right)|,\ |f_p\left(t,x,p,r\right)|,\ |f_{r_i}\left(t,x,p,r\right)|&\le M_1^{(1)}\left(q_1,q_2\right),\\ \|g\left(t,x,p,r\right)\|&\le M_2\left(q_1,q_2\right),\\ \|g_x\left(t,x,p,r\right)\|,\ \|g_p\left(t,x,p,r\right)\|,\ \|g_{r_i}\left(t,x,p,r\right)\|&\le M_2^{(1)}\left(q_1,q_2\right),\end{aligned}$$

$$
\begin{aligned}
\|g(t,x,p,r) - g(\bar{t},x,p,r)\| &\le H_2(q_1,q_2)\,|t-\bar{t}|^{\alpha}, \\
\|g_x(t,x,p,r) - g_x(t,\bar{x},\bar{p},\bar{r})\| &\le H_2^{(1)}(q_1,q_2)\,[|x-\bar{x}| + |p-\bar{p}| + \|r-\bar{r}\|]^{\alpha}, \\
\|g_p(t,x,p,r) - g_p(t,\bar{x},\bar{p},\bar{r})\| &\le H_2^{(1)}(q_1,q_2)\,[|x-\bar{x}| + |p-\bar{p}| + \|r-\bar{r}\|]^{\alpha}, \\
\|g_{r_i}(t,x,p,r) - g_{r_i}(t,\bar{x},\bar{p},\bar{r})\| &\le H_2^{(1)}(q_1,q_2)\,[|x-\bar{x}| + |p-\bar{p}| + \|r-\bar{r}\|]^{\alpha}.
\end{aligned}
$$

Assumption $\mathrm{H}_3[Q]$. Parameters Q_i, $Q_i^{(j)}$, $i,j=1,2$ fulfill the inequalities

$$
\begin{aligned}
&Q_1 > \Lambda_1, && \\
&Q_1^{(1)} > \Lambda_1^{(1)}, && \\
&Q_1^{(2)} > 2\Lambda_1^{(2)}, && \alpha \in (0,1), \\
&Q_1^{(2)} > M_1^* + \frac{c^2}{4}Q_1 + \frac{c^2}{4}\Lambda_1 + \frac{3}{2}c\Lambda_1^{(1)} + 2\Lambda_1^{(2)}, && \alpha = 1, \\
&Q_2 > \Lambda_2, && \\
&Q_2^{(1)} \ge M_2^*, \quad Q_2^{(1)} > \Lambda_2^{(1)}, && \\
&Q_2^{(2)} > H_2^*, \quad Q_2^{(2)} > \Lambda_2^{(2)}, && \alpha \in (0,1), \\
&Q_2^{(2)} \ge M_2^{(1)*}\left[1 + 2\left(Q_1^{(1)} + nQ_2^{(1)}\right)\right] + H_2^*, && \alpha = 1, \\
&Q_2^{(2)} > M_2^{(1)*}\left(1 + Q_1^{(1)} + nQ_2^{(1)}\right) + \Lambda_2^{(2)}, && \alpha = 1,
\end{aligned}
$$

where $M_i^* = M_i(Q_1,Q_2)$, $M_i^{(1)*} = M_i^{(1)}(Q_1,Q_2)$, $H_2^* = H_2(Q_1,Q_2)$, $H_2^{(1)*} = H_2^{(1)}(Q_1,Q_2)$, $i=1,2$.

We define the set $C_{b,\tau}^{1,\alpha}(Q)$ parametrized by the time $\tau \in (0,T]$ and the constants Q_i, $Q_i^{(j)} > 0$, $i,j=1,2$ as follows

$$
\begin{aligned}
C_{b,\tau}^{1,\alpha}(Q) = \Big\{&(u,v) \in C_{loc}^{1+\alpha}\left([0,\tau]\times\mathbb{R},\mathbb{R}^{1+k}\right) : \\
&u(0,x) = u_0(x),\ v(0,x) = v_0(x),\ u_t(0,x) = u_1(x), \\
&\|u\|_0 \le Q_1,\ \|u_t\|_0 \le Q_1^{(1)},\ \|u_x\|_0 \le Q_1^{(1)}, [u_t]_{H,\alpha,\Delta(x,\tau)} \le Q_1^{(2)},\ [u_x]_{H,\alpha,\Delta(x,\tau)} \le Q_1^{(2)}, \\
&\|v\|_0 \le Q_2,\ \|v_t\|_0 \le Q_2^{(1)},\ \|v_x\|_0 \le Q_2^{(1)}, [v_t]_{H,\alpha,\Delta(x,\tau)} \le Q_2^{(2)},\ [v_x]_{H,\alpha,\Delta(x,\tau)} \le Q_2^{(2)},\ x \in \mathbb{R}\Big\}.
\end{aligned}
\tag{100}
$$

Theorem 16 ([A2], Thm. 4.1). *If Assumptions $H_1[u_0,v_0,u_1]$, $H_2[f,g]$, $H_3[Q]$ are satisfied and $c \ge 0$, then there is $\tau \in (0,T]$ such that the problem* (92), (93) *has a unique solution $(u,v) \in C_{b,\tau}^{1,\alpha}(Q)$ and $u \in C^2([0,\tau]\times\mathbb{R},\mathbb{R})$.*

I proved Theorem 16 using the Banach fixed point theorem, and using integral Lemma 3.1 and Arzeli-Ascoli lemma as auxiliaries. Let us stress that in Theorem 16 the assumption is that f,g can only be locally Lipschitzian with respect to $p \in \mathbb{R}$, $r \in \mathbb{R}^k$, which allows to consider in particular equations with polynomial terms with respect to u and v. Moreover, they can be all polynomials if the right-hand side of the equations does not depend on t,x. Theorem 16 is also true when the ordinary part in (92) is excluded and $f = f(t,x,p)$. Let us add that $C_{b,\tau}^{1,\alpha}(Q)$ is not a closed ball, but it is a closed subset of a closed ball in $C_b\big([0,\tau]\times\mathbb{R},\mathbb{R}^{1+k}\big)$. It is this form of the set $C_{b,\tau}^{1,\alpha}(Q)$ that allowed for the selection of parameters and guaranteed the existence of $\tau > 0$ such that the appropriate operator $H = (F,G)$ was internal, i.e. $H\big(C_{b,\tau}^{1,\alpha}(Q)\big) \subset C_{b,\tau}^{1,\alpha}(Q)$ and narrowing.

[A3] In this paper, I proved Theorems 4.3 and 4.6 about the existence, uniqueness and estimate of global in time classical solutions of the one-dimensional weakly coupled nonlinear hyperbolic initial problem (92), (93) studied in [A2]. But now the interval $[0,T]$ in (92) is replaced by the ray $\mathbb{R}_0^+ = [0,\infty)$, and the initial functions are denoted by $\varphi_0, \psi_0, \varphi_1$ instead of u_0, v_0, u_1. I also proved the auxiliary Theorem 2.2 about weak hyperbolic differential inequalities and Lemma 3.1 about the equivalence of the differential problem with a certain integral system, in a slightly different class of functions than in [A2]. Moreover, I proposed a method of constructing lower and upper solutions in the case of bounded f, g, u_0, u_1, v_0. It consists in solving the appropriate associated ordinary differential equations with the initial condition. Such a differential method is more convenient to use than, for example, the integral method using Green's function described in [11] for parabolic equations.

Theorem 17 ([A3], Thm. 4.3). *Assume that*

(1) $f \in C^1\left(\mathbb{R}_0^+ \times \mathbb{R}^{2+k}, \mathbb{R}\right)$, $g \in C^1\left(\mathbb{R}_0^+ \times \mathbb{R}^{2+k}, \mathbb{R}^k\right)$,

(2) f, g *are Lipschitz continuous with respect to* p, r *in* $\mathbb{R}_0^+ \times \mathbb{R}^{2+k}$ *with a constant* L,

(3) g_x, g_p, g_{r_i}, $i = 1, ..., k$ *are Lipschitz continuous with respect to* x, p, r *in* $\mathbb{R}_0^+ \times \mathbb{R}^{2+k}$ *with a constant* L_1,

(4) $\varphi_0 \in C^2(\mathbb{R}, \mathbb{R})$, $\varphi_1 \in C^1(\mathbb{R}, \mathbb{R})$, $\psi_0 \in C^1\left(\mathbb{R}, \mathbb{R}^k\right)$,

(5) $(\psi_0)_x$ *is Lipschitz continuous in* $\mathbb{R}$ *with a constant* L_0.

Then there exists a unique solution $(u,v) \in C^2\left(\mathbb{R}_0^+ \times \mathbb{R}, \mathbb{R}\right) \times C^1\left(\mathbb{R}_0^+ \times \mathbb{R},\ \mathbb{R}^k\right)$ *of the problem* (92), (93).

A function $(u,v) \in C^2\left(\mathbb{R}_0^+ \times \mathbb{R}, \mathbb{R}\right) \times C^1\left(\mathbb{R}_0^+ \times \mathbb{R},\ \mathbb{R}^k\right)$ satisfying the system of inequalities

$$\begin{cases} u_{tt} - u_{xx} + cu_t \le f(t,x,u,v), & (t,x) \in \mathbb{R}_0^+ \times \mathbb{R}, \\ v_t \le g(t,x,u,v), & (t,x) \in \mathbb{R}_0^+ \times \mathbb{R}, \\ \varphi_0(x) \ge u(0,x), & x \in \mathbb{R}, \\ \psi_0(x) \ge v(0,x), & x \in \mathbb{R}, \\ \varphi_1(x) \ge u_t(0,x), & x \in \mathbb{R}, \end{cases} \tag{101}$$

is called a lower solution of (92), (93) in $\mathbb{R}_0^+ \times \mathbb{R}$. If the inequalities are inverse, we call it an upper solution of this problem.

Assumption A. There exists at least one pair of lower and upper solutions $(\underline{u}_0, \underline{v}_0)$, $(\overline{u}_0, \overline{v}_0)$ of (92), (93) such that

$$\underline{u}_0 \le \overline{u}_0,\ \underline{v}_0 \le \overline{v}_0 \ \text{ w } \ \mathbb{R}_0^+ \times \mathbb{R}. \tag{102}$$

For a given pair of lower and upper solutions $(\underline{u}_0, \underline{v}_0)$, $(\overline{u}_0, \overline{v}_0)$ of (92), (93) satisfying Assumption A, we define the sector

$$\langle (\underline{u}_0, \underline{v}_0), (\overline{u}_0, \overline{v}_0) \rangle = \left\{ (u,v) \in C^2\left(\mathbb{R}_0^+ \times \mathbb{R}, \mathbb{R}\right) \times C^1\left(\mathbb{R}_0^+ \times \mathbb{R}, \mathbb{R}^k\right) : \right.$$
$$\left. \underline{u}_0(t,x) \le u(t,x) \le \overline{u}_0(t,x), \underline{v}_0(t,x) \le v(t,x) \le \overline{v}_0(t,x), (t,x) \in \mathbb{R}_0^+ \times \mathbb{R} \right\}$$

and the interval

$$\langle m, M \rangle = \left\{ (u,v) \in \mathbb{R}^{1+k} :\ m_0 \le u \le M_0,\ m \le v \le M \right\},$$

where $m = (m_1, ..., m_k)$, $M = (M_1, ..., M_k)$,

$$m_0 = \inf \left\{ \underline{u}_0(t,x) :\ (t,x) \in \mathbb{R}_0^+ \times \mathbb{R} \right\},$$

$$
\begin{aligned}
m_i &= \inf\left\{\underline{v}_{0i}(t,x):\ (t,x)\in\mathbb{R}_0^+\times\mathbb{R}\right\},\\
M_0 &= \sup\left\{\overline{u}_0(t,x):\ (t,x)\in\mathbb{R}_0^+\times\mathbb{R}\right\},\\
M_i &= \sup\left\{\overline{v}_{0i}(t,x):\ (t,x)\in\mathbb{R}_0^+\times\mathbb{R}\right\},
\end{aligned}
$$

$\underline{v} = (\underline{v}_{01},...,\underline{v}_{0k})$, $\overline{v} = (\overline{v}_{01},...,\overline{v}_{0k})$, $i = 1,...,k$. Define two sequences $(\underline{u}_n,\underline{v}_n)$, $(\overline{u}_n,\overline{v}_n)$ of functions $\underline{u}_n,\overline{u}_n : \mathbb{R}_0^+\times\mathbb{R}\to\mathbb{R}$, $\underline{v}_n,\overline{v}_n : \mathbb{R}_0^+\times\mathbb{R}\to\mathbb{R}^k$, $n\in\mathbb{N}_0 := \mathbb{N}\cup\{0\}$ by the linear reccurence formulas

$$
\begin{cases}
\mathcal{L}\underline{u}_{n+1} = f\left(t,x,\underline{u}_n(t,x),\underline{v}_n(t,x)\right) + \frac{c^2}{4}\underline{u}_n(t,x), & (t,x)\in\mathbb{R}_0^+\times\mathbb{R},\\
\left(\underline{v}_{n+1}\right)_t = g\left(t,x,\underline{u}_n(t,x),\underline{v}_n(t,x)\right), & (t,x)\in\mathbb{R}_0^+\times\mathbb{R},\\
\underline{u}_{n+1}(0,x) = \varphi_0(x), & x\in\mathbb{R},\\
\underline{v}_{n+1}(0,x) = \psi_0(x), & x\in\mathbb{R},\\
\left(\underline{u}_{n+1}\right)_t(0,x) = \varphi_1(x), & x\in\mathbb{R},
\end{cases}
\tag{103}
$$

$$
\begin{cases}
\mathcal{L}\overline{u}_{n+1} = f\left(t,x,\overline{u}_n(t,x),\overline{v}_n(t,x)\right) + \frac{c^2}{4}\overline{u}_n(t,x), & (t,x)\in\mathbb{R}_0^+\times\mathbb{R},\\
\left(\overline{v}_{n+1}\right)_t = g\left(t,x,\overline{u}_n(t,x),\overline{v}_n(t,x)\right), & (t,x)\in\mathbb{R}_0^+\times\mathbb{R},\\
\overline{u}_{n+1}(0,x) = \varphi_0(x), & x\in\mathbb{R},\\
\overline{v}_{n+1}(0,x) = \psi_0(x), & x\in\mathbb{R},\\
\left(\overline{u}_{n+1}\right)_t(0,x) = \varphi_1(x), & x\in\mathbb{R},
\end{cases}
\tag{104}
$$

where $\mathcal{L} = u_{tt} - u_{xx} + cu_t + \frac{c^2}{4}u$ is an operator acting on functions $u\in C^2\left(\mathbb{R}_0^+\times\mathbb{R},\mathbb{R}\right)$.

Theorem 18 ([A3], Thm. 4.6). *Suppose that Assumption A is satisfied and*

(1) $f\in C^1\left(\mathbb{R}_0^+\times\mathbb{R}\times\langle m,M\rangle,\mathbb{R}\right)$, $g\in C^1\left(\mathbb{R}_0^+\times\mathbb{R}\times\langle m,M\rangle,\mathbb{R}^k\right)$,

(2) f,g *are Lipschitz continuous with respect to* p,r *in* $\mathbb{R}_0^+\times\mathbb{R}\times\langle m,M\rangle$ *with a constant* L,

(3) g_x, g_p, g_{r_i}, $i=1,...,k$ *are Lipschitz continuous with respect to* x,p,r *in* $\mathbb{R}_0^+\times\mathbb{R}\times\langle m,M\rangle$ *with a constant* L_1,

(4) $f(t,x,p,r)+\frac{c^2}{4}p$, *are nondecreasing with respect to* p,r *in* $\mathbb{R}_0^+\times\mathbb{R}\times\langle m,M\rangle$,

(5) $c\geq 0$,

(6) $\varphi_0\in C^2(\mathbb{R},\mathbb{R})$, $\varphi_1\in C^1(\mathbb{R},\mathbb{R})$, $\psi_0\in C^1\left(\mathbb{R},\mathbb{R}^k\right)$,

(7) $(\psi_0)_x$ *is Lipschitz continuous in* $\mathbb{R}$ *with a constant* L_0.

Then

(i) there exist unique solutions $(\underline{u}_n,\underline{v}_n),(\overline{u}_n,\overline{v}_n)\in C^2\left(\mathbb{R}_0^+\times\mathbb{R},\mathbb{R}\right)\times C^1\left(\mathbb{R}_0^+\times\mathbb{R},\mathbb{R}^k\right)$, $n\in\mathbb{N}_0$ *of* (103), (104), *respectively,*

(ii) the inequalities hold in $\mathbb{R}_0^+\times\mathbb{R}$,

$$\underline{u}_0\leq\underline{u}_1\leq\underline{u}_2\leq...\leq\overline{u}_2\leq\overline{u}_1\leq\overline{u}_0,$$

$$\underline{v}_0\leq\underline{v}_1\leq\underline{v}_2\leq...\leq\overline{v}_2\leq\overline{v}_1\leq\overline{v}_0,$$

(iii) $(\underline{u}_n,\underline{v}_n),(\overline{u}_n,\overline{v}_n)$, $n\in\mathbb{N}_0$ *are lower and upper solutions of* (92), (93) *in* $\mathbb{R}_0^+\times\mathbb{R}$,

(iv) $\lim_{n\to\infty}\left(\overline{u}_n(t,x)-\underline{u}_n(t,x)\right)=0$, $\lim_{n\to\infty}\left(\overline{v}_n(t,x)-\underline{v}_n(t,x)\right)=0$ *almost uniformly in* $\mathbb{R}_0^+\times\mathbb{R}$,

(v) the function

$$\left(u\left(t,x\right),v\left(t,x\right)\right)=\lim_{n\to\infty}\left(\underline{u}_n\left(t,x\right),\underline{v}_n\left(t,x\right)\right)=\lim_{n\to\infty}\left(\overline{u}_n\left(t,x\right),\overline{v}_n\left(t,x\right)\right)$$

$\in C^2\left(\mathbb{R}_0^+\times\mathbb{R},\mathbb{R}\right)\times C^1\left(\mathbb{R}_0^+\times\mathbb{R},\mathbb{R}^k\right)$ *is a unique solution of* (92), (93) *in the sector* $\left\langle\left(\underline{u}_0,\underline{v}_0\right),\ \left(\overline{u}_0,\overline{v}_0\right)\right\rangle$.

I proved Theorem 17 using Picard's iterative method, with the help of Lemma 3.1 on an integral form, lemma 4.1 on an estimate, Lemma 4.2 on a passing to the limit and the Arzeli-Ascola lemma. Then I proved Theorem 18 using the monotone method of lower and upper solutions, and using Lemmas 3.1, 4.1, 4.2, the Arzeli-Ascola lemma and Theorem 2.2 about weak hyperbolic differential inequalities as auxiliaries. Let us stress that in Theorem 17, the global Lipschitz condition on f,g,g_x,g_p,g_r with respect to p,r is assumed, while in Theorem 18 only the local Lipschitz condition, i.e. for p,r belonging to the interval $\langle m,M\rangle$. Therefore, Theorem 18 allows equations with polynomials with respect to u and v. It is also worth noting that Theorems 17, 18 are also true when the ordinary part in the system (92) is excluded and $f=f(t,x,p)$.

5 Difference methods for local and nonlocal diffusion models, [A1], [A5]

In Sections 2, 3 and 4, I presented the results of some specific systems of differential equations. But there are many more complicated physical phenomena to describe which ones constructs equations and systems of differential equations with nonlocal terms. Such equations are often called differential-functional equations. For example, these can be reaction-diffusion equations with the delayed time or space arguments and differential-integral equations. The first equations describe issues from biology, biophysics, biochemistry, chemistry, medicine, ecology, economics, control theory, nuclear reactions, and the second ones take into account the so-called integral sources [84, 89]. In this section, I will not focus on a specific model, but consider the general or abstract situation, while giving some important examples of both differential and differential-function equations for which all the assumptions I have made are fulfilled. I will present theorems concerning the convergence and stability of explicit and implicit difference methods and properties of discrete solutions for the mentioned equations with the initial condition and boundary conditions of the Dirichlet and Robin types. I would also like to point out that mixed spatial derivatives that occur in the equations studied can be used for more accurate modeling of phenomena in anisotropic media. But even equations with only pure derivatives, such as the heat equation, often generate mixed derivatives after a change of variables. In the theory of difference methods, variables are changed in order to transform the domain of an unknown function most frequently into a cuboid, which facilitates the approximation and increases the computational accuracy.

Consider the differential equation

$$\partial_t z\left(t,x\right)=\sum_{i=1}^{n}\partial_{x_ix_i}a\left(z\left(t,x\right)\right)+\sum_{i=1}^{n}\partial_{x_i}b\left(z\left(t,x\right)\right)+c\left(z\left(t,x\right)\right),\tag{105}$$

where the functions $a,b,c:\mathbb{R}\to\mathbb{R}$ are given. In applications, the right-hand second derivative component in (105) corresponds to diffusion or dispersion, the first-order derivative component represents convection or advection, and the last component describes reaction processes such as sorption, source or sink. The unknown function z is usually a non-negative biological, medical, physical, or chemical quantity, such as density, saturation, or concentration. Many of the known equations of the form (105) with right-hand polynomials are described in [1, 36, 42, 69]. It is in particular the one-dimensional generalized Burgers–Huxley equation

$$\partial_t z\,(t,x) = \kappa \partial_{xx} z\,(t,x) + \alpha (z(t,x))^p \partial_x z(t,x) + \beta z\,(t,x)\left[1 - (z\,(t,x))^p\right]\left[(z\,(t,x))^p - \gamma\right], \quad (106)$$

the one-dimensional generalized Burgers–Fisher equation

$$\partial_t z\,(t,x) = \kappa \partial_{xx} z\,(t,x) + \alpha (z(t,x))^p \partial_x z(t,x) + \beta z\,(t,x)\left[1 - (z\,(t,x))^p\right] \quad (107)$$

and the multidimensional reaction diffusion equation

$$\partial_t z\,(t,x) = \sum_{i=1}^{n} \partial_{x_i x_i} (z\,(t,x))^m - \beta\,(z\,(t,x))^\delta, \quad (108)$$

where $\kappa > 0$, $\alpha \in \mathbb{R}$, $\beta \geq 0$, $\gamma \in (0,1)$, $p \in \mathbb{N}$, $m > 0$, $\delta > 0$. The equation (106) covers many models from mathematical biology and physics, including several equations from population dynamics and nuclear physics. Putting $\alpha = 0$, $\kappa = \beta = p = 1$ in (107), we get the Fisher equation which is an archetypal deterministic model of the evolution of a beneficial gene in a population of diploid individuals living in a one-dimensional environment. The equation (108) is a simple and widely used model for various physical, chemical and biological problems related to dispersion, source or absorption, e.g. it is used to model filtration in porous media, transport of thermal energy in plasma, the flow of chemically reacting fluid from the surface and the evolution of the population. The equations (106), (107), (108) for certain parameter values satisfy all the assumptions in my theorems in [A5] or [A1], which I will present below. It is also worth noting that the Newell–Whitehead, Zeldovich, KPP and other equations studied in [36, 69] are also of the form (105) and fulfill these assumptions.

An example of a nonlocal equation that fulfills the assumptions of the theorems in [A5] is the integral form of the FitzHugh-Nagumo system (87)

$$u_t - u_{xx} = -f(u) - b\int_0^t u(s,x)\,ds - v_0(x), \quad (109)$$

where v_0 is the given initial condition for the kinetic equation [68].

[A1] In this article, I proved Theorems 6.1 and 6.2 about the error estimate and uniform convergence of explicit difference methods for nonlinear and quasi-linear parabolic in Walter's sense differential functional equations with the initial condition and the Dirichlet type boundary condition. Moreover, from Remark 6.5 we conclude on the error asymptotics and from Remark 6.2 it follows that the methods are stable. The equations may be in particular strongly nonlinear, i.e. nonlinear with respect to the second derivatives. I generalized the Perron condition (see (118)) assumed in all previous works from the Kamont's [15, 16, 46, 47, 48] group and its special case, i.e. the Lipschitz condition assumed in all previous works from Malec's [64, 65, 66] and Pao's [73] groups. This allowed to extend the class of nonlinear equations with those with the quasi-linear terms $\sum_{i,j=1}^n a_{ij}(t,x,z)\partial_{x_i x_j} z$, where the functions $a_{ij} : E \times \mathbb{R} \to \mathbb{R}$ are given, and allowed systems of strongly nonlinear and quasi-linear equations, based on Remark 6.3. As is known, quasi-linear terms often appear in diffusion modeling equations. I also analyzed, proving Lemmas 6.2 and 6.3, the speed of approximation of the functional term in the differential equations using the step operator S_h defined by Malec [64] and the interpolation operator T_h defined by Kamont [47]. The conclusion is that in the function class $z \in C^1(\Omega, \mathbb{R})$, the order of approximation is equal to one in both cases, but in the class $z \in C^2(\Omega, \mathbb{R})$, the order of approximation with T_h is two, while with S_h remains one. It is the results obtained in this article that inspired me to continue working with the general equations [B6], [B7], [B8], [B9],

[A5], as well as with very specific onces, modeling diffusion and transport phenomena, which I described in Sections 2, 3 and 4.

Let $T>0$, $T_0\geq 0$, $X=(X_1,...,X_n)$, $\tau=(\tau_1,...,\tau_n)$, where $X_i>0$, $\tau_i\geq 0$ for $i=1,...,n$, be given. We define the sets

$$\begin{aligned}
\Xi &= (-X_1,X_1)\times ...\times(-X_n,X_n)\subset\mathbb{R}^n,\\
\overline{\Xi} &= [-X-\tau,X+\tau],\quad \partial\Xi=\overline{\Xi}\setminus\Xi,\\
E &= [0,T]\times\Xi\subset\mathbb{R}^{1+n},\\
E_0 &= [-T_0,0]\times\overline{\Xi}\subset\mathbb{R}^{1+n},\\
\partial_0 E &= (0,T]\times\partial\Xi\subset\mathbb{R}^{1+n},\\
\Omega &= E\cup E_0\cup\partial_0 E,\\
\Omega_t &= \Omega\cap([-T_0,t]\times\mathbb{R}^n)\,,\quad t\in[0,T]\,.
\end{aligned}$$

We denote by $M_{n\times n}$ the set of all $n\times n$ symmetric real matrices. We define also the sets

$$\begin{aligned}
\Delta_f &= E\times B(\Omega,\mathbb{R})\times\mathbb{R}^n\times M_{n\times n},\\
\Delta_{f1} &= E\times B^2(\Omega,\mathbb{R})\times\mathbb{R}^{2n}\times M^2_{n\times n},
\end{aligned}$$

where

$$\begin{aligned}
&B(\Omega,\mathbb{R})=\big\{z:\Omega\to\mathbb{R}\mid\sup\{|z(t,x)|:\ (t,x)\in\Omega\}<\infty,\\
&\exists\ k\in\mathbb{N}\ \exists\ \Omega_1,...,\Omega_k\ \exists\ a^{(1)},...,a^{(k)},a\in\mathbb{R}\ \exists\ b^{(1)},...,b^{(k)},b\in\mathbb{R}^n:\\
&\Omega_i=\Omega\cap\left(\left[a^{(i)},a^{(i)}+a\right)\times\left[b^{(i)},b^{(i)}+b\right)\right),\\
&\Omega=\bigcup_{i=1}^{k}\Omega_i,\ \ \Omega_i\cap\Omega_j=\emptyset\text{ for }i\neq j,\ \ z|_{\Omega_i}\in C(\Omega_i,\mathbb{R})\,,\ \ i,j=1,...,k\big\}
\end{aligned}$$

is the space of Lebesgue-measurable functions, bounded and piecewise continuous on Ω. The maximum norms in $\mathbb{R}^n$ and $M_{n\times n}$ we denote by $\|\cdot\|$, while in $B(\Omega,\mathbb{R})$ by $\|\cdot\|_\Omega$. For a fixed $t\in[0,T]$, the formula

$$\|z\|_{\Omega_t}=\max\left\{\left|z\left(\tilde t,x\right)\right|:\ \left(\tilde t,x\right)\in\Omega_t\right\},\quad z\in B(\Omega,\mathbb{R})$$

stands for a seminorm in $B(\Omega,\mathbb{R})$. Let functions $f:\Delta_f\to\mathbb{R}$ and $\varphi:E_0\cup\partial_0E\to\mathbb{R}$ be given. Consider a nonlinear second-order partial differential functional equation of the form

$$\partial_t z(t,x)=f(t,x,z,\partial_x z(t,x),\partial_{xx}z(t,x))\,,\quad (t,x)\in E \tag{110}$$

with the initial condition and the Dirichlet boundary condition

$$z(t,x)=\varphi(t,x)\,,\quad (t,x)\in E_0\cup\partial_0E, \tag{111}$$

where $\partial_x z=(\partial_{x_1}z,...,\partial_{x_n}z)$, $\partial_{xx}z=\left[\partial_{x_ix_j}z\right]_{i,j=1}^n$. We say that the equation (110) is *parabolic in Walter's sense* if for all matrices $q,\tilde q\in M_{n\times n}$ and each $(t,x)\in E$, $z\in B(\Omega,\mathbb{R})$, $p\in\mathbb{R}^n$, the implication is true

$$q\leq\tilde q\Rightarrow f(t,x,z,p,q)\leq f(t,x,z,p,\tilde q)\,,$$

where the inequality $q\leq\tilde q$ means that the matrix $\tilde q-q$ is positive semi-defined (see [86], §23). A functional f satisfies *the Volterra condition* if for each $(t,x)\in E$, $z,\bar z\in B(\Omega,\mathbb{R})$ and $p\in\mathbb{R}^n$, $q\in M_{n\times n}$, the implication holds

$$z|_{\Omega_t}=\bar z|_{\Omega_t}\Rightarrow f(t,x,z,p,q)=f(t,x,\bar z,p,q).$$

We discretize Ω. Let $(h_0, h') = h$, $h' = (h_1, ..., h_n)$ be the steps of a mesh. Denote by H the set of all steps h such that there are $N_0 \in \mathbb{Z}$ and $N = (N_1, ..., N_n) \in \mathbb{N}^n$ with the properties: $N_0 h_0 = T_0$, $N_i h_i = X_i + \tau_i$, $i = 1, ..., n$. The numbers $K_0 \in \mathbb{N}$ and $K = (K_1, ..., K_n) \in \mathbb{Z}^n$ are such that $K_0 h_0 \le T < (K_0 + 1) h_0$, $K_i h_i < X_i \le (K_i + 1) h_i$, $i = 1, ..., n$. The nodal points $\left(t^{(\mu)}, x^{(m)}\right)$, $x^{(m)} = \left(x_1^{(m_1)}, ..., x_n^{(m_n)}\right)$ we define in the following way: $t^{(\mu)} = \mu h_0$, $x_i^{(m_i)} = m_i h_i$, $i = 1, ..., n$. For $h \in H$ we define the discrete sets

$$\begin{aligned}
R_h^{1+n} &= \left\{ \left(t^{(\mu)}, x^{(m)}\right) : (\mu, m) \in \mathbb{Z}^{1+n} \right\}, \\
E_h &= E \cap R_h^{1+n}, \\
E_{0.h} &= E_0 \cap R_h^{1+n}, \\
\partial_0 E_h &= \partial_0 E \cap R_h^{1+n}, \\
\Omega_h &= E_h \cup E_{0.h} \cup \partial_0 E_h, \\
\Omega_{h.\mu} &= \Omega_h \cap \left(\left[-T_0, t^{(\mu)}\right] \times \mathbb{R}^n \right), \quad \mu = 0, ..., K_0, \\
E_h^+ &= \left\{ \left(t^{(\mu)}, x^{(m)}\right) \in E_h : \ 0 \le \mu \le K_0 - 1 \right\}.
\end{aligned}$$

For a mesh function $z : \Omega_h \supset \tilde{\Omega}_h \to \mathbb{R}$ and a point $\left(t^{(\mu)}, x^{(m)}\right) \in \tilde{\Omega}_h$, we put $z^{(\mu,m)} := z\left(t^{(\mu)}, x^{(m)}\right)$, $|z|^{(\mu,m)} := |z^{(\mu,m)}|$. The symbol $z|_{\tilde{\Omega}_h}$ is the restricton of z to $\tilde{\Omega}_h$. The space of all mesh functions we denote by $\mathfrak{F}\left(\tilde{\Omega}_h, \mathbb{R}\right)$ and introduce the maximum norm

$$\|z\|_{\tilde{\Omega}_h} = \max\left\{ |z|^{(\mu,m)} : \ \left(t^{(\mu)}, x^{(m)}\right) \in \tilde{\Omega}_h \right\}, \quad z \in \mathfrak{F}\left(\tilde{\Omega}_h, \mathbb{R}\right). \tag{112}$$

For a fixed $\mu \in \{0, 1, ..., K_0\}$, the relation

$$\|z\|_{\Omega_{h.\mu}} = \max\left\{ |z|^{(\tilde{\mu},m)} : \ \left(t^{(\tilde{\mu})}, x^{(m)}\right) \in \Omega_{h.\mu} \right\}, \quad z \in \mathfrak{F}\left(\Omega_h, \mathbb{R}\right) \tag{113}$$

is a seminorm in $\mathfrak{F}\left(\Omega_h, \mathbb{R}\right)$. We define the set of indices

$$\Gamma = \{(i,j) : \ 1 \le i, j \le n, \ i \ne j\}$$

and assume that $\Gamma_+, \Gamma_- \subset \Gamma$ are such that $\Gamma_+ \cup \Gamma_- = \Gamma$, $\Gamma_+ \cap \Gamma_- = \emptyset$ (in particular, it may happen that $\Gamma_+ = \emptyset$ or $\Gamma_- = \emptyset$). We assume that $(i,j) \in \Gamma_+$ when $(j,i) \in \Gamma_+$ and $(i,j) \in \Gamma_-$ when $(j,i) \in \Gamma_-$. Let $z \in \mathfrak{F}\left(\Omega_h, \mathbb{R}\right)$ and $\left(t^{(\mu)}, x^{(m)}\right) \in E_h$. We define the forward and backward difference quotients, respectively

$$\begin{aligned}
\delta_0 z^{(\mu,m)} &= \frac{1}{h_0}\left[z^{(\mu+1,m)} - z^{(\mu,m)}\right], \\
\delta_i^+ z^{(\mu,m)} &= \frac{1}{h_i}\left[z^{(\mu,m+e_i)} - z^{(\mu,m)}\right], \quad i = 1, ..., n, \\
\delta_i^- z^{(\mu,m)} &= \frac{1}{h_i}\left[z^{(\mu,m)} - z^{(\mu,m-e_i)}\right], \quad i = 1, ..., n,
\end{aligned} \tag{114}$$

where $e_i = (0, ..., 0, 1, 0, ..., 0)$ with 1 in the ith entry. And then we define the central and the so-called seven-point difference quotients $\delta = (\delta_1, ..., \delta_n)$, $\delta^{(2)} = [\delta_{ij}]_{i,j=1}^n$,

$$\begin{aligned}
\delta_i z^{(\mu,m)} &= \frac{1}{2}\left[\delta_i^+ z^{(\mu,m)} + \delta_i^- z^{(\mu,m)}\right], \quad i = 1, ..., n, \\
\delta_{ii} z^{(\mu,m)} &= \delta_i^+ \delta_i^- z^{(\mu,m)}, \quad i = 1, ..., n, \\
\delta_{ij} z^{(\mu,m)} &= \frac{1}{2}\left[\delta_i^+ \delta_j^- z^{(\mu,m)} + \delta_i^- \delta_j^+ z^{(\mu,m)}\right], \quad (i,j) \in \Gamma_-, \\
\delta_{ij} z^{(\mu,m)} &= \frac{1}{2}\left[\delta_i^+ \delta_j^+ z^{(\mu,m)} + \delta_i^- \delta_j^- z^{(\mu,m)}\right], \quad (i,j) \in \Gamma_+.
\end{aligned} \tag{115}$$

Let a function $\varphi_h \in \mathfrak{F}(E_{0.h} \cup \partial_0 E_h, \mathbb{R})$ be given. We define the explicit difference functional scheme

$$\begin{cases} \delta_0 z^{(\mu,m)} = f(t^{(\mu)}, x^{(m)}, G_h[z], \delta z^{(\mu,m)}, \delta^{(2)} z^{(\mu,m)}), & \left(t^{(\mu)}, x^{(m)}\right) \in E_h, \\ z^{(\mu,m)} = \varphi_h^{(\mu,m)}, & \left(t^{(\mu)}, x^{(m)}\right) \in E_{0.h} \cup \partial_0 E_h, \end{cases} \tag{116}$$

where $G_h = S_h$ or $G_h = T_h$.

Assumption F$[f, u]$.

(F_1) The function f of variables $(t, x, z, p, q) \in \Delta_f$ is continuous.

(F_2) The exist bounded functions $\alpha = (\alpha_1, ..., \alpha_n)$, $\beta = [\beta_{ij}]_{i,j=1}^n$ with $\alpha_i,\ \beta_{ij} : \Delta_{f1} \to \mathbb{R}$ such that for any $(t, x, z, p, q), (t, x, z, \bar{p}, \bar{q}) \in \Delta$,

$$f(t, x, z, p, q) - f(t, x, z, \bar{p}, \bar{q}) = \sum_{i=1}^n \alpha_i(P)(p_i - \bar{p}_i) + \sum_{i,j=1}^n \beta_{ij}(P)(q_{ij} - \bar{q}_{ij}),$$

where $P = (t, x, z, z, p, \bar{p}, q, \bar{q}) \in \Delta_{f1}$.

(F_3) The matrix β is symmetric and

$$\beta_{ij}(P) \geq 0 \quad \text{and} \quad \beta_{ij}(P) \not\equiv 0, \quad (i,j) \in \Gamma_+,$$

$$\beta_{ij}(P) \leq 0, \quad (i,j) \in \Gamma_-,$$

at each $P \in \Delta_{f1}$.

(F_4) There are functions $\sigma : [0, T] \times \mathbb{R}_+ \to \mathbb{R}_+$, $\rho : \mathbb{R}_+ \to \mathbb{R}_+$ such that:

(1) σ is continuous and nondecreasing with respect to both variables, $\sigma(t, 0) = 0$ for $t \in [0, T]$;

(2) ρ is nondecreasing;

(3) for each $c \geq 0$, $\varepsilon, \varepsilon_0 \geq 0$, the maximal solution of the Cauchy problem

$$\omega'(t) = c\sigma(t, \omega(t)) + \varepsilon, \quad \omega(0) = \varepsilon_0 \tag{117}$$

is defined on $[0, T]$ and the function $\tilde{\omega}(t) = 0$, $t \in [0, T]$ is the maximal solution of (117) for each $c \geq 0$ and $\varepsilon, \varepsilon_0 = 0$;

(4) *the generalized Perron type condition* holds

$$|f(t, x, z, p, q) - f(t, x, \bar{z}, p, q)| \leq \rho(\|q\|)\, \sigma\left(t, \|z - \bar{z}\|_{\Omega_t}\right) \tag{118}$$

for each $(t, x, z, p, q), (t, x, \bar{z}, p, q) \in \Delta_f$.

(F_5) $u \in C(\Omega, \mathbb{R}) \cap C^{1,2}(\overline{E}, \mathbb{R})$ is a solution of (110), (111).

Assumption S $[f, h]$

(S_1) The steps $h = (h_0, h') \in H$ are such that

$$1 - 2h_0 \sum_{i=1}^n \frac{1}{h_i^2} \beta_{ii}(P) + h_0 \sum_{(i,j) \in \Gamma} \frac{1}{h_i h_j} |\beta_{ij}(P)| \geq 0, \tag{119}$$

$$-\frac{h_i}{2} |\alpha_i(P)| + \beta_{ii}(P) - h_i \sum_{\substack{j=1 \\ j \neq i}}^n \frac{1}{h_j} |\beta_{ij}(P)| \geq 0, \tag{120}$$

at each $P \in \Delta_{f1}$, $i = 1, ..., n$.

(S_2) There is $c_0 > 0$ such that $h_i h_j^{-1} \leq c_0$, $i, j = 1, ..., n$.

Theorem 19 ([A1], Thm. 6.1). *Let Assumptions $F[f,u]$, $S[f,h]$ hold and there is $\gamma_0 : H \to \mathbb{R}_+$ such that*

$$\left|\varphi^{(\mu,m)} - \varphi_h^{(\mu,m)}\right| \leq \gamma_0(h), \ (t^{(\mu(}, x^{(m)}) \in E_{0.h} \cup \partial_0 E_h, \quad \lim_{h\to 0} \gamma_0(h) = 0. \tag{121}$$

Then

(i) *for any $h \in H$ there exists a unique solution $v \in \mathfrak{F}(\Omega_h, \mathbb{R})$ of* (116),

(ii) *there is $\alpha : H \to \mathbb{R}_+$ such that*

$$\|U - v\|_{\Omega_{h.\mu}} \leq \alpha(h), \ 0 \leq \mu \leq K_0, \quad \lim_{h\to 0} \alpha(h) = 0, \tag{122}$$

where $U := u|_{\Omega_h}$, i.e. the difference method is uniformly convergent.

I proved Theorem 19 about the convergence of the difference method using the discrete comparison Theorem 5.1. In $(F3)$, which is also the definition of Γ_+ and Γ_-, the sign of the function β_{ij} is assumed to be constant in Δ_{f1} for a fixed $(i,j) \in \Gamma$. For quasi-linear equations, i.e. those generated by the function

$$f(t,x,z,p,q) = \sum_{i,j=1}^{n} a_{ij}(t,x,z)q_{ij} + F(t,x,z,p), \quad (t,x,z,p,q) \in \Delta_f,$$

the assumption of sign constancy, in this case the coefficients a_{ij}, can be ignored. For this purpose, we modify the definition of the seven-point quotients, specifying them during the calculation process with the formula

$$\delta_{ij} z^{(\mu,m)} = \frac{1}{2}\left[\delta_i^+ \delta_j^- z^{(\mu,m)} + \delta_i^- \delta_j^+ z^{(\mu,m)}\right], \quad \text{jeśli } a_{ij}\left(t^{(\mu)}, x^{(m)}, G_h[z]\right) < 0, \tag{123}$$

$$\delta_{ij} z^{(\mu,m)} = \frac{1}{2}\left[\delta_i^+ \delta_j^+ z^{(\mu,m)} + \delta_i^- \delta_j^- z^{(\mu,m)}\right], \quad \text{jeśli } a_{ij}\left(t^{(\mu)}, x^{(m)}, G_h[z]\right) \geq 0.$$

Then the same theorem as Theorem 19 is true (see Theorem 6.2).

[A5] In this paper, I proved Theorem 4.1 about the estimate of solutions of a nonlinear parabolic in Walter's sense differential functional equation with the initial condition and the Robin type boundary condition, Theorem 4.2 about the existence, uniqueness and uniform estimate with respect to meshes (i.e. independent of the meshes) of solutions of associated implicit difference schemes as well as Theorem 5.1 about the error estimate and uniform convergence of the constructed difference method. Moreover, from Remark 5.3 we conclude about the error asymptotics, and from Remark 5.4 it follows that the method is stable. They may be in particular strongly nonlinear equations, quasi-linear equations, and systems of strongly nonlinear and quasi-linear equations, as noted in Remark 5.5. Remark 6.1 shows that the analogous theorems are true for quasi-linear equations with the seven-point difference quotients modified by the formula (123) at the level $\mu + 1$, as in [A1]. I also proved the auxiliary Theorem 3.1 about the existence, uniqueness and estimate of solutions to some discrete implicit functional equation with the initial-boundary condition, and the comparison Theorem 3.2. The important novelty in this article is the local assumption on the mesh steps, i.e. on the set Δ_f^*, in the construction of which the key is to determine the interval $R \subset \mathbb{R}$, which is realized by solving the comparison ordinary initial problems (128) and (132). In all previous works on this subject, this assumption was adopted globally, i.e. on the set Δ_f [15, 16, 46, 47, 48, 49, 50, 64, 65, 66, 72, 73]. Generalized Perron's condition (137) on the set Δ_f^* I introduced in [B8], and in the less general version, i.e. with $\rho_1(\|q\|)$ instead of $\rho_1(\|p\|, \|q\|)$ in [B7]. In this way, we allow in particular important equations with polynomial terms with respect to z and $\partial_{x_i} z$, e.g. with $z\partial_{x_i} z$ and with the quasi-linear terms $\sum_{i,j=1}^{n} a_{ij}(t,x,z)\partial_{x_i x_j} z$, where the functions $a_{ij} : E \times \mathbb{R} \to \mathbb{R}$ are given, which are typical in diffusion models. As I wrote earlier, for example the equations (106), (107), (108) for the appropriate parameter values fulfill all the assumptions in the theorems in this paper. In diffusion models, the Robin type boundary conditions are often assumed on the boundary of Ω, and even their nonlinear modifications, as was the case in Sections 2 and 3.

We complete the notation introduced in [A1]. We assume that $\tau = 0$, which means that we do not bold the boundery $\partial_0 E$. This is because now there are derivatives in the boundary condition. We split the boundary $\partial_0 E$ into the separable sets

$$\begin{gathered}
\partial\Xi_i = \{x \in \partial\Xi : \ x_i = X_i\}, \quad \partial\Xi_{n+i} = \{x \in \partial\Xi : \ x_i = -X_i\}, \\
S_i^+ = \partial\Xi_i \setminus \bigcup_{j=1}^{i-1} \partial\Xi_j, \quad S_i^- = \partial\Xi_{n+i} \setminus \bigcup_{j=1}^{n+i-1} \partial\Xi_j, \\
\partial_0 E_i^+ = (0,T] \times S_i^+, \quad \partial_0 E_i^- = (0,T] \times S_i^-, \quad i = 1, ..., n.
\end{gathered}$$

The set of bounded functions $B(\Omega,\mathbb{R})$ in the definition of the sets Δ_f, Δ_{f1}, we replace with the set of continuous functions $C(\Omega,\mathbb{R})$ and define also the sets

$$\begin{gathered}
C(\Omega, R) = \{z : \Omega \to R\} \cap C(\Omega,\mathbb{R}), \\
\mathfrak{F}\left(\tilde{\Omega}_h, R\right) = \{z : \tilde{\Omega}_h \to R\} \cap \mathfrak{F}\left(\tilde{\Omega}_h, \mathbb{R}\right),
\end{gathered}$$

where $R \subset \mathbb{R}$ is a given interval and $\tilde{\Omega}_h \subset \Omega_h$ is any subset. Let functions $f : \Delta_f \to \mathbb{R}$, $\varphi : E_0 \to \mathbb{R}$, $a, b, \psi : \partial_0 E \to \mathbb{R}$ be given. Consider the nonlinear second-order partial differential functional equation

$$\partial_t z(t,x) = f(t,x,z,\partial_x z(t,x), \partial_{xx} z(t,x)), \quad (t,x) \in E, \tag{124}$$

with the initial condition and the Robin boundary condition

$$z(t,x) = \varphi(t,x), \quad (t,x) \in E_0, \tag{125}$$

$$\begin{aligned}
a(t,x)z(t,x) + b(t,x)\partial_{x_i} z(t,x) = \psi(t,x), \quad (t,x) \in \partial_0 E_i^+, \ i = 1, ..., n, \\
a(t,x)z(t,x) - b(t,x)\partial_{x_i} z(t,x) = \psi(t,x), \quad (t,x) \in \partial_0 E_i^-, \ i = 1, ..., n.
\end{aligned} \tag{126}$$

We discretize the boundary sets

$$\partial_0 E_{h.i}^+ = \partial_0 E_i^+ \cap R_h^{1+n}, \quad \partial_0 E_{h.i}^- = \partial_0 E_i^- \cap R_h^{1+n}, \quad i = 1, ..., n.$$

We also define the interpolation operator $G_h : \mathfrak{F}(\Omega_h,\mathbb{R}) \to C(\Omega,\mathbb{R})$ that has the properties:

(1) for all $z \in C(\Omega,\mathbb{R}) \cap C^{1,2}(\bar{E},\mathbb{R})$

$$\lim_{h\to 0} \|G_h[Z] - z\|_\Omega = 0,$$

where $Z := z|_{\Omega_h}$ is the restriction of z to Ω_h,

(2) the Lipschitz condition with a constant $D_1 > 0$ holds

$$\left\|G_h[z] - G_h[\bar{z}]\right\|_{\Omega_{t(\mu)}} \leq D_1 \left\|z - \bar{z}\right\|_{\Omega_{h.\mu}}, \quad z, \bar{z} \in \mathfrak{F}(\Omega_h, \mathbb{R}), \ \mu = 0, ..., K_0,$$

(3) for each $z, \bar{z} \in \mathfrak{F}(\Omega_h, \mathbb{R})$ if $z|_{\Omega_{h.\mu}} = \bar{z}|_{\Omega_{h.\mu}}$, then $G_h[z]|_{\Omega_{t(\mu)}} = G_h[\bar{z}]|_{\Omega_{t(\mu)}}$, $\mu = 0, ..., K_0$,

(4) the growth condition is true

$$\|G_h[z]\|_{\Omega_{t(\mu)}} \leq \|z\|_{\Omega_{h.\mu}}, \quad z \in \mathfrak{F}(\Omega_h, \mathbb{R}), \ \mu = 0, ..., K_0.$$

The special case of G_h is T_h with $D_1 = 1$. Let functions $\varphi_h \in \mathfrak{F}(E_{0.h}, \mathbb{R})$, $\psi_h \in \mathfrak{F}(\partial_0 E_h, \mathbb{R})$ be given and let $A_h := a|_{\partial_0 E_h}$, $B_h := b|_{\partial_0 E_h}$. We define the implicit difference functional scheme

$$\begin{cases} \delta_0 z^{(\mu,m)} = f(t^{(\mu)}, x^{(m)}, G_h[z], \delta z^{(\mu+1,m)}, \delta^{(2)} z^{(\mu+1,m)}), & \left(t^{(\mu)}, x^{(m)}\right) \in E_h, \\ z^{(\mu,m)} = \varphi_h^{(\mu,m)}, & \left(t^{(\mu)}, x^{(m)}\right) \in E_{0.h}, \\ A_h^{(\mu,m)} z^{(\mu,m)} + B_h^{(\mu,m)} \delta_i^- z^{(\mu,m)} = \psi_h^{(\mu,m)}, & \left(t^{(\mu)}, x^{(m)}\right) \in \partial_0 E_{h.i}^+, \ i = 1, ..., n, \\ A_h^{(\mu,m)} z^{(\mu,m)} - B_h^{(\mu,m)} \delta_i^+ z^{(\mu,m)} = \psi_h^{(\mu,m)}, & \left(t^{(\mu)}, x^{(m)}\right) \in \partial_0 E_{h.i}^-, \ i = 1, ..., n. \end{cases} \tag{127}$$

Assumption G$[f, a, b, \varphi]$.

(G_1) There is a function $\sigma : [0, T] \times \mathbb{R}_+ \to \mathbb{R}_+$ such that:

(1) σ is continuous and nondecreasing with respect to both variables;

(2) the maximal solution $\tilde{\omega}$ of the Cauchy problem

$$\omega'(t) = \sigma(t, \omega(t)), \quad \omega(0) = \|\varphi\|_{E_0} \tag{128}$$

is defined on $[0, T]$;

(3) the growth condition holds

$$|f(t, x, z, 0, 0)| \leq \sigma\left(t, \|z\|_{]\Omega_t}\right) \tag{129}$$

for all $(t, x) \in E$, $z \in C(\Omega, \mathbb{R})$.

(G_2) The equation (124) is parabolic in Walter's sense.

(G_3) a, b are continuous, $a > 0$, $b \geq 0$.

Theorem 20 ([A5], Thm. 4.1). *If Assumption G$[f, a, b, \varphi]$ is satisfied, $u \in C(\Omega, \mathbb{R}) \cap C^{1,2}\left(\bar{E}, \mathbb{R}\right)$ a solution of* (124)–(126) *and*

$$|\psi(t, x)| \leq a(t, x)\tilde{\omega}(t), \quad (t, x) \in \partial_0 E, \tag{130}$$

then the estimate is true

$$|u(t, x)| \leq \tilde{\omega}(t), \quad (t, x) \in \Omega, \tag{131}$$

where $\tilde{\omega}$ is the maximal solution of (128).

Assumption F$[f, a, b, \varphi, \varphi_h, \psi_h]$.

(F_1) The function f of variables $(t, x, z, p, q) \in \Delta_f$ is of the Volterra type.

(F_2) There is a constant $\Phi \geq 0$ such that for all $h \in H$

$$\max\{\|\varphi_h\|_{E_{0.h}}, \|\psi_h/A_h\|_{\partial_0 E_h}\} \le \Phi.$$

(F_3) $G[f, a, b, \varphi]$ is satisfied and the maximal solution $\bar{\omega}$ of the Cauchy problem

$$\omega'(t) = \sigma(t, \omega(t)), \quad \omega(0) = \Phi \tag{132}$$

is defined on $[0, T]$.

(F_4) There exist bounded partial derivatives

$$\partial_p f = (\partial_{p_1} f, ..., \partial_{p_n} f), \quad \partial_q f = [\partial_{q_{ij}} f]_{i,j=1}^n$$

on $\Delta_f^* = E \times C(\Omega, R) \times \mathbb{R}^n \times M_{n\times n}$, where

$$R := [-\omega^*(T), \omega^*(T)], \quad \omega^*(T) := \max\{\tilde{\omega}(T), \bar{\omega}(T)\}. \tag{133}$$

(F_5) The matrix $\partial_q f$ is symmetric and

$$\partial_{q_{ij}} f(P) \ge 0 \quad \text{and} \quad \partial_{q_{ij}} f(P) \not\equiv 0, \quad (i,j) \in \Gamma_+,$$

$$\partial_{q_{ij}} f(P) \le 0, \quad (i,j) \in \Gamma_-,$$

at each $P \in \Delta_f^*$.

Assumption S $[f, h]$.

(S_1) The steps $h = (h_0, h') \in H$ are such that

$$-\frac{h_i}{2} |\partial_{p_i} f(P)| + \partial_{q_{ii}} f(P) - h_i \sum_{\substack{j=1 \\ j\neq i}}^{n} \frac{1}{h_j} \left|\partial_{q_{ij}} f(P)\right| \ge 0 \tag{134}$$

at each $P \in \Delta_f^*$, $i = 1, ..., n$.

(S_2) $\lim_{h\to 0} \frac{h_i}{h_0} = 0$, $i = 1, ..., n$.

(S_3) There is $c_0 > 0$ such that $h_i h_j^{-1} \le c_0$, $i, j = 1, ..., n$.

Theorem 21 ([A5], Thm. 4.2). *If Assumptions F$[f, a, b, \varphi, \varphi_h, \psi_h]$, S$[f, h]$ hold, then for each $h \in H$ there exists a unique solution $v \in \mathfrak{F}(\Omega_h, \mathbb{R})$ of* (127) *and the estimate is true*

$$\|v\|_{\Omega_{h.\mu}} \le \bar{\omega}(t^{(\mu)}) \le \bar{\omega}(T), \quad \mu = 0, ..., K_0, \tag{135}$$

where $\bar{\omega}$ is the maximal solution of (132).

Assumption $\hat{\mathbf{F}}$ $[f, u]$.

$(\hat{F}_1)$ F$[f, a, b, \varphi, \varphi_h, \psi_h]$ is satisfied. Moreover, there are functions $\sigma_1 : [0, T] \times \mathbb{R}_+ \to \mathbb{R}_+$, $\rho : \mathbb{R}_+^2 \to \mathbb{R}_+$ such that:

(1) σ_1 is continuous and nondecreasing with respect to both variables, $\sigma_1(t, 0) = 0$ for $t \in [0, T]$;

(2) ρ_1 is nondecreasing with respect to both variables;

(3) for each $c \ge 0$, $\varepsilon, \varepsilon_0 \ge 0$, the maximal solution of the Cauchy problem

$$\omega'(t) = c\sigma_1(t, D_1\omega(t)) + \varepsilon, \quad \omega(0) = \varepsilon_0 \tag{136}$$

is defined on $[0,T]$ and $\tilde{\omega}_1(t)=0$, $t\in[0,T]$ is the maximal solution of (136) for each $c\geq 0$ and $\varepsilon,\varepsilon_0=0$, where D_1 appears in the definition of the interpolating operator G_h;

(4) *the generalized Perron condition* holds

$$|f(t,x,z,p,q)-f(t,x,\bar{z},p,q)|\leq\rho_1(\|p\|,\|q\|)\,\sigma_1\left(t,\|z-\bar{z}\|_{\Omega_t}\right) \tag{137}$$

for each $(t,x,z,p,q),(t,x,\bar{z},p,q)\in\Delta_f^*$.

$(\hat{F}_2)$ $u\in C(\Omega,\mathbb{R})\cap C^{1,2}\left(\bar{E},\mathbb{R}\right)$ is a solution of (124)–(126).

Theorem 22 ([A5], Thm. 5.1). *Let Assumptions* $F[f,a,b,\varphi,\varphi_h,\psi_h]$, $\tilde{S}[f,h]$, $\hat{F}[f,u]$ *and* (130) *hold, there are constants* $\tilde{a}>0$, $\tilde{b}\geq 0$ *such that* $a(t,x)\geq\tilde{a}$, $b(t,x)\leq\tilde{b}$, $(t,x)\in\partial E_h$, *and there are functions* $\gamma_0,\gamma_1:H\to\mathbb{R}_+$ *such that*

$$\left|\varphi^{(\mu,m)}-\varphi_h^{(\mu,m)}\right|\leq\gamma_0(h),\ \ (t^{(\mu(},x^{(m)})\in E_{0.h},\quad\lim_{h\to 0}\gamma_0(h)=0, \tag{138}$$

$$\left|\psi^{(\mu,m)}-\psi_h^{(\mu,m)}\right|\leq h_0\gamma_1(h),\ \ (t^{(\mu(},x^{(m)})\in\partial_0 E_h,\quad\lim_{h\to 0}\gamma_1(h)=0. \tag{139}$$

Then

(i) *for each* $h\in H$ *there exists a unique solution* $v\in\mathfrak{F}(\Omega_h,R)$ *of* (127)*,*

(ii) *there is* $\alpha:H\to\mathbb{R}_+$ *such that*

$$\|U-v\|_{\Omega_{h.\mu}}\leq\alpha(h),\ \ 0\leq\mu\leq K_0,\quad\lim_{h\to 0}\alpha(h)=0, \tag{140}$$

where $U:=u|_{\Omega_h}$*, i.e. the difference method is uniformly convergent.*

Theorem 20 results from the ordinary differential inequalities, while Theorems 21, 22 I proved using Theorems 3.1, 3.2. The auxiliary Theorems 3.1, 3.2 I proved with the help of Banach's fixed point theorem and mathematical induction. I used the comparison technique from the proof of Theorem 22 to justify Theorem 6 in Section 2 of this dissertation. Let us note that the set $B(\Omega,\mathbb{R})$ in the definition of the domain Δ_f of the function f was replaced with $C(\Omega,\mathbb{R})$, and I only considered the functions f differentiable with respect to p,q due to the application and approximation of the equation (124). I came to this conclusion after the publication of [A1], when I started to deal with diffusion issues in more depth.

6 Other scientific achievements

6.1 List of publications

6.1.1 Publications before PhD

[B1] L. Sapa, *A finite-difference method for a parabolic-elliptic system*, Opuscula Mathematica 17 (1997), 57–66.

[B2] L. Sapa, *A finite-difference method for a non-linear parabolic-elliptic system with Dirichlet conditions*, Universitatis Iagellonicae Acta Mathematica 37 (1999), 363–376.

[B3] J. Artymiuk, E. Artymiuk, L. Sapa, *Construction calculations in the design of bite drilling tools*, Wiertnictwo, Nafta, Gaz 19 (2002), 27–34.

6.1.2 Publications after PhD

[B4] L. Sapa, *Existence and uniqueness of a classical solution of Fourier's first problem for nonlinear parabolic-elliptic systems*, Universitatis Iagellonicae Acta Mathematica 44 (2006), 83–95.

[B5] M. Malec, L. Sapa, *A finite difference method for nonlinear parabolic-elliptic systems of second-order partial differential equations*, Opuscula Mathematica 27 (2007), 259–289.

[B6] L. Sapa, *A finite difference method for quasi-linear and nonlinear differential functional parabolic equations with Neumann's condition*, Commentationes Mathematicae 49 (2009), 83–106.

[B7] K. Kropielnicka, L. Sapa, *Estimate of solutions for differential and difference functional equations with applications to difference methods*, Applied Mathematics and Computation 217 (2011), 6206–6218.

[B8] L. Sapa, *Estimates of solutions for parabolic differential and difference functional equations and applications*, Opuscula Mathematica 32 (2012), 529–549.

[B9] L. Sapa, *Implicit difference methods for differential functional parabolic equations with Dirichlet's condition*, Zeitschrift fur Analysis und ihre Anwendungen 32 (2013), 313–337.

[B10] K. Tkacz-Śmiech, B. Bożek, L. Sapa, M. Danielewski, *Viscosity controlled interdiffusion in nitriding*, Diffusion Foundations 10 (2016), 28–38.

[B11] M. Danielewski, L. Sapa, *Nonlinear Klein-Gordon equation in Cauchy-Navier elastic solid*, Cherkasy University Bulletin, Physical and Mathematical Sciences 1 (2017), 22–29.

[B12] L. Sapa, B. Bożek, M. Danielewski, *Weak solutions to interdiffusion models with Vegard rule*, AIP Conference Proceedings 1926, 020039 (2018), 020039-1–020039-9.

[B13] M. Danielewski, L. Sapa, *Foundations of the quaternion quantum mechanics*, Entropy 22, 1424 (2020), 1–20.

[B14] M. Danielewski, L. Sapa, *Diffusion in Cauchy elastic solid*, Diffusion Fundamentals 33 (2020), 1–14.

[B15] M. Danielewski, L. Sapa, *Quaternions and Cauchy classical theory of elasticity*, Advances in Manufacturing Science and Technology 44 (2020), 67–70.

[B16] B. Bożek, L. Sapa, K. Tkacz-Śmiech, M. Zajusz, M. Danielewski, *Compendium about multicomponent interdiffusion in 2 dimensions*, Metallurgical and Materials Transactions A (2021), doi 10.1007/s11661-021-06267-9.

6.2 Description of the results obtained

6.2.1 Diffusive and diffusive-free mass transport, [B10], [B11], [B12], [B13], [B14], [B15] [B16]

The articles B[12], B[16] are strongly related to my research on diffusive mass transport in solids, the results of which are presented in Section 2 of this dissertation. The work [B12] is a conference material. We presented here mathematical models of interdiffusion in solids for one- and multidimensional cases, (20)-(22) and (41)-(43), respectively. Moreover, we formulated Theorems 1, 2, 3 which are proved in [A6]. In [A7], [A8] we developed implicit difference methods conserving the Vegard rule for the parabolic-elliptic problem (41)-(43) and proved some of their properties in 1D and 2D. The main advantage of the work [B16] is the description of the laboratory experiment of diffusion in a sample composed of cobalt, iron and nickel in 2D geometry and the comparison of the obtained results with the numerical simulations obtained using the difference method from [A8] for the model (41)-(43). The conducted analysis confirms the correctness of the mathematical model, the difference method and theoretical results from [A8], and therefore in particular the correctness of the adopted postulate (15) about the drift velocity potential v^D. This work is currently an important compendium on interdiffusion in solids at high temperatures. The paper [B10] concerns a special form of interdiffusion in solids, which is the nitriding of metals and alloys at low temperatures. In this case, in addition to the concentrations and drift, the chemical potentials and pressure must also be taken into account. For the construction of the mathematical model, we used two continuity equations, the Vegard rule, the viscoelastic Maxwell equation for drift and pressure, and the Gibbs-Duhem equation for chemical potentials. In the one-dimensional case, we developed an implicit difference method and performed a series of numerical experiments for the Robin boundary condition with one moving end of the interval (Stefan's problem).

At the other extreme of the transport processes are the issues of completely diffusion-free mass transfer in an ideally elastic medium. The theoretical foundations of this problem were created by Cauchy, and later used by Navier. In the article [B13] we showed that quaternion quantum mechanics has well-established mathematical roots and can be derived from the elastic medium model, i.e. it can be considered to represent the physical reality of the elastic medium. Starting from the classical Navier-Cauchy equilibrium

$$u_{tt} = 3c^2\nabla(\mathrm{div}u) - c^2\mathrm{rot}(\mathrm{rot}u) \tag{141}$$

and the formula for energy

$$e = \frac{1}{2}u_t \circ u_t + \frac{3}{2}c^2(\mathrm{div}u)^2 + \frac{1}{2}c^2\mathrm{rot}u \circ \mathrm{rot}u, \tag{142}$$

and using the Helmholtz theorem on the decomposition of the velocity field $u \in \mathbb{R}^3$ and the quaternion algebra [37], we derived the system of Klein-Gordon and Poisson quaternion wave equations, as well as the quaternion Schrödinger equation, stationary and non-stationary. We obtained the quaternion stationary Schrödinger equation using the calculus of variations, minimizing the corresponding real integral functional from the lagrangian generated by the Cauchy-Riemann quaternion differential operator. The work [B13] extends the results from [B11], [B14] and [B15]. In [B11] we derived the system of Klein-Gordon and Poisson quaternion wave equations in a slightly poorer version for an ideally elastic medium, which is the Planck-Kleinert crystal. We also obtained nonlocal boundary conditions using the continuity equation for the quaternion diffusive energy flux. In turn, in [B14] we obtained the quaternion Schrödinger equation for the Planck-Kleinert crystal. The work [B15] is a short review of the results concerning the quaternion field theory described above.

6.2.2 Difference methods, [B1], [B2], B[5], [B6], [B7], [B8], [B9]

The works [B1], [B2] and [B5] concern the construction and properties of implicit difference methods for multidimensional nonlinear weakly coupled differential parabolic-elliptic systems with the initial condition and different boundary conditions. The articles [B1], [B2] I wrote before my PhD in mathematics. The article [B5] is an abbreviation of my PhD thesis, which was supplemented with one more chapter described below in [B4]. I will now characterize briefly [B2], [B5]. In these papers I studied parabolic-elliptic systems in the general form

$$\begin{cases} \partial_t z_l\,(t,x) = f_l\,(t,x,z(t,x),\partial_x z_l\,(t,x)\,,\partial_{xx} z_l\,(t,x))\,, & (t,x)\in E, \quad l=1,...,q, \\ f_l\,(t,x,z(t,x),\partial_x z_l\,(t,x)\,,\partial_{xx} z_l\,(t,x)) = 0, & (t,x)\in E, \quad l=q+1,...,p, \end{cases} \tag{143}$$

where the functions $f_l : E \times \mathbb{R}^p \times \mathbb{R}^n \times M_{n\times n} \to \mathbb{R}$, $l = 1, ..., p$ are given, $z = (z_1, ..., z_p)$, $E = [0, T] \times (0, \delta)^n \subset \mathbb{R}^{1+n}$. The system (143) I considered with the initial and boundary conditions, but in [B2] it is the Dirichlet condition, and in [B5] - the general nonlinear coupled one

$$\begin{cases} \varphi_l\left(t, x, \tilde{z}(t, x), \partial_{x_i} z_l\left(t, x\right)\right) = 0, & (t, x) \in \partial_0 E, \quad l = 1, ..., q, \\ \psi_l\left(t, x, z(t, x), \partial_{x_i} z_l\left(t, x\right)\right) = 0, & (t, x) \in \partial_0 E, \quad l = q+1, ..., p, \end{cases} \tag{144}$$

where the function $\varphi_l : \partial_0 E \times \mathbb{R}^q \times \mathbb{R} \to \mathbb{R}$, $l = 1, ..., q$ and $\psi_l : \partial_0 E \times \mathbb{R}^p \times \mathbb{R} \to \mathbb{R}$, $l = q+1, ..., p$ are given, $\tilde{z} = (z_1, ..., z_q)$, $E = [0, T] \times \partial(0, \delta)^n$. In [B2] I proved, with the help of Lemmas 4.1, 5.2 about discrete inequalities and Lemma 5.1 about consistency of the difference method, Theorem 6.1 about the error estimate and uniform convergence. In turn, in [B5], using Lemmas 5.1, 5.2, I proved Theorem 5.1 about the existence and uniqueness of solutions of the difference scheme. The important Lemma 5.2 I justified using the Banach fixed point theorem. Moreover, I proved Theorem 5.3 about the error estimate and uniform convergence of the difference method. In the proof, I used Lemmas 5.3, 5.4, 5.5 about discrete inequalities and Theorem 5.2 about consistency of the method. It is worth noting that to justify Theorem 5.3, I used discrete inequalities with nonlocal terms, even though the differential equations do not have nonlocal terms. The regularity assumptions for the functions $f_l = f_l(t, x, z, p, q)$, $\varphi_l = \varphi_l(t, x, z, p)$ and $\psi_l = \psi_l(t, x, z, p)$ generating the equations (143) and the boundary conditions (144) state that they are Lipschitzian with respect to z, p, q in their domain.

The papers [B6], [B7], [B8] and [B9] are devoted to the construction and study of properties of explicit and implicit difference methods for multidimensional nonlinear and quasi-linear non-local parabolic equations with the initial condition and boundary conditions of the Dirichlet or Neumann type. We consider the equations, parabolic in Walter's sense with a functional dependence of the Volterra type of the form

$$\partial_t z\left(t, x\right) = f\left(t, x, z, \partial_x z\left(t, x\right), \partial_{xx} z\left(t, x\right)\right), \quad (t, x) \in E, \tag{145}$$

where the function $f : E \times B(\Omega, \mathbb{R}) \times \mathbb{R}^n \times M_{n\times n} \to \mathbb{R}$ is given. In the works [B8], [B9], the set $B(\Omega, \mathbb{R})$ was replaced with the set $C(\Omega, \mathbb{R})$ (see Section 5). The article [B6] is an equivalent of the work [A1] with the difference that the boundary condition here is of the Neumann type. The assumptions, theorems and the proofing technique are analogous to those in [A1], but its realization was possible thanks to the formulation and proof of the discrete comparison Theorem 3.1. The article [B7], similarly to [A1], concerns the convergence and stability of explicit difference methods for equations with the Dirichlet condition. It initiated the important idea of finding estimates of differential and discrete solutions, independently of grid steps, which allows for a significant weakening of the Perron condition assumption, i.e. we assume it on the set Δ_f^* instead of the set Δ_f - I described it in detail in Section 5, analyzing the work [A5]. I used this idea later in [B8], and in [A5] I went even further and made assumptions for the grid steps only on Δ_f^*. The papers [B8], [B9] are devoted to implicit difference methods for equations with the Dirichlet condition. They prove the same statements as in the above mentioned articles, that is, about the existence and uniqueness of solutions to difference schemes, and about the convergence and stability. But it was possible thanks to the formulation and proof in [B9] of Theorem 3.1 about the existence and uniqueness of solutions to the implicit discrete functional equation with the initial-boundary condition and the discrete comparison Theorem 3.2. As mentioned before, in [B8] I introduced Perron's most general condition (137).

6.2.3 Other articles, [B3], [B4]

The article [B3] was written before my PhD im mathematics and is purely applicative. With the help of elementary mathematical calculations, we characterized some constructional relationships in the design of bite drilling tools.

The article [B4] is written on the basis of one chapter in my PhD thesis. In it, I proved Theorem 1 about the existence and uniqueness of the global in time classical solutions of a one-dimensional weakly coupled nonlinear nonlocal parabolic-elliptic system with the initial condition and the Dirichlet boundary condition. I proved this theorem using the monotone method of lower and upper solutions using the properties of the Green function for the Stourm-Liouville operator and the corresponding Nemytskii operator.

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5. **Scientific activity in more than one university or research institution:**

- I cooperate with mathematicians from the Jagiellonian University (dr. hab. P. Kalita). It resulted in the important article [A4].
- I cooperate with mathematicians from the University of Gdańsk (dr. hab. K. Kropielnicka, prof. H. Leszczyński, previously prof. Z. Kamont). It resulted in the important article [B7]. I gave several lectures at the seminar headed by H. Leszczyński, previously by Z. Kamont.
- For many years I have been participating in the seminar Partial Differential Equations, headed by prof. P. Zgliczyński and dr hab. A. Ochal at the Jagiellonian University. I gave several lectures there, in particular: 8 March 2011, Difference methods for parabolic equations; 28 January 2014, Existence and uniqueness of solutions to the evolutionary system with the initial condition, and the problem of stability of stationary and wave solutions; 26 May 2014, Orbital stability study by the method of the finite dimensional reduction of the spectral problem; 15, 26 March 2016, Multicomponent diffusion; 21, 28 March 2017, Differential recurrence inequalities and estimates for the Navier-Stokes system; 9 May 2018, Mathematical, numerical and physical analysis of interdiffusion models with a drift.
- For 1 year I participated in the seminar headed by prof. F. Barański at the Cracow University of Technology. I gave several lectures there. In 2018, for 1 semester, I participated in the seminar headed by prof. J. Koroński at the Cracow University of Technology. I gave a lecture there.

- On June 19, 2020, I gave the lecture, Parabolic-elliptic systems in diffusion models, at the seminar Nonlinear Analysis, headed by dr. hab. M. Galewski and prof. W. Kryszewski at the Lodz University of Technology.
- On March 4, 2021, I gave the lecture, Parabolic-elliptic and parabolic systems in diffusion models, at the seminar Equations of Mathematical Physics, headed by prof. G. Łukaszewicz at the University of Warsaw. I am attending this seminar which is conducted online.
- For 10 years I have been cooperating with scientists from the Faculty of Materials Science and Ceramics of AGH (prof. M. Danielewski, prof. R. Filipek, prof. K. Tkacz-Śmiech, dr. K. Szyszkiewicz-Warzecha, dr. M. Zajusz). This resulted in many articles: [A4], [A6], [A7], [A8], [B10] - [B16]. I was a contractor in 3 grants, 2 headed by prof. M. Danielewski (MAESTRO, No. 2011/02/A/ST8/00280; OPUS 13, No. 2017/25/B/ST8/02549) and 1 headed by prof. R. Filipek (INNOTECH-K1/IN1/25/153217/NCBR/12). Cooperation with practitioners gives me the opportunity to verify the constructed mathematical models describing diffusion in solids by comparing mathematical theorems and numerical simulations with the results of laboratory experiments. The effects of such a comparison are particularly visible in [A8] and [B16]. I believe that in the future, the analysis of experiments will help me prove new mathematical theorems concerning the properties of solutions to differential equations generated by these models. I also hope that appropriate experiments can be carried out with ion channels, biological channels or their artificial equivalents.

6. **Achievements in teaching, organization and science popularization:**

   a) Teaching activities:

   - I was a supervisor of 18 defended master's theses. Currently, I have 3 graduate students. I was also a supervisor of 11 defended bachelor's theses. I reviewed many bachelor's and master's theses.
   - In the second year, I conduct the important course lecture Differential Equations for the second year of first-cycle studies at the Faculty of Applied Mathematics. For many years I have been conducting the monographic lecture (currently a seminar) Numerical Methods of Partial Differential Equations for second-cycle studies at the Faculty of Applied Mathematics - it is compulsory for the specialty computational and computer mathematics. In addition, for several years I conducted the monographic lecture, Iterative Methods for Nonlinear Equations, and lectures and tutorials in Mathematical Analysis and Functional Analysis, and also for one year - bachelor's seminar, at the Faculty of Applied Mathematics.
   - I conducted lectures and tutorials in mathematics at AGH for the following fields of study: electrical engineering, electronics, informatics, telecommunications, energy, technology chemical. Since the beginning of my employment in 1993, I have been giving lectures and tutorials in mathematics in part-time studies, in the fields of study: electrical engineering, informatics. In the years 1993-2015 I conducted lectures and tutorials in mathematics and from mathematical statistics in Local Teaching Centers AGH in Krosno, Nowa Sól, Bolesławiec and Jastrzębie Zdrój.
   - In 2014, I was awarded the Medal of the National Education Commission.

b) Organizational activities:

    - For the last 3 terms of office, I was a member of the Council of the Faculty of Applied Mathematics of AGH. During this period, I was a member of the Faculty Teaching Committee and the AGH University of Science and Technology Disciplinary Committee for Students. For 2 terms I was a member of the Faculty Committee for Awards and Decorations. Currently, I am a member of the Faculty Teaching Committee, the Committee for Specialty Mathematics in Technical and Natural Sciences, and the Committee for the Bachelor's Examination and Second-Cycle Entrance Examination.
    - In 2008 and 2009, I participated in the works of the Faculty Admissions Committee.
    - As part of recruitment at AGH, I have been taking part in the organization of the AGH Diamond Index Olympiad for many years, conducting the second stage of this Olympiad in Nowa Sól.
    - For the last term of office I was a member of the Audit Committee of the Cracow Branch of the Polish Mathematical Society.

c) Activities popularizing science:

    - For many years I have been taking part in the organization of the Science Festival in Cracow.

7. **Other informations:**

- According to the Web of Science database, my Hirsch index is equel to 5, there are 14 of my articles in this database ([A9] and [B16] are not yet included), the number of citations is equel to 51, including 22 without self citations; the number of citing articles is equel to 27, including 17 without self citing ones.
- I participated in 30 international scientific conferences, including 5 foreign ones: 2 times in Latvia, 1 time in Hungary, Ukraine and Bulgaria. I delivered 26 talks, including 1 plenary (Latvia, 2018) and presented 2 posters. Moreover, I was a co-author of 11 talks at international scientific conferences, including 8 foreign ones: 4 times in Austria, 1 time in South Korea, Greece, Croatia and Ukraine.
- I was a contractor in 3 grants:
    1) MAESTRO, No. 2011/02/A/ST8/00280, Diffusion in solids revisited; the unification of the bi-velocity and phase field methods for designing new materials, Head: prof. M. Danielewski, The project was implemented in: 30.04.2012 - 30.04.2017,
    2) INNOTECH-K1/IN1/25/153217/NCBR/12, Innovative non-destructive method of corrosion diagnosis of reinforced concrete structures, Head: prof. R. Filipek, The project was implemented in: 1.05.2012 - 30.09.2015.
    3) OPUS 13, No. 2017/25/B/ST8/02549, New generation solid electrolytes - influence of impurities on oxide properties high entropy materials, Head: prof. M. Danielewski, The project was implemented in: 23.11.2017 - 23.11.2020, extended until September 2021.
- I reviewed 19 scientific articles for the following journals: Mathematics (6), Journal of Computational and Applied Mathematics (2), Annales Polonici Mathematici (2), Opuscula Mathematica (2), Universitatis Iagellonicae Acta Mathematica (2), Mathematical Biosciences (2), Symmetry (1), Mathematical Bulletin of the Shevchenko Scientific Society (1), Machines (1).

- In 2015, I reviewed the book by prof. J. Myjak, Differential Equations, for AGH Publishing House.
- I was awarded the 3rd degree individual Rector's Award for my scientific activity, in 2012 and 2019.