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Difference Methods to One and Multidimensional Interdiffusion Models with Vegard Rule

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Abstract. In this work we consider the one and multidimensional diffusional transport in an s-component solid solution. The new model is expressed by the nonlinear parabolic-elliptic system of strongly coupled differential equations with the initial and the nonlinear coupled boundary conditions. It is obtained from the local mass conservation law for fluxes which are a sum of the diffusional and Darken drift terms, together with the Vegard rule. The considered boundary conditions allow the physical system to be not only closed but also open. We construct the implicit finite difference methods (FDM) generated by some linearization idea, in the one and two-dimensional cases. The theorems on existence and uniqueness of solutions of the implicit difference schemes, and the theorems concerned convergence and stability are proved. We present the approximate concentrations, drift and its potential for a ternary mixture of nickel, copper and iron. Such difference methods can be also generalized on the three-dimensional case. The agreement between the theoretical results, numerical simulations and experimental data is shown.

Keywords: interdiffusion, Darken method, Vegard rule, parabolic-elliptic nonlinear differential system, implicit finite difference method, existence and uniqueness of solutions to difference scheme, convergence, stability.

AMS Subject Classification: 65M06; 65M22; 35M33; 35Q70.

1 Introduction

Quantitative description of the diffuse mass transport is particularly essential for materials processing and hydrodynamics. It is important for the Navier–Stokes problem, where it allows considering diffusion in multicomponent fluids [13]. An inspiring effort dedicated to the rigorous mathematical treatment of the flows occurring in multicomponent systems has begun with the work of Darken [10] on the modeling of diffusive flows. In the case of the one-dimensional binary closed mixture with constant concentration, $c_1+c_2 = \text{const}$, the Darken method allows to transform the system of two partial differential equations modeling the process

$$\partial_t c_i = -\partial_x\big(-D_i(c_1,c_2)\partial_x c_i + c_i v^d\big) \quad \text{for} \quad i = 1,2,$$

to one quasi-linear diffusion equation

$$\partial_t c_1 = \partial_x\big(\tilde{D}(c_1)\partial_x c_1\big), \tag{1.1}$$

with the initial and the simple boundary conditions (semi-infinite only), where v^d means a drift velocity. Equation (1.1) allows using the Boltzmann–Matano transformation [3]. It introduces a similarity parameter $\lambda = (x-x_0)/\sqrt{t}$, where x_0 is the position of the so-called Matano interface [18]. This ansatz transforms, in a not equivalent way, the governing partial differential diffusion equation (1.1) to a nonlinear ordinary differential equation. But in a multicomponent case (three or more components, $s \geq 3$) such the Darken reduction is not effective, because leads to a system of equations. Analogous procedure is used in a case of the Onsager phenomenological equations, where the fluxes are coupled by interdiffusion coefficients $D_i(c_1,\dots,c_{s-1})$ for $i = 1,\dots,s$.

The drift velocity v^d is concerned with the Kirkendall effect [23]. It is the motion of the boundary between two metals that occurs as a consequence of the difference in diffusion rates of the metal atoms. The effect can be observed for example by placing insoluble markers at the interface between a pure metal and an alloy containing that metal, and heating to a temperature where atomic diffusion is possible; the boundary will move relative to the markers. The Kirkendall effect has important practical consequences. One of these is the prevention or suppression of voids formed at the boundary interface in various kinds of alloy to metal bondings. These are referred to as Kirkendall voids.

The Darken method was extended for multicomponent systems in [16]. Later it was proved that it is self-consistent with the Onsager phenomenological description [4]. Several attempts to solve the problem in liquid mixtures were little effective due to arbitrary selection of the reference frame for diffusion. The most fundamental approach is given in [6], where a volume transport is considered.

In the paper we study the model of interdiffusion introduced in [22] and in some special case in [24], in the one-dimensional and the multidimensional cases. The model is expressed by the strongly coupled nonlinear parabolic-

elliptic system

$$\begin{cases} \partial_t c_i + \operatorname{div}\big(-D_i(c_1,\ldots,c_s)\nabla c_i + c_i \nabla F\big) = 0, \\ \triangle F = \operatorname{div}\big(\sum_{k=1}^{s} \Omega_k D_k(c_1,\ldots,c_s)\nabla c_k\big), \\ \int_\Omega F dx = 0, \end{cases} \tag{1.2}$$

for $i = 1,\ldots,s$, where Ω_k means the partial molar volume of the kth component (see Section 2), with the initial and the nonlinear coupled boundary conditions. It is obtained from the local mass conservation law for fluxes which are a sum of the diffusional and Darken drift terms, together with the Vegard rule. This rule is a straight application of the Euler homogeneous function theorem [12]. The strong coupling of the equations is caused by the potential F of the drift velocity v^d. In the one-dimensional case our model implies the well-known evolutional model studied in [7, 8, 16, 21, 22]

$$\partial_t c_i + \partial_x\big(-D_i(c_1,\ldots,c_s)\partial_x c_i + c_i\big(\sum_{k=1}^{s} \Omega_k D_k(c_1,\ldots,c_s)\partial_x c_k + K(t)\big)\big) = 0, \tag{1.3}$$

for $i = 1,\ldots,s$. Note that the three-dimensional generalization of (1.3) has been studied for example in [5, 9]. But in those papers it is assumed that a some vector field equals zero because the divergence of this field equals zero. It is not a mathematical way and physically a part of information from fluxes is neglected. We omit this assumption by a postulate that the field of the drift is potential. A detailed analysis of a concept of the drift velocity, a choice of the reference frame, as well as the other physical, mathematical and numerical consequences of the proposed formalism can be found in [4,7,8,11,16,25,26] and in the references therein. In those papers concentration of a mixture must be constant, while the Vegard rule assumed by us admits the overall concentration depending on time and a space. We do not use the Darken reduction method and the not equivalent Boltzmann–Matano substitution mentioned above.

The aim of the paper is giving the implicit finite difference methods (FDM) of approximate solving of system (1.2) with the initial-boundary conditions in the one and two-dimensional cases, and theirs mathematical analysis. In the construction of the numerical methods an idea od some linearization is used. The agreement between the theoretical results, numerical simulations and experimental data is shown.

Let us stress that such strongly coupled systems as (1.2) or (1.3) (i.e., by the second derivatives) mathematically have been seldom investigated. The system (1.2) is a little similar in the structure to the Nernst–Planck–Poisson system (NPP) [1, 2, 14, 15]. We suppose after analysis of the papers mentioned above, concerned the NPP model that if the initial concentrations and the fluxes on the boundaries are sufficiently regular, then system (1.2) has a unique regular solution. It is a completely new model and our analytical investigations are not finished.

In the paper we prove that the convergence and stability of our method with respect to the concentrations are equivalent to the convergence and stability with respect to the potential, in the suitable difference maximum norms. In the proofs we use a technique studied in [17, 19, 20]. We assume additionally

that some difference quotients are uniformly bounded with respect to meshes. This property is observed in numerical experiments. Since our differential system is parabolic–elliptic strongly nonlinear system, theoretical convergence and stability analysis for the proposed numerical method is a challenge task. The same problem is open for the NPP model.

The paper is organized in the following way. In Section 2 the initial-boundary differential problem is formulated. Sections 3 and 4 deal with the construction of the implicit finite difference methods, the theorems on existence, uniqueness of solutions to the suitable difference schemes and some convergence and stability properties in the one and two-dimensional cases, respectively. Moreover, the examples of physical problems and numerical experiments are given in these sections.

2 Strong formulation of an interdiffusion model

In [22] the following model of interdiffusion is constructed. Let an open and bounded set $\Omega \subset \mathbb{R}^n$ with a piecewise smooth boundary $\partial\Omega$, $T > 0$ and $s \in \mathbb{N} \setminus \{1\}$ be fixed, and denote $\mathbb{R}_+ = (0, \infty)$. The symbol $\overline{\Omega}$ means the closure of Ω.

The following data are given:

1. $\Omega_i = \text{const} \in \mathbb{R}_+ -$ the partial molar volume of the ith component of the mixture, $i = 1, \dots, s$.
2. $D_i : \left[0, \frac{1}{\Omega_1}\right] \times \dots \times \left[0, \frac{1}{\Omega_s}\right] \to \mathbb{R}_+ -$ the diffusion coefficient of the ith component of the mixture, $i = 1, \dots, s$.
3. $c_{0i} : \Omega \to \mathbb{R}_+ -$ the initial concentration of the ith component of the mixture, $i = 1, \dots, s$.
4. $j_i : [0, T] \times \partial\Omega \to \mathbb{R} -$ the evolution of a mass flow of the ith component of the mixture through the boundary $\partial\Omega$, $i = 1, \dots, s$.

The following functions are unknown:

1. $c_i : [0, T] \times \Omega \to \mathbb{R}_+ -$ the concentration of the ith component of the mixture, $i = 1, \dots, s$.
2. $v^d : [0, T] \times \Omega \to \mathbb{R}^n -$ the drift velocity.

We assume that each component of the mixture is a continuous medium, i.e. it satisfies the local mass conservation law (continuity equation)

$$\partial_t c_i + \operatorname{div} J_i = 0 \quad \text{on} \quad [0, T] \times \Omega, \quad i = 1, \dots, s, \tag{2.1}$$

where

$$J_i = -D_i(c_1, \dots, c_s)\nabla c_i + c_i v^d \quad \text{on} \quad [0, T] \times \Omega, \quad i = 1, \dots, s \tag{2.2}$$

is a flux of the ith component of the mixture, and it is a sum of the diffusional and Darken drift fluxes. Note that (2.2) is a generalization of the Fick flux

formula. Moreover, we postulate the constant partial molar volumes and the noncompressible transport (Vegard rule)

$$\sum_{i=1}^{s} \Omega_i c_i = 1 \quad \text{on} \quad [0,T] \times \Omega. \tag{2.3}$$

Consider the initial condition on the concentrations

$$c_i(0,x) = c_{0i}(x) \quad \text{on} \quad \overline{\Omega}, \tag{2.4}$$

and the boundary conditions

$$J_i \circ \mathbf{n} = j_i(t,x) \quad \text{on} \quad [0,T] \times \partial\Omega, \quad i = 1, \ldots, s, \tag{2.5}$$

where $\mathbf{n}$ is the outside normal to the boundary $\partial\Omega$.

Multiplying (2.1) by Ω_i, adding its by sides and using (2.2), (2.3) we obtain the volume continuity equation

$$\operatorname{div}\big(-\sum_{i=1}^{s} \Omega_i D_i(c_1, \ldots, c_s)\nabla c_i + v^d\big) = 0 \quad \text{on} \quad [0,T] \times \Omega.$$

We postulate that there exists a potential F of the drift v^d:

$$\nabla F = v^d. \tag{2.6}$$

In consequence

$$\triangle F = \operatorname{div}\big(\sum_{i=1}^{s} \Omega_i D_i(c_1, \ldots, c_s)\nabla c_i\big) \quad \text{on} \quad [0,T] \times \Omega.$$

Moreover, multiplying (2.2) by Ω_i and $\mathbf{n}$, adding its by sides and using (2.3), (2.5) we get

$$\frac{\partial F}{\partial \mathbf{n}} = \sum_{i=1}^{s} \Omega_i \big(D_i(c_1, \ldots, c_s)\frac{\partial c_i}{\partial \mathbf{n}} + j_i(t,x)\big) \quad \text{on} \quad [0,T] \times \partial\Omega.$$

The solution of the problem of interdiffusion in the s-component solid solution are the functions c_i, $i = 1, \ldots, s$ and F which fulfill the strongly coupled nonlinear parabolic-elliptic system

$$\begin{cases} \partial_t c_i + \operatorname{div}\big(-D_i(c_1, \ldots, c_s)\nabla c_i + c_i \nabla F\big) = 0 \quad \text{on} \quad [0,T] \times \Omega, \\ \triangle F = \operatorname{div}\big(\sum_{k=1}^{s} \Omega_k D_k(c_1, \ldots, c_s)\nabla c_k\big) \quad \text{on} \quad [0,T] \times \Omega, \\ \int_\Omega F dx = 0 \quad \text{on} \quad [0,T], \end{cases} \tag{2.7}$$

with the initial condition

$$c_i(0,x) = c_{0i}(x) \quad \text{on} \quad \overline{\Omega}, \tag{2.8}$$

and the coupled nonlinear boundary conditions

$$\begin{cases} -D_i(c_1,\dots,c_s)\frac{\partial c_i}{\partial \mathbf{n}} + c_i\frac{\partial F}{\partial \mathbf{n}} = j_i(t,x) \quad \text{on} \quad [0,T]\times\partial\Omega, \\ \frac{\partial F}{\partial \mathbf{n}} = \sum_{k=1}^{s}\Omega_k\big(D_k(c_1,\dots,c_s)\frac{\partial c_k}{\partial \mathbf{n}} + j_k(t,x)\big) \quad \text{on} \quad [0,T]\times\partial\Omega, \end{cases} \tag{2.9}$$

$i = 1,\dots,s$. We assume the constant volume

$$\int_{\partial\Omega}\sum_{i=1}^{s}\Omega_i j_i(t,x)dS = 0$$

for $t \in [0,T]$. It can be treated as the compatibility condition to the elliptic subsystem be well posed. This condition follows immediately from the Gauss theorem. Moreover, we assume the Vegard rule on the initial concentrations

$$\sum_{i=1}^{s}\Omega_i c_{0i}(x) = 1 \quad \text{on} \quad \Omega,$$

(see (2.3), (2.4)).

Remark 1. If $n = 1$ and v^d is continuous, then there exists F in (2.6). Moreover, in this case system (2.7) with the boundary conditions (2.9) imply by integration of the elliptic equation on F, the strongly coupled nonlinear evolution system

$$\begin{aligned} &\partial_t c_i + \partial_x\big(-D_i(c_1,\dots,c_s)\partial_x c_i \\ &\quad + c_i\Big(\sum_{k=1}^{s}\Omega_k D_k(c_1,\dots,c_s)\partial_x c_k + K(t)\big)\Big) = 0, \quad \text{on} \quad [0,T]\times\Omega, \end{aligned} \tag{2.10}$$

and the coupled nonlinear boundary conditions

$$\begin{aligned} &- D_i(c_1,\dots,c_s)\frac{\partial c_i}{\partial \mathbf{n}} + c_i\Big(\sum_{k=1}^{s}\Omega_k D_k(c_1,\dots,c_s)\frac{\partial c_k}{\partial \mathbf{n}} \\ &\qquad + K(t)\mathbf{n}\Big) = j_i(t,x), \quad \text{on} \quad [0,T]\times\partial\Omega, \end{aligned} \tag{2.11}$$

$i = 1,\dots,s$, where

$$K(t) = \sum_{i=1}^{s}\Omega_i j_i(t,\Lambda) = -\sum_{i=1}^{s}\Omega_i j_i(t,-\Lambda),$$

$\Omega = (-\Lambda,\Lambda)$. The one dimensional model (2.10), (2.8), (2.11) is well-known for many years [7, 8, 16, 21, 22].

Remark 2. If $n = 2$ or $n = 3$, Ω is a connected region and rot $v^d = 0$, then there exists F also in (2.6). Nearly all of the diffusion processes in solids show negligible turbulence, thus it can be neglected and the postulate about rot $v^d = 0$ is appropriate.

3 Implicit difference method and example, case n=1

Let $\Omega = (-\Lambda, \Lambda)$. We assume to test our model that the diffusion coefficients D_i are constant and the physical system is closed, i.e. $j_i(t, \Lambda) = j_i(t, -\Lambda) \equiv 0$ for $t \in [0, T]$, $i = 1, \ldots, s$. The initial-boundary differential problem (2.7)–(2.9) takes now a form

$$\begin{cases} \partial_t c_i = D_i \partial_{xx} c_i - \partial_x c_i \partial_x F - c_i \partial_{xx} F \quad \text{on} \quad [0,T] \times \Omega, \\ \partial_{xx} F = \sum_{k=1}^{s} \Omega_k D_k \partial_{xx} c_k \quad \text{on} \quad [0,T] \times \Omega, \\ \int_\Omega F dx = 0 \quad \text{on} \quad [0,T], \end{cases} \tag{3.1}$$

$$c_i(0,x) = c_{0i}(x) \quad \text{on} \quad \overline{\Omega}, \tag{3.2}$$

$$\begin{cases} -D_i \partial_x c_i + c_i \sum_{k=1}^{s} \Omega_k D_k \partial_x c_k = 0 \quad \text{on} \quad [0,T] \times \partial\Omega, \\ \partial_x F = \sum_{k=1}^{s} \Omega_k D_k \partial_x c_k \quad \text{on} \quad [0,T] \times \partial\Omega, \end{cases} \tag{3.3}$$

$i = 1, \ldots, s$. Taking into account the Vegard rule (2.3), we calculate

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

and then (3.1)–(3.3) are reduced as follows

$$\begin{cases} \partial_t c_i = D_i \partial_{xx} c_i - \partial_x c_i \partial_x F - c_i \partial_{xx} F \quad \text{on} \quad [0,T] \times \Omega, \\ \partial_{xx} F = \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_{xx} c_k \quad \text{on} \quad [0,T] \times \Omega, \\ \int_\Omega F dx = 0 \quad \text{on} \quad [0,T], \end{cases} \tag{3.4}$$

$$c_i(0,x) = c_{0i}(x) \quad \text{on} \quad \bar{\Omega}, \tag{3.5}$$

$$\begin{cases} -D_i \partial_x c_i + c_i \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_x c_k = 0 \quad \text{on} \quad [0,T] \times \partial\Omega, \\ \partial_x F = \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_x c_k \quad \text{on} \quad [0,T] \times \partial\Omega, \end{cases} \tag{3.6}$$

$i = 1, \ldots, s-1$. We assume additionally that

$$\sum_{i=1}^{s-1} \Omega_i c_{0i}(x) \leq 1 \quad \text{on} \quad \Omega.$$

3.1 Implicit difference method

Define a mesh on Ω in the following way. Let $h = 2\Lambda/(M+1)$ and $\tau = T/K$ stand for the space and time steps of the mesh, respectively, where $M, K \in \mathbb{N}$ are given. Define nodal points (t^μ, x_m) as follows

$$\begin{aligned} x_m &= -\Lambda + mh, \quad m = 0, 1, \ldots, M+1, \\ t^\mu &= \mu\tau, \quad \mu = 0, 1, \ldots, K. \end{aligned}$$

We define an implicit difference scheme for the elliptic subsystem on F in

(3.4)–(3.6). It is a system of linear algebraic equations of the form

$$\begin{cases} -F_0^{\mu+1} + F_1^{\mu+1} = P_0^\mu(c) := \sum_{k=1}^{s-1} \Omega_k\big(D_k - D_s\big)\big(-c_{k,0}^\mu + c_{k,1}^\mu\big), \\ F_{m-1}^{\mu+1} - 2F_m^{\mu+1} + F_{m+1}^{\mu+1} = P_m^\mu(c) \\ \qquad := \sum_{k=1}^{s-1} \Omega_k\big(D_k - D_s\big)\big(c_{k,m-1}^\mu - 2c_{k,m}^\mu + c_{k,m+1}^\mu\big), \\ F_M^{\mu+1} - F_{M+1}^{\mu+1} = P_{M+1}^\mu(c) := \sum_{k=1}^{s-1} \Omega_k\big(D_k - D_s\big)\big(c_{k,M}^\mu - c_{k,M+1}^\mu\big), \\ F_0^{\mu+1} + 2\sum_{m=1}^{M} F_m^{\mu+1} + F_{M+1}^{\mu+1} = 0, \end{cases} \tag{3.7}$$

for $m = 1, \dots, M$, $\mu = 0, \dots, K-1$. For each μ it is the system of $M+3$ equations with $M+2$ unknowns.

Then we define an *implicit difference scheme* for the concentrations c_i, $i = 1, \dots, s-1$ as a system of linear algebraic equations of the form

$$\begin{cases} q_{i,0}^\mu c_{i,0}^{\mu+1} + q_{i,1}^\mu c_{i,1}^{\mu+1} = Q_{i,0}^\mu := 0, \\ d_{i,m-1}^\mu c_{i,m-1}^{\mu+1} + v_{i,m}^\mu c_{i,m}^{\mu+1} + u_{i,m+1}^\mu c_{i,m+1}^{\mu+1} = Q_{i,m}^\mu := e_{i,m}^\mu c_{i,m}^\mu, \\ q_{i,M}^\mu c_{i,M}^{\mu+1} + q_{i,M+1}^\mu c_{i,M+1}^{\mu+1} = Q_{i,M+1}^\mu := 0, \end{cases} \tag{3.8}$$

where

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

for $m = 1, \dots, M$, $i = 1, \dots, s-1$ and $\mu = 0, \dots, K-1$. For each μ and i it is the system of $M+2$ equations with $M+2$ unknowns.

If $v_{i,m}^{\mu(m)} \neq 0$, then we make a sequence of the Gauss substitutions

$$\begin{aligned} &v_{i,k}^{\mu(0)} = q_{i,k}^\mu, \quad k = 0, 1, \quad v_{i,m}^{\mu(m)} = v_{i,m}^\mu - d_{i,m-1}^\mu\big(v_{i,m-1}^{\mu(m-1)}\big)^{-1} v_{i,m}^{\mu(m-1)}, \\ &v_{i,m-1}^{\mu(m)} = 0, \quad v_{i,m+1}^{\mu(m)} = u_{i,m+1}^\mu, v_{i,M+1}^{\mu(M+1)} = q_{i,M+1}^\mu - q_{i,M}^\mu\big(v_{i,M}^{\mu(M)}\big)^{-1} v_{i,M+1}^{\mu(M)}, \\ &v_{i,M}^{\mu(M+1)} = 0, \quad Q_{i,0}^{\mu(0)} = Q_{i,0}^\mu, \quad Q_{i,m}^{\mu(m)} = Q_{i,m}^\mu - d_{i,m-1}^\mu\big(v_{i,m-1}^{\mu(m-1)}\big)^{-1} Q_{i,m-1}^{\mu(m-1)}, \\ &Q_{i,M+1}^{\mu(M+1)} = Q_{i,M+1}^\mu - q_{i,M}^\mu\big(v_{i,M}^{\mu(M)}\big)^{-1} Q_{i,M}^{\mu(M)}, \end{aligned} \tag{3.9}$$

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

Theorem 1. *(i) For all the steps h, τ, system (3.7) has exactly one solution*

$F^{\mu+1}$ for given concentrations $(c_1^\mu,\dots,c_{s-1}^\mu)$ of the form

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

$$F_m^{\mu+1}=F_{m+1}^{\mu+1}-\sum_{k=1}^{s-1}\Omega_k(D_k-D_s)(c_{k,m+1}^\mu-c_{k,m}^\mu),\ m=M,\dots,0. \tag{3.10}$$

(ii) System (3.8) has exactly one solution $(c_1^{\mu+1},\dots,c_{s-1}^{\mu+1})$ for given concentrations $(c_1^\mu,\dots,c_{s-1}^\mu)$ and potential $F^{\mu+1}$ if and only if the steps h, τ are such small that $v_{i,m}^{\mu(m)}\neq 0$, $m=0,\dots,M+1$, $i=1,\dots,s-1$. It has the formula

$$\begin{aligned} c_{i,M+1}^{\mu+1}&=\left(v_{i,M+1}^{\mu(M+1)}\right)^{-1}Q_{i,M+1}^{\mu(M+1)},\\ c_{i,m}^{\mu+1}&=\left(v_{i,m}^{\mu(m)}\right)^{-1}\left(Q_{i,m}^{\mu(m)}-v_{i,m+1}^{\mu(m)}c_{i,m+1}^{\mu+1}\right),\quad m=M,\dots,0, \end{aligned} \tag{3.11}$$

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

Proof. We will prove firstly point (i). Let any μ be fixed and let concentrations $(c_1^\mu,\dots,c_{s-1}^\mu)$ be known. Adding the first equation to the second one, the new second equation to the third one, and so on, leads to the system

$$\begin{pmatrix} -1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0\\ 0 & -1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0\\ 0 & 0 & -1 & 1 & \cdots & 0 & 0 & 0 & 0\\ \vdots & & & & \ddots & & & & \vdots\\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 1\\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0\\ 1 & 2 & 2 & 2 & \cdots & 2 & 2 & 2 & 1 \end{pmatrix}\begin{pmatrix} F_0^{\mu+1}\\ F_1^{\mu+1}\\ F_2^{\mu+1}\\ \vdots\\ F_M^{\mu+1}\\ F_{M+1}^{\mu+1}\end{pmatrix}=\begin{pmatrix} \sum_{j=0}^{0}P_j^\mu(c)\\ \sum_{j=0}^{1}P_j^\mu(c)\\ \sum_{j=0}^{2}P_j^\mu(c)\\ \vdots\\ \sum_{j=0}^{M}P_j^\mu(c)\\ \sum_{j=0}^{M+1}P_j^\mu(c)\\ 0\end{pmatrix}.$$

It follows from elementary calculations that $\sum_{j=0}^{M+1}P_j^\mu(c)=0$. Hence, the last equation but one can be omitted and after next eliminations we get the equivalent system, where the $(M+1)$th equation is defined as

$$2(M+1)F_{M+1}^{\mu+1}=\sum_{l=0}^{M}(1+2l)\sum_{j=0}^{l}P_j^\mu(c),$$

with the square $(M+2)\times(M+2)$ nonsingular matrix. It has a unique solution of the form (3.10), because

$$\begin{aligned} &\sum_{j=0}^{l}P_j^\mu(c)=\sum_{k=1}^{s-1}\Omega_k(D_k-D_s)(c_{k,l+1}^\mu-c_{k,l}^\mu),\ \ \sum_{l=0}^{M}(1+2l)\sum_{j=0}^{l}P_j^\mu(c)\\ &\quad=\sum_{k=1}^{s-1}\Omega_k(D_k-D_s)\big[-c_{k,0}^\mu-2\sum_{l=1}^{M}c_{k,l}^\mu+(1+2M)c_{k,M+1}^\mu\big],\ \ l=0,\dots,M. \end{aligned}$$

Now we will prove point (ii). Let any μ and i be fixed and let concentrations $(c_1^\mu,\dots,c_{s-1}^\mu)$ and potential $F^{\mu+1}$ be known. We see that the matrix in (3.8) has

a tridiagonal form. Assume that the steps h, τ are such small that $v_{i,m}^{\mu(m)} \neq 0$, $m = 0, \ldots, M+1$ in (3.9). In consequence, after the use of the Gauss elimination method (3.9), system (3.8) has the equivalent form

$$\begin{pmatrix} v_{i,0}^{\mu(0)} & v_{i,1}^{\mu(0)} & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & v_{i,1}^{\mu(1)} & v_{i,2}^{\mu(1)} & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & v_{i,2}^{\mu(2)} & v_{i,3}^{\mu(2)} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & v_{i,M}^{\mu(M)} & v_{i,M+1}^{\mu(M)} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & v_{i,M+1}^{\mu(M+1)} \end{pmatrix} \begin{pmatrix} c_{i,0}^{\mu+1} \\ c_{i,1}^{\mu+1} \\ \vdots \\ c_{i,M+1}^{\mu+1} \end{pmatrix} = \begin{pmatrix} Q_{i,0}^{\mu(0)} \\ Q_{i,1}^{\mu(1)} \\ \vdots \\ Q_{i,M+1}^{\mu(M+1)} \end{pmatrix}.$$

It has a unique solution of the form (3.11). □

Remark 3. Unfortunately we are not able till now to give an effective formula on the steps h, τ, independent on $F_{i,m-1}^{\mu+1}$, $F_{i,m}^{\mu+1}$, $F_{i,m+1}^{\mu+1}$, in order to the matrix generating system (3.8) be nonsingular.

Let (c, F), $c = (c_1, \ldots, c_{s-1})$ be the solution of (3.4)–(3.6) and let (w, G), $w = (w_1, \ldots, w_{s-1})$ be the solution of (3.7), (3.8). Define the errors of the difference method

$$r = c - w, \quad R = F - G,$$

the maximum norms

$$\|r\|_0 = \max\big\{|r_{i,m}^{\mu}| : \ \mu = 0, \ldots, K, \ i = 1, \ldots, s-1, \ m = 0, \ldots, M+1\big\},$$
$$\|R\|_0 = \max\big\{|R_m^{\mu}| : \ \mu = 1, \ldots, K, \ m = 0, \ldots, M+1\big\},$$

and the seminorms

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

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

$$\delta^+ r_{i,m}^{\mu} = \frac{r_{i,m+1}^{\mu} - r_{i,m}^{\mu}}{h}, \quad \delta^- r_{i,m}^{\mu} = \frac{r_{i,m}^{\mu} - r_{i,m-1}^{\mu}}{h},$$
$$\delta r_{i,m}^{\mu} = \frac{r_{i,m+1}^{\mu} - r_{i,m-1}^{\mu}}{2h}, \quad \delta^{(2)} r_{i,m}^{\mu} = \frac{r_{i,m-1}^{\mu} - 2r_{i,m}^{\mu} + r_{i,m+1}^{\mu}}{h^2},$$

and analogously δR_m^{μ}, $\delta^{(2)} R_m^{\mu}$. We introduce the following seminorms

$$\|\delta r\|_0 = \max\big\{|\delta r_{i,m}^{\mu}| : \ \mu = 0, \ldots, K, \ i = 1, \ldots, s-1, \ m = 1, \ldots, M\big\},$$
$$\|\delta^{(2)} r\|_0 = \max\big\{|\delta^{(2)} r_{i,m}^{\mu}| : \ \mu = 0, \ldots, K, \ i = 1, \ldots, s-1, \ m = 1, \ldots, M\big\},$$
$$\|\delta R\|_0 = \max\big\{|\delta R_m^{\mu}| : \ \mu = 1, \ldots, K, \ m = 1, \ldots, M\big\},$$
$$\|\delta^{(2)} R\|_0 = \max\big\{|\delta^{(2)} R_m^{\mu}| : \ \mu = 1, \ldots, K, \ m = 1, \ldots, M\big\}.$$

Moreover, we consider the maximum norms

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

Theorem 2. *Assume that* $(c, F) \in C^{1,2}([0,T] \times \overline{\Omega}, \mathbb{R}^s)$, $c = (c_1, \ldots, c_{s-1})$ *is the solution of (3.4)–(3.6) and* (w, G), $w = (w_1, \ldots, w_{s-1})$ *is the solution of (3.7), (3.8). Then there exist real valued functions* $\alpha_i(\tau, h)$, $i = 0, 1, 2$ *such that*

$$\|R\|_0 \le 2 \sum_{k=1}^{s-1} \Omega_k |D_k - D_s| \|r\|_0 + \alpha_0(\tau, h), \tag{3.12}$$
$$\|\delta R\|_0 \le \sum_{k=1}^{s-1} \Omega_k |D_k - D_s| \|\delta r\|_0 + \alpha_1(\tau, h),$$
$$\|\delta^{(2)} R\|_0 \le \sum_{k=1}^{s-1} \Omega_k |D_k - D_s| \|\delta^{(2)} r\|_0 + \alpha_2(\tau, h),$$

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

Proof. We define discrete functions $\varepsilon_m^{\mu+1}$, $\varepsilon^{\mu+1}$ as follows

$$\begin{cases} -F_0^{\mu+1} + F_1^{\mu+1} = P_0^\mu(c) + h\varepsilon_0^{\mu+1}, \\ F_{m-1}^{\mu+1} - 2F_m^{\mu+1} + F_{m+1}^{\mu+1} = P_m^\mu(c) + h^2 \varepsilon_m^{\mu+1}, \\ F_M^{\mu+1} - F_{M+1}^{\mu+1} = P_{M+1}^\mu(c) + h\varepsilon_{M+1}^{\mu+1}, \\ F_0^{\mu+1} + 2\sum_{m=1}^{M} F_m^{\mu+1} + F_{M+1}^{\mu+1} = \frac{1}{h}\varepsilon^{\mu+1}, \end{cases} \tag{3.13}$$

for $m = 1, \ldots, M$, $i = 1, \ldots, s-1$, $\mu = 0, \ldots, K-1$. The regularity of the differential solution (c, F) implies the existence of a real valued function $\varepsilon(\tau, h)$ such that for $m = 0, \ldots, M+1$, $i = 1, \ldots, s-1$, $\mu = 0, \ldots, K-1$,

$$|\varepsilon_m^{\mu+1}|, |\varepsilon^{\mu+1}| \le \varepsilon(\tau, h), \qquad \lim_{(\tau,h)\to(0,0)} \varepsilon(\tau, h) = 0. \tag{3.14}$$

Let $\mu \in \{0, \ldots, K-1\}$ be fixed. Observe that the elliptic error $R^{\mu+1}$ is the solution of the system of algebraic equations

$$\begin{cases} -R_0^{\mu+1} + R_1^{\mu+1} = P_0^\mu(r) + h\varepsilon_0^{\mu+1}, \\ R_{m-1}^{\mu+1} - 2R_m^{\mu+1} + R_{m+1}^{\mu+1} = P_m^\mu(r) + h^2 \varepsilon_m^{\mu+1}, \\ R_M^{\mu+1} - R_{M+1}^{\mu+1} = P_{M+1}^\mu(r) + h\varepsilon_{M+1}^{\mu+1}, \\ R_0^{\mu+1} + 2\sum_{m=1}^{M} R_m^{\mu+1} + R_{M+1}^{\mu+1} = \frac{1}{h}\varepsilon^{\mu+1}, \end{cases} \tag{3.15}$$

$m = 1, \ldots, M$, where the parabolic error r^μ is treated as given. Reasoning similarly as in the proof of Theorem 1 we get

$$R_{M+1}^{\mu+1} = \frac{\sum_{k=1}^{s-1} \Omega_k (D_k - D_s)\big[-r_{k,0}^\mu - 2\sum_{l=1}^{M} r_{k,l}^\mu + (1+2M) r_{k,M+1}^\mu\big] + \bar{\varepsilon}^{\mu+1}}{2(M+1)},$$

$$R_m^{\mu+1} = R_{m+1}^{\mu+1} - \sum_{k=1}^{s-1} \Omega_k (D_k - D_s)(r_{k,m+1}^\mu - r_{k,m}^\mu) - \bar{\varepsilon}_m^{\mu+1}, \; m = M, \ldots, 0, \tag{3.16}$$

where

$$\overline{\varepsilon}^{\mu+1}=\sum_{l=0}^{M}(1+2l)\big(h\varepsilon_0^{\mu+1}+h^2\sum_{j=1}^{l}\varepsilon_j^{\mu+1}\big)+\frac{1}{h}\varepsilon^{\mu+1},\quad \overline{\varepsilon}_m^{\mu+1}=h\varepsilon_0^{\mu+1}+h^2\sum_{j=1}^{m}\varepsilon_j^{\mu+1}.$$

Note that

$$\delta R_m^{\mu+1}=\sum_{k=1}^{s-1}\Omega_k(D_k-D_s)\delta r_{k,m}^{\mu}+\overline{\overline{\varepsilon}}_m^{\mu+1},\quad m=1,\dots,M, \tag{3.17}$$

$$\delta^{(2)}R_m^{\mu+1}=\sum_{k=1}^{s-1}\Omega_k(D_k-D_s)\delta^{(2)}r_{k,m}^{\mu}+\varepsilon_m^{\mu+1},\quad m=1,\dots,M,$$

where

$$\overline{\overline{\varepsilon}}_m^{\mu+1}=-\varepsilon_0^{\mu+1}-h\sum_{l=1}^{m-1}\varepsilon_l^{\mu+1}-\frac{1}{2}h\varepsilon_m^{\mu+1}.$$

Put

$$\alpha_0(\tau,h)=\big[(1+2\Lambda)h+\Lambda^2+\Lambda+\frac{1}{\Lambda}\big]\varepsilon(\tau,h), \tag{3.18}$$

$$\alpha_1(\tau,h)=\big(\frac{1}{2}h+1+2\Lambda\big)\varepsilon(\tau,h),\quad \alpha_2(\tau,h)=\varepsilon(\tau,h).$$

It follows from (3.14), (3.16)–(3.18) that

$$\big|R_m^{\mu+1}\big|\le 2\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\|r\|_0+\alpha_0(\tau,h),\quad m=0,\dots,M+1,$$

$$\big|\delta R_m^{\mu+1}\big|\le \sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\|\delta r\|_0+\alpha_1(\tau,h),\quad m=1,\dots,M,$$

$$\big|\delta^{(2)}R_m^{\mu+1}\big|\le \sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\|\delta^{(2)}r\|_0+\alpha_2(\tau,h),\quad m=1,\dots,M,$$

and in consequence (3.12). □

Theorem 3. *Assume that* $(c,F)\in C^{1,2}([0,T]\times\overline{\Omega},\mathbb{R}^s)$, $c=(c_1,\dots,c_{s-1})$ *is the solution of (3.4)–(3.6) and* (w,G), $w=(w_1,\dots,w_{s-1})$ *is the solution of (3.7), (3.8). Let moreover*

$$\big|\delta G_m^{\mu}\big|\le A,\quad \big|\delta^{(2)}G_m^{\mu}\big|\le B,\quad \big|\delta^{+}w_{i,0}^{\mu}\big|,\quad \big|\delta^{-}w_{i,M+1}^{\mu}\big|\le C, \tag{3.19}$$

$$Ah\le 2D_i,\quad \frac{h}{\tau}\le D,\quad \lim_{(\tau,h)\to(0,0)}\frac{h}{\tau}=0, \tag{3.20}$$

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

$$\|r\|_0\le\frac{e^{LT}-1}{L}\big[\big(1+h\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\big)d\ \big(\|\delta R\|_0+\|\delta^{(2)}R\|_0\big)+\beta(\tau,h)\big] \tag{3.21}$$

and $\lim\limits_{(\tau,h)\to(0,0)} \beta(\tau,h)=0$, *where*

$$L=\frac{CD}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|+\big(1+2\Lambda\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\big)B.$$

Proof. We define discrete functions $\gamma_m^{\mu+1}$ as follows

$$\begin{cases} q_{i,0}^{\mu}c_{i,0}^{\mu+1}+q_{i,1}^{\mu}c_{i,1}^{\mu+1}=Q_{i,0}^{\mu}+h\gamma_{i,0}^{\mu+1},\\ d_{i,m-1}^{\mu}c_{i,m-1}^{\mu+1}+v_{i,m}^{\mu}c_{i,m}^{\mu+1}+u_{i,m+1}^{\mu}c_{i,m+1}^{\mu+1}=Q_{i,m}^{\mu}+\tau\gamma_{i,m}^{\mu+1},\\ q_{i,M}^{\mu}c_{i,M}^{\mu+1}+q_{i,M+1}^{\mu}c_{i,M+1}^{\mu+1}=Q_{i,M+1}^{\mu}+h\gamma_{i,M+1}^{\mu+1}, \end{cases}$$

for $i=1,\dots,s-1$, $m=1,\dots,M$, $\mu=0,\dots,K-1$. The regularity of the differential solution (c,F) implies the existence of a real valued function $\gamma(\tau,h)$ such that for $i=1,\dots,s-1$, $m=0,\dots,M+1$, $\mu=0,\dots,K-1$,

$$|\gamma_{i,m}^{\mu+1}|\le\gamma(\tau,h),\qquad \lim_{(\tau,h)\to(0,0)}\gamma(\tau,h)=0. \tag{3.22}$$

Moreover, by this regularity there is a constant $d\ge 0$ such that

$$\big|c_{i,m}^{\mu}\big|,\ \big|\delta c_{i,m}^{\mu}\big|,\ \big|\delta^{+}c_{i,0}^{\mu}\big|,\ \big|\delta^{-}c_{i,M+1}^{\mu}\big|\le d \tag{3.23}$$

for $i=1,\dots,s-1$, $m=1,\dots,M$, $\mu=0,\dots,K$.

Suppose that $\mu\in\{0,\dots,K-1\}$ is fixed. In the case $m\in\{1,\dots,M\}$ we have

$$\begin{aligned} r_{i,m}^{\mu+1}=&\big(1-\tau\delta^{(2)}G_m^{\mu+1}\big)r_{i,m}^{\mu}+\tau\big(D_i\delta^{(2)}r_{i,m}^{\mu+1}-\delta G_m^{\mu+1}\delta r_{i,m}^{\mu+1}\big)\\ &+\tau\big(-\delta c_{i,m}^{\mu+1}\delta R_m^{\mu+1}-c_{i,m}^{\mu}\delta^{(2)}R_m^{\mu+1}\big)+\tau\gamma_{i,m}^{\mu+1}. \end{aligned}$$

The above relation and (3.19), (3.20), (3.22), (3.23) give the estimates

$$\begin{aligned} &(1+2D_i\kappa)\big|r_{i,m}^{\mu+1}\big|\le(1+\tau B)\big|r_{i,m}^{\mu}\big|+\kappa\big|D_i-\frac{h}{2}\delta G_m^{\mu+1}\big|\big|r_{i,m+1}^{\mu+1}\big|\\ &\quad+\kappa\big|D_i+\frac{h}{2}\delta G_m^{\mu+1}\big|\big|r_{i,m-1}^{\mu+1}\big|+\tau d\big(\big|\delta R_m^{\mu+1}\big|+\big|\delta^{(2)}R_m^{\mu+1}\big|\big)+\tau\gamma(\tau,h),\\ &(1+2D_i\kappa)\big|r_{i,m}^{\mu+1}\big|\le(1+\tau B)\big\|r\big\|_{(\mu)}+2D_i\kappa\big\|r\big\|_{(\mu+1)}\\ &\quad+\tau d\big(\big\|\delta R\big\|_0+\big\|\delta^{(2)}R\big\|_0\big)+\tau\gamma(\tau,h),\\ &\big|r_{i,m}^{\mu+1}\big|\le(1+\tau B)\big\|r\big\|_{(\mu)}+\tau d\big(\big\|\delta R\big\|_0+\big\|\delta^{(2)}R\big\|_0\big)+\tau\gamma(\tau,h). \end{aligned} \tag{3.24}$$

Now consider the case $m=0$. Using (3.19), (3.22), (3.23) we can write

$$\begin{aligned} r_{i,0}^{\mu+1}=&\Big(1-\frac{h}{D_i}\sum_{k=1}^{s-1}\Omega_k(D_k-D_s)\delta^{+}w_{k,0}^{\mu}\Big)r_{i,1}^{\mu+1}\\ &-c_{i,1}^{\mu+1}\frac{h}{D_i}\sum_{k=1}^{s-1}\Omega_k(D_k-D_s)\delta^{+}r_{k,0}^{\mu}+\frac{h}{D_i}\gamma_{i,0}^{\mu+1}, \end{aligned}$$

$$|r_{i,0}^{\mu+1}|\le \big(1+h\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\big)|r_{i,1}^{\mu+1}|+h\frac{d(C+d)}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|$$
$$+h\frac{1}{D_i}\gamma(\tau,h). \tag{3.25}$$

Put

$$\beta(\tau,h)=\frac{h}{\tau}\frac{d(C+d)}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|+\big(1+h\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|+\frac{D}{D_i}\big)\gamma(\tau,h).$$

The formulas(3.24), (3.25) imply the estimate

$$|r_{i,0}^{\mu+1}|\le \big(1+\tau L\big)\|r\|_{(\mu)}+\tau\Big(1+h\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\Big)$$
$$\times d\big(\|\delta R\|_0+\|\delta^{(2)}R\|_0\big)+\tau\beta(\tau,h). \tag{3.26}$$

Analogously we obtain the same estimate in the case $m=M+1$,

$$|r_{i,M+1}^{\mu+1}|\le \big(1+\tau L\big)\|r\|_{(\mu)}+\tau\Big(1+h\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\Big)$$
$$\times d\big(\|\delta R\|_0+\|\delta^{(2)}R\|_0\big)+\tau\beta(\tau,h). \tag{3.27}$$

From (3.24), (3.26), (3.27) we get the recurrence inequality

$$\|r\|_{(\mu+1)}\le \big(1+\tau L\big)\|r\|_{(\mu)}+\tau\Big(1+h\frac{C}{D_i}\sum_{k=1}^{s-1}\Omega_k|D_k-D_s|\Big)$$
$$\times d\big(\|\delta R\|_0+\|\delta^{(2)}R\|_0\big)+\tau\beta(\tau,h). \tag{3.28}$$

The recurrence inequality (3.28) gives

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

$\mu=0,\dots,K$, and finally (3.21) holds. □

Remark 4. It follows from Theorem 2 that the convergence of the difference method with respect to the concentrations implies the convergence with respect to the potential in the norms $\|\ \|_i$, $i=0,1,2$, respectively. On the other hand, it follows from Theorem 3 that the convergence of the difference method with respect to the potential in the norm $\|\ \|_2$ implies the convergence with respect to the concentrations in the norm $\|\ \|_0$. Moreover, if the initial concentrations are of such regularity that the solution (c,F) of (3.4)–(3.6) belongs to $C^{2,3}([0,T]\times\overline{\Omega},\mathbb{R}^s)$, then the truncation errors $r,R=O(\tau+h)$.

Remark 5. It can be proved that the difference method studied is stable in the similar manner as it is convergent, that is the stability with respect to the concentrations is equivalent to the stability with respect to the potential. The proof is analogous to the proofs of Theorems 2, 3.

3.2 Example and numerical experiments

To illustrate a class of problems which can be treated with our method, we consider an example of a ternary mixture of nickel (Ni), copper (Cu) and iron (Fe) with constants D_i, $i = 1, 2, 3$. The examples with D_i depending on densities c_i (the dependence is of a polynomial type) are given in [25, 27].

Let the physical data be given:

$$
\begin{aligned}
&s = 3, \quad Ni - Cu - Fe, \quad \Lambda = 0.035, \quad (\Omega_1, \Omega_2, \Omega_3) = (6.5, 7.0, 7.1),\\
&(D_1, D_2, D_3) = (1.58 \cdot 10^{-13}, 5.73 \cdot 10^{-12}, 2.99 \cdot 10^{-11}),\\
&(c_{01}, c_{02}, c_{03}) = (0.069846, 0.047244, 0.030175) \quad \text{in} \quad [-\Lambda, 0],\\
&(c_{01}, c_{02}, c_{03}) = (0.0, 0.047244, 0.094119) \quad \text{in} \quad (0, \Lambda].
\end{aligned}
$$

For the times 0, 7 and 28 days we obtain with the finite difference method (FDM) given in Subsection 3.1 the following results (in Figures (1–2) the calculations are made on the mesh with 150 space nodal points):

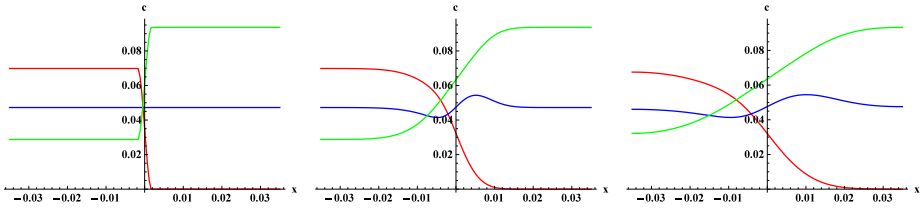

Figure 1. Distributions of concentrations c_i $(i = 1, 2, 3)$ for the times 0, 7 and 28 days respectively: c_1 – blue, c_2 – red, c_3 – green.

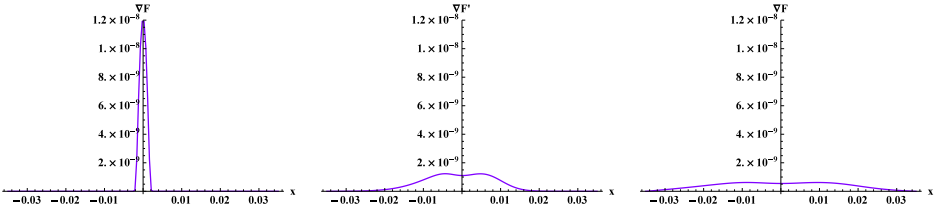

Figure 2. Distributions of dryft $v^d = \nabla F$ for the times 0, 7 and 28 days respectively.

4 Implicit difference method and example, case n=2

Let $\Omega = (-\Lambda, \Lambda) \times (-\Lambda, \Lambda)$. We assume to test our model that the diffusion coefficients D_i are constant and the physical system is closed, i.e. $j_i(t, x) \equiv 0$ for $(t, x) \in [0, T] \times \partial\Omega$, $i = 1, ..., s$. Reasoning similarly as in Section 2, the initial-boundary differential problem (2.7)–(2.9) takes a form

$$\begin{cases} \partial_t c_i = D_i(\partial_{x_1x_1} c_i + \partial_{x_2x_2} c_i) - \partial_{x_1} c_i \partial_{x_1} F \\ \qquad -\partial_{x_2} c_i \partial_{x_2} F - c_i(\partial_{x_1x_1} F + \partial_{x_2x_2} F) \quad \text{on} \quad [0,T]\times\Omega, \\ \partial_{x_1x_1} F + \partial_{x_2x_2} F = \\ \qquad \sum_{k=1}^{s-1} \Omega_k (D_k - D_s)(\partial_{x_1x_1} c_k + \partial_{x_2x_2} c_k) \quad \text{on} \quad [0,T]\times\Omega, \\ \int_\Omega F dx = 0 \quad \text{on} \quad [0,T], \end{cases} \tag{4.1}$$

$$c_i(0,x) = c_{0i}(x) \quad \text{on} \quad \overline{\Omega}, \tag{4.2}$$

$$\begin{cases} -D_i \partial_{x_j} c_i + c_i \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_{x_j} c_k = 0 \quad \text{on} \quad [0,T]\times\partial\Omega, \\ \partial_{x_j} F = \sum_{k=1}^{s-1} \Omega_k (D_k - D_s) \partial_{x_j} c_k \quad \text{on} \quad [0,T]\times\partial\Omega, \end{cases} \tag{4.3}$$

$j = 1, 2$, $i = 1, ..., s-1$. The concentration c_s we calculate from the formula

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

We assume additionally that

$$\sum_{i=1}^{s-1} \Omega_i c_{0i}(x) \le 1 \quad \text{on} \quad \Omega.$$

4.1 Implicit difference method

We define a mesh on Ω in the similar way as in Section 2. Let $h = 2\Lambda/(M+1)$ and $\tau = T/K$ stand for the space and time steps of the mesh, respectively, where $M, K \in \mathbb{N}$ are given. Define nodal points (t^μ, x_{1l}, x_{2m}) as follows

$$\begin{aligned} &x_{1l} = -\Lambda + lh,\ x_{2m} = -\Lambda + mh, \quad l,\ m = 0, 1, \dots, M+1, \\ &t^\mu = \mu\tau, \quad \mu = 0, 1, \dots, K. \end{aligned}$$

We define an *implicit difference scheme* for the elliptic subsystem on F in (4.1)–(4.3). It is a system of linear algebraic equations of the form

$$\begin{cases} F^{\mu+1}_{0,0} - \frac{1}{2}F^{\mu+1}_{0,1} - \frac{1}{2}F^{\mu+1}_{1,0} = P^\mu_{0,0}(c) := 0, \\ F^{\mu+1}_{l,0} - F^{\mu+1}_{l,1} = P^\mu_{l,0}(c) := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(c^\mu_{k,l,0} - c^\mu_{k,l,1}\big), \\ F^{\mu+1}_{M+1,0} - \frac{1}{2}F^{\mu+1}_{M+1,1} - \frac{1}{2}F^{\mu+1}_{M,0} = P^\mu_{M+1,0}(c) := 0, \\ F^{\mu+1}_{0,m} - F^{\mu+1}_{1,m} = P^\mu_{0,m}(c) := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(c^\mu_{k,0,m} - c^\mu_{k,1,m}\big), \\ 4F^{\mu+1}_{l,m} - F^{\mu+1}_{l+1,m} - F^{\mu+1}_{l-1,m} - F^{\mu+1}_{l,m+1} - F^{\mu+1}_{l,m-1} = P^\mu_{l,m}(c) \\ := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(4c^\mu_{k,l,m} - c^\mu_{k,l+1,m} - c^\mu_{k,l-1,m} - c^\mu_{k,l,m+1} - c^\mu_{k,l,m-1}\big), \\ F^{\mu+1}_{M+1,m} - F^{\mu+1}_{M,m} = P^\mu_{M+1,m}(c) := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(c^\mu_{k,M+1,m} - c^\mu_{k,M,m}\big), \\ F^{\mu+1}_{0,M+1} - \frac{1}{2}F^{\mu+1}_{0,M} - \frac{1}{2}F^{\mu+1}_{1,M+1} = P^\mu_{0,M+1}(c) := 0, \\ F^{\mu+1}_{l,M+1} - F^{\mu+1}_{l,M} = P^\mu_{l,M+1}(c) := \sum_{k=1}^{s-1} \Omega_k \big(D_k - D_s\big)\big(c^\mu_{k,l,M+1} - c^\mu_{k,l,M}\big), \\ F^{\mu+1}_{M+1,M+1} - \frac{1}{2}F^{\mu+1}_{M+1,M} - \frac{1}{2}F^{\mu+1}_{M,M+1} = P^\mu_{M+1,M+1}(c) := 0, \\ \frac{1}{4}\Big(F^{\mu+1}_{0,0} + F^{\mu+1}_{0,M+1} + F^{\mu+1}_{M+1,0} + F^{\mu+1}_{M+1,M+1}\Big) \\ + \frac{1}{2}\sum_{k=1}^{M}\Big(F^{\mu+1}_{0,k} + F^{\mu+1}_{M+1,k} + F^{\mu+1}_{k,0} + F^{\mu+1}_{k,M+1}\Big) \\ + \sum_{j=1}^{M}\sum_{k=1}^{M} F^{\mu+1}_{j,k} = P^\mu_{M+2,0}(c) := 0, \end{cases}$$

for $l, m = 1, \ldots, M$, $\mu = 0, \ldots, K-1$. For each μ it is the system of M^2+4M+5 equations with M^2+4M+4 unknowns.

Then we define an *implicit difference scheme* for the concentrations c_i, $i = 1, \ldots, s-1$ as a system of linear algebraic equations of the form

$$
\begin{cases}
c^{\mu+1}_{i,0,0} - \frac{1}{2}c^{\mu+1}_{i,0,1} - \frac{1}{2}c^{\mu+1}_{i,1,0} = Q^{\mu}_{i,0,0} := 0, \\
s^{\mu}_{i,l,0}c^{\mu+1}_{i,l,0} + s^{\mu}_{i,l,1}c^{\mu+1}_{i,l,1} = Q^{\mu}_{i,l,0} := 0, \\
c^{\mu+1}_{i,M+1,0} - \frac{1}{2}c^{\mu+1}_{i,M+1,1} - \frac{1}{2}c^{\mu+1}_{i,M,0} = Q^{\mu}_{M+1,0} := 0, \\
q^{\mu}_{i,0,m}c^{\mu+1}_{i,0,m} + q^{\mu}_{i,1,m}c^{\mu+1}_{i,1,m} = Q^{\mu}_{i,0,m} := 0, \\
v^{\mu}_{i,l,m}c^{\mu+1}_{i,l,m} + r^{\mu}_{i,l+1,m}c^{\mu+1}_{i,l+1,m} + l^{\mu}_{i,l-1,m}c^{\mu+1}_{i,l-1,m} + u^{\mu}_{i,l,m+1}c^{\mu+1}_{i,l,m+1} \\
\quad + d^{\mu}_{i,l,m-1}c^{\mu+1}_{i,l,m-1} = Q^{\mu}_{i,l,m} := e^{\mu}_{i,l,m}c^{\mu}_{i,l,m}, \\
q^{\mu}_{i,M+1,m}c^{\mu+1}_{i,M+1,m} + q^{\mu}_{i,M,m}c^{\mu+1}_{i,M,m} = Q^{\mu}_{i,M+1,m} := 0, \\
c^{\mu+1}_{i,0,M+1} - \frac{1}{2}c^{\mu+1}_{i,0,M} - \frac{1}{2}c^{\mu+1}_{i,1,M+1} = Q^{\mu}_{i,0,M+1} := 0, \\
s^{\mu}_{i,l,M+1}c^{\mu+1}_{i,l,M+1} + s^{\mu}_{i,l,M}c^{\mu+1}_{i,l,M} = Q^{\mu}_{i,l,M+1} := 0, \\
c^{\mu+1}_{i,M+1,M+1} - \frac{1}{2}c^{\mu+1}_{i,M+1,M} - \frac{1}{2}c^{\mu+1}_{i,M,M+1} = Q^{\mu}_{i,M+1,M+1} := 0,
\end{cases}
$$

where

$$
\begin{aligned}
&\kappa = \frac{\tau}{h^2}, \quad v^{\mu}_{i,l,m} = 1 + 4\kappa D_i, \\
&p^{\mu}_{i,l-1,m} = -\kappa D_i - 0.25\kappa\big(F^{\mu+1}_{l+1,m} - F^{\mu+1}_{l-1,m}\big), \\
&r^{\mu}_{i,l+1,m} = -\kappa D_i + 0.25\kappa\big(F^{\mu+1}_{l+1,m} - F^{\mu+1}_{l-1,m}\big), \\
&d^{\mu}_{i,l,m-1} = -\kappa D_i - 0.25\kappa\big(F^{\mu+1}_{l,m+1} - F^{\mu+1}_{l,m-1}\big), \\
&u^{\mu}_{i,l,m+1} = -\kappa D_i + 0.25\kappa\big(F^{\mu+1}_{l,m+1} - F^{\mu+1}_{l,m-1}\big), \\
&e^{\mu}_{i,l,m} = 1 - \kappa\big(F^{\mu+1}_{l+1,m} + F^{\mu+1}_{l-1,m} - 4F^{\mu+1}_{l,m} + F^{\mu+1}_{l,m+1} + F^{\mu+1}_{l,m-1}\big), \\
&q^{\mu}_{i,0,m} = q^{\mu}_{i,M+1,m} = s^{\mu}_{i,l,0} = s^{\mu}_{i,l,M+1} = D_i, \\
&q^{\mu}_{i,1,m} = -D_i + \sum_{k=1}^{s-1} \Omega_k\big(D_k - D_s\big)\Big(c^{\mu}_{k,1,m} - c^{\mu}_{k,0,m}\Big), \\
&q^{\mu}_{i,M,m} = -D_i + \sum_{k=1}^{s-1} \Omega_k\big(D_k - D_s\big)\Big(c^{\mu}_{k,M,m} - c^{\mu}_{k,M+1,m}\Big), \\
&s^{\mu}_{i,l,1} = -D_i + \sum_{k=1}^{s-1} \Omega_k\big(D_k - D_s\big)\Big(c^{\mu}_{k,l,1} - c^{\mu}_{k,l,0}\Big), \\
&s^{\mu}_{i,l,M} = -D_i + \sum_{k=1}^{s-1} \Omega_k\big(D_k - D_s\big)\Big(c^{\mu}_{k,l,M} - c^{\mu}_{k,l,M+1}\Big),
\end{aligned}
$$

$l, m = 1, \ldots, M$, $i = 1, \ldots, s-1$ and $\mu = 0, \ldots, K-1$. For each μ and i it is the system of M^2+4M+4 equations with M^2+4M+4 unknowns.

Remark 6. Similar theorems and remarks to Theorems 1–3 and Remarks 3–5 are true. The proofs are analogous.

4.2 Example and numerical experiments

To illustrate a class of problems which can be treated with our method, we consider an example of a ternary mixture of nickel (Ni), copper (Cu) and iron (Fe) with constants D_i, $i = 1, 2, 3$.

Let the physical data be given:

$$
\begin{aligned}
&s = 3, \quad Ni - Cu - Fe, \quad \Lambda = 0.035, \quad (\Omega_1, \Omega_2, \Omega_3) = (6.5, 7.0, 7.1),\\
&(D_1, D_2, D_3) = (1.58 \cdot 10^{-13}, 5.73 \cdot 10^{-12}, 2.99 \cdot 10^{-11}),\\
&(c_{01}, c_{02}, c_{03}) = (0.03, 0.064857, 0.0908451)\\
&\qquad \text{in} \quad Z_1 = \left\{(x_1, x_2) : \left(x_1 - \Lambda/4\right)^2 + \left(x_1 - \Lambda/4\right)^2 \le \left(\Lambda/\sqrt{5}\right)^2\right\},\\
&(c_{01}, c_{02}, c_{03}) = (0.04, 0.0, 0.0366197)\\
&\qquad \text{in} \quad Z_2 = \left\{(x_1, x_2) : \left(x_1 + \Lambda/4\right)^2 + \left(x_1 + \Lambda/4\right)^2 \le \left(\Lambda/\sqrt{5}\right)^2\right\} \setminus Z_1,\\
&(c_{01}, c_{02}, c_{03}) = (0.01, 0.08285715, 0.0908451)\\
&\qquad \text{in} \quad Z_3 = \left([-\Lambda, \Lambda] \times [-\Lambda, \Lambda]\right) \setminus (Z_1 \cup Z_2).
\end{aligned}
$$

For the times 0, 7 and 28 days we obtain with the finite difference method (FDM) given in Subsection 4.1 the following results (in Figures 3–8 the calculations are made on the mesh with 21×21 space nodal points):

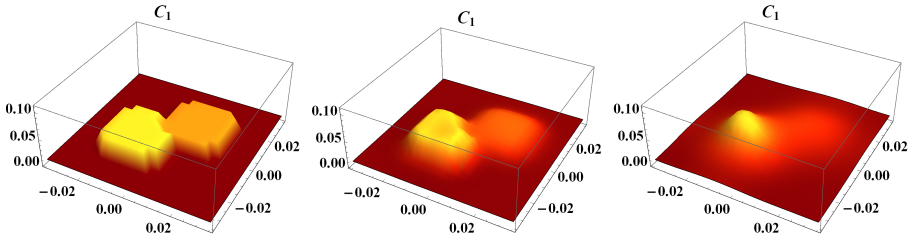

Figure 3. Distributions of Ni concentration c_1 for the times 0, 7 and 28 days respectively.

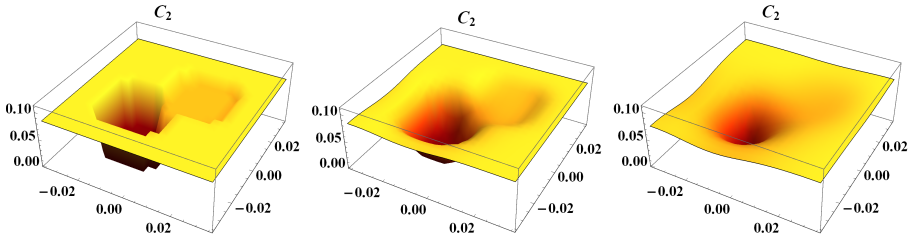

Figure 4. Distributions of Cu concentration c_2 for the times 0, 7 and 28 days respectively.

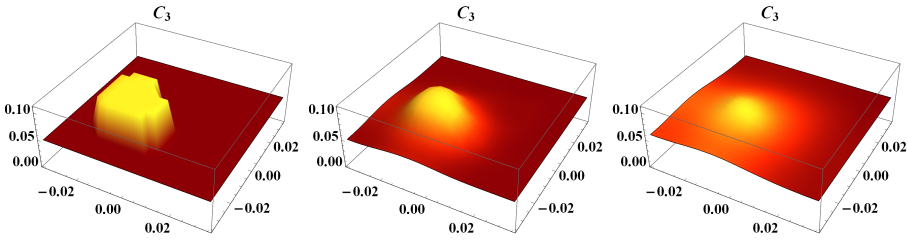

Figure 5. Distributions of Fe concentration c_3 for the times 0, 7 and 28 days respectively.

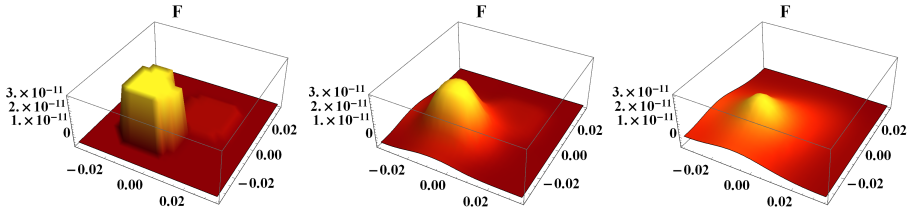

Figure 6. Evolution of the potential F distribution for the times 0, 7 and 28 days respectively.

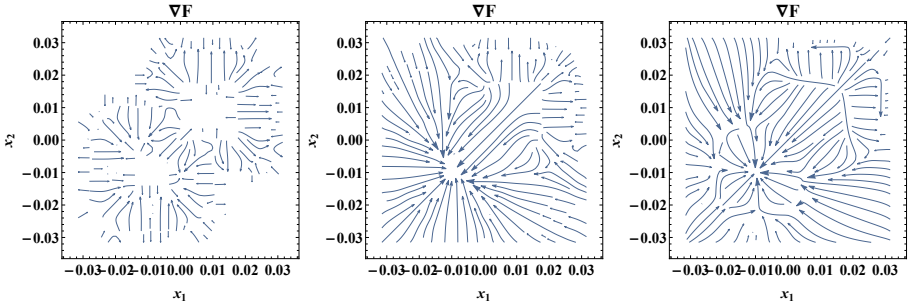

Figure 7. Evolution of the field ∇F for the times 0, 7 and 28 days respectively.

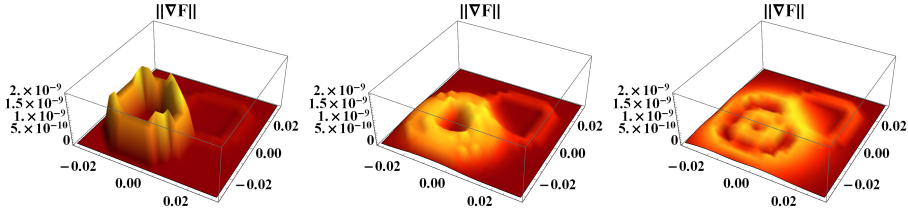

Figure 8. Evolution of the norm $\|\nabla F\|$ for the times 0, 7 and 28 days respectively.

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