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Iterative methods for ternary diffusions

Henryk Leszczyński* and Monika Wrzosek

*Correspondence:
hleszcz@mat.ug.edu.pl
Institute of Mathematics, University of Gdańsk, Wita Stwosza 57, Gdańsk, 80-952, Poland

Abstract

We apply iterative methods to three-component diffusion equations and study their convergence in L^2 and in the Sobolev space $W^{1,\infty}$. The system is parabolic and mass-conservative. Newton's method converges very fast and its iterations do not leave the set of admissible functions.

MSC: 35K51; 35K57; 65M12; 65M80

Keywords: diffusion; iterative method; Newton's method

1 Introduction

Since its discovery and later analysis by Darken [1], the Kirkendall effect [2] has been found in various alloy systems, and studies on lattice defects and diffusion developed significantly. The Danielewski-Holly method [3] extends the Darken standard theory of interdiffusion and describes the process in the bounded mixture showing constant concentration. Under certain regularity assumptions and quantitative condition Danielewski and Holly proved the existence and uniqueness of solution to PDE describing the interdiffusion phenomena. Further developments have been presented in numerous articles; *e.g.* [4, 5].

In the paper we apply Newton's method (see [6–8]) to three-component diffusion equations and study the convergence in L^2 and Sobolev space $W^{1,\infty}$. The system of equations is strongly coupled, however, the maximum principle presented in Section 1 confirms its parabolic type. Parabolicity is additionally confirmed by our convergence result for iterative methods. This falsifies the nonparabolicity hypothesis by Danielewski and Holly [3], where they construct an initial concentration whose L^2 norm increases in time, at least on some interval. The Newton method, known as *quasilinearization method*, is very useful in modern numerical methods for solving PDE's; see [9]. We apply this method to strongly coupled parabolic systems describing diffusing mixtures. This strong parabolicity might have caused weird phenomena, but we have discovered a kind of maximum principle and some conservation laws in this system, hence the iterative methods proposed here behave very well. Our result is very useful in numerical simulations when one wants to construct reliable and fast convergent approximations. Since Newton's method produces linear PDE's satisfying maximum principles and *a priori* estimates of the respective Green functions or Cauchy kernels, one can find errors estimates much better than those obtained from the Newton-Kantorovich theorem, cf. [10, 11].

Consider a mixture composed of three different components. Let $t \geq 0$, $x \in [-L, L]$, $v_i : [0,\infty) \times [-L, L] \to \mathbb{R}$ denote the velocity field of the ith component and $c_i : [0,\infty) \times [-L, L] \to \mathbb{R}$ its molar density or molar concentration. It is a measure of the number of particles contained in any volume, $c_1 + c_2 + c_3 \equiv \text{const}$. The component diffusion flux is a Fickian flow:

$$J_i^d(t,x) := -D_i \operatorname{grad} c_i,$$

where D_i is the intrinsic diffusitivity of the ith component which we assume to satisfy $D_1 > D_2 > D_3 > 0$. Denote $D_i' := D_i - D_3$ for $i = 1, 2$. The overall ith component flux is a sum of diffusion and convection fluxes:

$$J_i := J_i^d + c_i v^D,$$

where v^D stands for a drift velocity. By the mass conservation law:

$$\frac{\partial c_i}{\partial t} = -\operatorname{div} J_i$$

and upon denoting $u = c_1$, $v = c_2$, $w = c_3$ we arrive at the following system of equations:

$$\begin{aligned} u_t &= D_1 u_{xx} - \left(u\left[D_1' u_x + D_2' v_x\right]\right)_x, \\ v_t &= D_2 v_{xx} - \left(v\left[D_1' u_x + D_2' v_x\right]\right)_x, \\ w_t &= D_3 w_{xx} - \left(w\left[D_1' u_x + D_2' v_x\right]\right)_x \end{aligned} \tag{1.1}$$

with the initial condition

$$u(0,x) = u_0(x), \qquad v(0,x) = v_0(x), \qquad w(0,x) = w_0(x) = 1 - u_0(x) - v_0(x) \tag{1.2}$$

for $x \in [-L, L]$ and the Neumann boundary condition

$$\frac{\partial u}{\partial n} = 0, \qquad \frac{\partial v}{\partial n} = 0, \qquad \frac{\partial w}{\partial n} = 0 \quad \text{for } t \geq 0, x \in \{-L, L\}. \tag{1.3}$$

Let $\mathcal{X}$ denote the space consisting of triples of functions (u, v, w) satisfying

$u, v, w \in C^{1,2}$,
u_x, u_{xx}, v_x, v_{xx} are bounded,
$u \geq 0$, $v \geq 0$, $w \geq 0$ for $t \geq 0$, $x \in [-L, L]$,
$u + v + w = 1$ for $t \geq 0$, $x \in [-L, L]$,
u, v, w obey the Neumann boundary condition.

Remark 1.1 If $(u, v, w) \in \mathcal{X}$ then the third equation of (1.1) is not necessary, since $w = 1 - u - v$. However, we keep it for a more convenient analysis of some properties of solutions.

Remark 1.2 We call

$$v^D = D_1' u_x + D_2' v_x = D_1 u_x + D_2 v_x + D_3 w_x$$

the drift velocity; it describes the marker position.

Lemma 1.3 (Mass conservation) *If* $(u,v,w) \in \mathcal{X}$ *satisfy* (1.1), (1.2) *then*

$$\int_{-L}^{L} u\,dx = const., \qquad \int_{-L}^{L} v\,dx = const., \qquad \int_{-L}^{L} w\,dx = const.$$

Proof The relation

$$\frac{d}{dt}\int_{-L}^{L} u\,dx = 0$$

can be shown by means of the Neumann boundary condition. □

Lemma 1.4 (Maximum principle) *Suppose that* $u(0,\cdot), v(0,\cdot), w(0,\cdot) \in C^2$ *and*

$$u(0,x) \ge 0, \qquad v(0,x) \ge 0, \qquad w(0,x) \ge 0, \qquad u(0,x) + v(0,x) + w(0,x) = 1$$

for $x \in [-L,L]$. *If* (u,v,w) *satisfy* (1.1)-(1.3) *then* $(u,v,w) \in \mathcal{X}$.

Proof Let $\tilde{u} = u + \varepsilon e^{\lambda t}$, $\tilde{v} = v + \varepsilon e^{\lambda t}$, $\tilde{w} = w + \varepsilon e^{\lambda t}$ for $\varepsilon > 0$. We have

$$\tilde{u}_t = u_t + \varepsilon\lambda e^{\lambda t}, \qquad \tilde{u}_x = u_x, \qquad \tilde{u}_{xx} = u_{xx},$$
$$\tilde{v}_t = v_t + \varepsilon\lambda e^{\lambda t}, \qquad \tilde{v}_x = v_x, \qquad \tilde{v}_{xx} = v_{xx}.$$

There exists $\lambda \in \mathbb{R}$ (sufficiently large) such that we have strong differential inequalities:

$$\tilde{u}_t > D_1\tilde{u}_{xx} - \tilde{u}\big[D_1'\tilde{u}_{xx} + D_2'\tilde{v}_{xx}\big] - \tilde{u}_x\big[D_1'\tilde{u}_x + D_2'\tilde{v}_x\big],$$
$$\tilde{v}_t > D_2\tilde{v}_{xx} - \tilde{v}\big[D_1'\tilde{u}_{xx} + D_2'\tilde{v}_{xx}\big] - \tilde{v}_x\big[D_1'\tilde{u}_x + D_2'\tilde{v}_x\big],$$
$$\tilde{w}_t > D_3\tilde{w}_{xx} - \tilde{w}\big[D_1'\tilde{u}_{xx} + D_2'\tilde{v}_{xx}\big] - \tilde{w}_x\big[D_1'\tilde{u}_x + D_2'\tilde{v}_x\big].$$

We claim that $\tilde{u} > 0$, $\tilde{v} > 0$, $\tilde{w} > 0$ in the whole domain. Suppose that this is not true and take the smallest $t^* > 0$ such that $\tilde{u}(t^*,x^*) = 0$, or $\tilde{v}(t^*,x^*) = 0$, or $\tilde{w}(t^*,x^*) = 0$ for some $x^* \in [-L,L]$. Without loss of generality we assume $\tilde{u}(t^*,x^*) = 0$. Since $\tilde{u}(t^*,x^*) = \min_{\{t\le t^*, x\in[-L,L]\}} \tilde{u}(t,x)$ we have $\tilde{u}_x(t^*,x^*) = 0$, $\tilde{u}_t(t^*,x^*) \le 0$ and $\tilde{u}_{xx}(t^*,x^*) \ge 0$. Hence

$$\begin{aligned} 0 \ge \tilde{u}_t(t^*,x^*) &> D_1\tilde{u}_{xx}(t^*,x^*) - \tilde{u}(t^*,x^*)\big[D_1'\tilde{u}_{xx}(t^*,x^*) + D_2'\tilde{v}_{xx}(t^*,x^*)\big] \\ &\quad - \tilde{u}_x(t^*,x^*)\big[D_1'\tilde{u}_x(t^*,x^*) + D_2'\tilde{v}_x(t^*,x^*)\big] \ge 0, \end{aligned}$$

which is a contradiction. Thus $\tilde{u} > 0$ for $t \ge 0$, $x \in [-L,L]$. If $\varepsilon \to 0^+$ then $\tilde{u} \to u$. Hence $u > 0$. Similarly, $v(t,x) \ge 0$ and $w(t,x) \ge 0$ for $t \ge 0$, $x \in [-L,L]$. □

2 Uniqueness

Let $\bar{\mathcal{X}}$ be the closure of $\mathcal{X}$ w.r.t. the L^2 norm. The existence and uniqueness of solutions to problem (1.1)-(1.3) in $\mathcal{X}$ w.r.t. the Sobolev norm $W^{1,2}$ is given in [3]. The following proposition concerns the uniqueness of solutions in L^2. Since the set of C^2-functions is dense in L^2, the proof is carried out in $\mathcal{X}$. The uniqueness is obtained for weak solutions.

Proposition 2.1 *Assume that* $(7-4\sqrt{3})D_2 \le D_1 \le (7+4\sqrt{3})D_2$ *and* $(u_0, v_0, w_0) \in \bar{\mathcal{X}}$. *Then a weak solution* $(u, v, w) \in \bar{\mathcal{X}}$ *to problem* (1.1)-(1.3) *is unique in* L^2.

Proof Since every L^2-function can be approximated by a sequence of $\mathcal{X}$-functions, it suffices to show the uniqueness of $\mathcal{X}$-solutions w.r.t. the L^2-norm. Let $(u, v, w) \in \mathcal{X}$ and $(\bar{u}, \bar{v}, \bar{w}) \in \mathcal{X}$ be solutions to (1.1)-(1.3). Denote

$$\Delta u = u - \bar{u}, \qquad \Delta v = v - \bar{v}, \qquad \Delta w = w - \bar{w}$$

and observe that

$$\begin{aligned}
\Delta u_t &= D_1 \Delta u_{xx} - \left(\Delta u\left[D_1' u_x + D_2' v_x\right]\right)_x - \left(\bar{u}\left[D_1' \Delta u_x + D_2' \Delta v_x\right]\right)_x, \\
\Delta v_t &= D_2 \Delta v_{xx} - \left(\Delta v\left[D_1' u_x + D_2' v_x\right]\right)_x - \left(\bar{v}\left[D_1' \Delta u_x + D_2' \Delta v_x\right]\right)_x, \\
\Delta w_t &= D_3 \Delta w_{xx} - \left(\Delta w\left[D_1' u_x + D_2' v_x\right]\right)_x - \left(\bar{w}\left[D_1' \Delta u_x + D_2' \Delta v_x\right]\right)_x.
\end{aligned}$$

We have

$$\begin{aligned}
\int_{-L}^{L} \Delta u \Delta u_t \, dx = D_1 \int_{-L}^{L} \Delta u \Delta u_{xx} \, dx - \int_{-L}^{L} \Delta u \left(\Delta u\left[D_1' u_x + D_2' v_x\right]\right)_x dx \\
- \int_{-L}^{L} \Delta u \left(\bar{u}\left[D_1' \Delta u_x + D_2' \Delta v_x\right]\right)_x dx.
\end{aligned}$$

Using integration by parts we obtain

$$\begin{aligned}
&2D_1 \int_{-L}^{L} \Delta u \Delta u_{xx} \, dx = -2D_1 \int_{-L}^{L} (\Delta u_x)^2 \, dx, \\
&2 \int_{-L}^{L} \Delta u \left(\Delta u\left[D_1' u_x + D_2' v_x\right]\right)_x dx = \int_{-L}^{L} (\Delta u)^2 \left[D_1' u_{xx} + D_2' v_{xx}\right] dx, \\
&2 \int_{-L}^{L} \Delta u \left(\bar{u}\left[D_1' \Delta u_x + D_2' \Delta v_x\right]\right)_x dx = -2 \int_{-L}^{L} \Delta u_x \bar{u}\left[D_1' \Delta u_x + D_2' \Delta v_x\right] dx.
\end{aligned}$$

Hence

$$\begin{aligned}
&\frac{d}{dt} \int_{-L}^{L} \left[(\Delta u)^2 + (\Delta v)^2 + (\Delta w)^2\right] dx \\
&\quad = 2 \int_{-L}^{L} (\Delta u \Delta u_t + \Delta v \Delta v_t + \Delta w \Delta w_t) \, dx \\
&\quad = -2 \int_{-L}^{L} \left(D_1 (\Delta u_x)^2 + D_2 (\Delta v_x)^2 + D_3 (\Delta w_x)^2\right) dx \\
&\qquad - \int_{-L}^{L} \left((\Delta u)^2 + (\Delta v)^2 + (\Delta w)^2\right)\left[D_1' u_{xx} + D_2' v_{xx}\right] dx \\
&\qquad + 2 \int_{-L}^{L} (\Delta u_x \bar{u} + \Delta v_x \bar{v} + \Delta w_x \bar{w})\left[D_1' \Delta u_x + D_2' \Delta v_x\right] dx.
\end{aligned}$$

By the fact that $\Delta w_x = -\Delta u_x - \Delta v_x$ we obtain

$$\begin{aligned}
&2\int_{-L}^{L} (\Delta u \Delta u_t + \Delta v \Delta v_t + \Delta w \Delta w_t)\,dx \\
&\quad = -\int_{-L}^{L} \big((\Delta u)^2 + (\Delta v)^2 + (\Delta w)^2\big)\big[D_1' u_{xx} + D_2' v_{xx}\big]\,dx \\
&\qquad - 2\int_{-L}^{L} \big(D_1 + D_3 - D_1'(\bar u - \bar w)\big)(\Delta u_x)^2\,dx \\
&\qquad - 2\int_{-L}^{L} \big(D_2 + D_3 - D_2'(\bar v - \bar w)\big)(\Delta v_x)^2\,dx \\
&\qquad - 2\int_{-L}^{L} \big(2D_3 - D_1'(\bar v - \bar w) - D_2'(\bar u - \bar w)\big)\Delta u_x \Delta v_x\,dx.
\end{aligned}$$

We examine the nonnegative definiteness of the matrix:

$$A = \begin{bmatrix} D_1 + D_3 - D_1'(\bar u - \bar w) & D_3 - \frac{1}{2}D_1'(\bar v - \bar w) - \frac{1}{2}D_2'(\bar u - \bar w) \\ D_3 - \frac{1}{2}D_1'(\bar v - \bar w) - \frac{1}{2}D_2'(\bar u - \bar w) & D_2 + D_3 - D_2'(\bar v - \bar w) \end{bmatrix}$$

i.e.

$$D_1 + D_3 - D_1'(\bar u - \bar w) \geq 0, \qquad D_2 + D_3 - D_2'(\bar v - \bar w) \geq 0, \quad \text{and} \quad \det(A) \geq 0.$$

The first two inequalities are true due to the relations:

$$-1 \leq \bar u - \bar w \leq 1, \qquad -1 \leq \bar v - \bar w \leq 1, \qquad D_1 > D_2 > D_3 > 0.$$

The condition

$$(7 - 4\sqrt{3})D_2 \leq D_1 \leq (7 + 4\sqrt{3})D_2$$

implies $\det(A) \geq 0$ for all admissible $\bar u$, $\bar w$. □

3 Iterative methods

Recall that

$$\begin{aligned}
&D_1' u_x + D_2' v_x = D_1 u_x + D_2 v_x + D_3 w_x, \\
&D_1' u_{xx} + D_2' v_{xx} = D_1 u_{xx} + D_2 v_{xx} + D_3 w_{xx}.
\end{aligned}$$

Assume that $(u^{(0)}, v^{(0)}, w^{(0)})$ coincides with (u_0, v_0, w_0) at $t = 0$ and formulate an iterative method for (1.1)-(1.3):

$$\begin{aligned}
&u_t^{(k+1)} = D_1 u_{xx}^{(k+1)} - \big(u^{(k)}\big[D_1 u_x^{(k+1)} + D_2 v_x^{(k+1)} + D_3 w_x^{(k+1)}\big]\big)_x, \\
&v_t^{(k+1)} = D_2 v_{xx}^{(k+1)} - \big(v^{(k)}\big[D_1 u_x^{(k+1)} + D_2 v_x^{(k+1)} + D_3 w_x^{(k+1)}\big]\big)_x, \\
&w_t^{(k+1)} = D_3 w_{xx}^{(k+1)} - \big(w^{(k)}\big[D_1 u_x^{(k+1)} + D_2 v_x^{(k+1)} + D_3 w_x^{(k+1)}\big]\big)_x,
\end{aligned} \tag{3.1}$$

with the initial condition

$$u^{(k+1)}(0,x) = u_0(x), \qquad v^{(k+1)}(0,x) = v_0(x), \qquad w^{(k+1)}(0,x) = w_0(x) \tag{3.2}$$

for $x \in [-L, L]$ and the Neumann boundary condition. Moreover, assume that

$$u_0(x) + v_0(x) + w_0(x) = 1 \tag{3.3}$$

for $x \in [-L, L]$. Denote

$$\Delta u^{(k)} = u^{(k+1)} - u^{(k)}, \qquad \Delta v^{(k)} = v^{(k+1)} - v^{(k)}, \qquad \Delta w^{(k)} = w^{(k+1)} - w^{(k)}.$$

Lemma 3.1 *Assume* $u_0, v_0, w_0 \in \mathcal{X}$, $(u^{(0)}, v^{(0)}, w^{(0)}) = (u_0, v_0, w_0)$ *at* $t = 0$ *and* $u^{(0)} + v^{(0)} + w^{(0)} = 1$. *If* $(u^{(k)}, v^{(k)}, w^{(k)})$ *fulfills* (3.1) *with* (3.2), *the Neumann boundary condition and* (3.3), *then* $u^{(k)} + v^{(k)} + w^{(k)} = 1$.

Proof It suffices to show $u^{(k)} + v^{(k)} + w^{(k)} = 1 \Rightarrow u^{(k+1)} + v^{(k+1)} + w^{(k+1)} = 1$. We assume the induction hypothesis $u^{(k)} + v^{(k)} + w^{(k)} = 1$. Thus

$$\begin{aligned}
&u_t^{(k+1)} + v_t^{(k+1)} + w_t^{(k+1)} \\
&\quad = D_1 u_{xx}^{(k+1)} + D_2 v_{xx}^{(k+1)} + D_3 w_{xx}^{(k+1)} \\
&\qquad - \bigl(u_x^{(k)} + v_x^{(k)} + w_x^{(k)}\bigr)\bigl[D_1 u_x^{(k+1)} + D_2 v_x^{(k+1)} + D_3 w_x^{(k+1)}\bigr] \\
&\qquad - \bigl(u^{(k)} + v^{(k)} + w^{(k)}\bigr)\bigl[D_1 u_{xx}^{(k+1)} + D_2 v_{xx}^{(k+1)} + D_3 w_{xx}^{(k+1)}\bigr] \equiv 0.
\end{aligned}$$

Hence the statement is proved. □

The following theorem establishes a convergence of the iterative method (3.1)-(3.2).

Theorem 3.2 *Suppose* $(u_0, v_0, w_0) \in \mathcal{X}$ *and* $(u^{(0)}, v^{(0)}, w^{(0)}) = (u_0, v_0, w_0)$ *at* $t = 0$. *If* $u_x^{(k)}$, $v_x^{(k)}$, $w_x^{(k)}$ *are* C^2 *and*

$$0 \le u^{(k)} \le 1, \qquad 0 \le v^{(k)} \le 1, \qquad 0 \le w^{(k)} \le 1 \quad \textit{for } k = 1, 2, \ldots$$

then the sequence $(u^{(k)}, v^{(k)}, w^{(k)})$ *defined by* (3.1), (3.2) *converges to the solution* (u, v, w) *of* (1.1), (1.2) *in the Sobolev space* $W^{1,\infty}$.

Proof As in the previous section denote the increments $\Delta u^{(k)} = u^{(k+1)} - u^{(k)}$, $\Delta v^{(k)} = v^{(k+1)} - v^{(k)}$, $\Delta w^{(k)} = w^{(k+1)} - w^{(k)}$. From (3.1) we have the following differential equations:

$$\begin{aligned}
\Delta u_t^{(k+1)} &= D_1 \Delta u_{xx}^{(k+1)} - \bigl(u^{(k+1)}\bigl[D_1' \Delta u_x^{(k+1)} + D_2' \Delta v_x^{(k+1)}\bigr]\bigr)_x \\
&\quad - \bigl(\Delta u^{(k)}\bigl[D_1' u_x^{(k+1)} + D_2' v_x^{(k+1)}\bigr]\bigr)_x, \\
\Delta v_t^{(k+1)} &= D_2 \Delta v_{xx}^{(k+1)} - \bigl(v^{(k+1)}\bigl[D_1' \Delta u_x^{(k+1)} + D_2' \Delta v_x^{(k+1)}\bigr]\bigr)_x \\
&\quad - \bigl(\Delta v^{(k)}\bigl[D_1 u_x^{(k+1)} + D_2 v_x^{(k+1)} + D_3 w_x^{(k+1)}\bigr]\bigr)_x.
\end{aligned}$$

Using the Green functions $G^{1,k}$, $G^{2,k}$ corresponding to the differential operators

$$\begin{bmatrix} \frac{\partial}{\partial t} - D_1 \frac{\partial^2}{\partial x^2} + u^{(k+1)} D_1' \frac{\partial^2}{\partial x^2} & D_2' \frac{\partial^2}{\partial x^2} \\ D_1' \frac{\partial^2}{\partial x^2} & \frac{\partial}{\partial t} - D_2 \frac{\partial^2}{\partial x^2} + v^{(k+1)} D_2' \frac{\partial^2}{\partial x^2} \end{bmatrix} \tag{3.4}$$

we have

$$\begin{bmatrix} \Delta u^{(k+1)}(t,x) \\ \Delta v^{(k+1)}(t,x) \end{bmatrix} = \int_0^t \int_{-L}^{L} \begin{bmatrix} G^{1,k}(t,s,x,y) P^{1,k}(s,y) \\ G^{2,k}(t,s,x,y) P^{2,k}(s,y) \end{bmatrix} dy\, ds,$$
$$\begin{bmatrix} \Delta u_x^{(k+1)}(t,x) \\ \Delta v_x^{(k+1)}(t,x) \end{bmatrix} = \int_0^t \int_{-L}^{L} \begin{bmatrix} G_x^{1,k}(t,s,x,y) P^{1,k}(s,y) \\ G_x^{2,k}(t,s,x,y) P^{2,k}(s,y) \end{bmatrix} dy\, ds,$$

where $P^{i,k}(s,y)$ depend on $\Delta u^{(k)}$, $\Delta v^{(k)}$, $\Delta u_x^{(k)}$, $\Delta v_x^{(k)}$, $\Delta u_x^{(k+1)}$, $\Delta v_x^{(k+1)}$ for $i = 1, 2$. The Green functions $G^{i,k}$ depend on $u^{(k)}$, $v^{(k)}$ and have the uniform estimates

$$\int_{-L}^{L} \left| G^{i,k}(t,s,x,y) \right| dy \le C, \qquad \int_{-L}^{L} \left| G_x^{i,k}(t,s,x,y) \right| dy \le \frac{C}{\sqrt{t-s}}, \tag{3.5}$$

with some generic constant C not depending on k. By Lemma 3.1 there exists $M \ge 0$ such that

$$\begin{aligned} &\left\| u_x^{(k+1)}(t,\cdot) \right\|_{L^\infty} \le M, \qquad \left\| v_x^{(k+1)}(t,\cdot) \right\|_{L^\infty} \le M, \\ &\left\| u_{xx}^{(k+1)}(t,\cdot) \right\|_{L^\infty} \le M, \qquad \left\| v_{xx}^{(k+1)}(t,\cdot) \right\|_{L^\infty} \le M. \end{aligned} \tag{3.6}$$

Since

$$\begin{aligned} \left\| P^{1,k}(t,\cdot) \right\|_{L^\infty} \le{}& M\left(D_1' + D_2'\right) \left\| \Delta u^{(k)}(t,\cdot) \right\|_{L^\infty} + M\left(D_1' + D_2'\right) \left\| \Delta u_x^{(k)}(t,\cdot) \right\|_{L^\infty} \\ &+ M D_1' \left\| \Delta u_x^{(k+1)}(t,\cdot) \right\|_{L^\infty} + M D_2' \left\| \Delta v_x^{(k+1)}(t,\cdot) \right\|_{L^\infty} \end{aligned}$$

we get

$$\begin{aligned} \left\| \left(\Delta u^{(k+1)}, \Delta v^{(k+1)}\right)(t,\cdot) \right\|_{W^{1,\infty}} :={}& \left\| \Delta u^{(k+1)}(t,\cdot) \right\|_{W^{1,\infty}} + \left\| \Delta v^{(k+1)}(t,\cdot) \right\|_{W^{1,\infty}} \\ \le{}& \int_0^t \frac{2C_1}{\sqrt{t-s}} \left\| \left(\Delta u^{(k)}, \Delta v^{(k)}\right)(s,\cdot) \right\|_{W^{1,\infty}} ds \\ &+ \int_0^t \frac{2C_1}{\sqrt{t-s}} \left\| \left(\Delta u^{(k+1)}, \Delta v^{(k+1)}\right)(s,\cdot) \right\|_{W^{1,\infty}} ds. \end{aligned}$$

Applying Lemma A.1 we have $\|(\Delta u^{(0)}, \Delta v^{(0)})(t,\cdot)\|_{W^{1,\infty}} \le K_0$ and by induction: $\|(\Delta u^{(k)}, \Delta v^{(k)})(t,\cdot)\|_{W^{1,\infty}} \le K_k t^{\frac{k}{2}}$ for $k = 1, 2, \ldots$. Hence

$$K_{k+1} = K_k \frac{C}{1 - 2CT^{1/2}} \int_0^1 \frac{\theta^k}{\sqrt{1-\theta}}\, d\theta.$$

Notice that

$$\frac{K_{k+1}}{K_k} = \frac{C}{1 - 2CT^{1/2}} \int_0^1 \frac{\theta^k}{\sqrt{1-\theta}}\, d\theta \to 0 \quad \text{as } k \to \infty.$$

By the d'Alembert's ratio test the convergence radius is $+\infty$. □

We give sufficient conditions for the successive approximations to remain in $\mathcal{X}$.

Proposition 3.3 *Assume that* $u_0, v_0 \in C^4$, $0 < \varepsilon_0 \le u_0(x) \le 1 - \varepsilon_0 < 1$, $0 < \varepsilon_0 \le v_0(x) \le 1 - \varepsilon_0 < 1$ *and the sequence* $(u^{(k)}, v^{(k)}, w^{(k)})$ *defined by* (3.1) *with the first element given by*

$$u^{(0)}(t,x) = u_0(x) + tk_u(x) \quad \text{and} \quad v^{(0)}(t,x) = v_0(x) + tk_v(x),$$

where $k_u, k_v \in \mathcal{X}$ *are of the form*

$$\begin{aligned} k_u(x) &= D_1 u_0''(x) - \bigl(u_0(x)\bigl[D_1' u_0'(x) + D_2' v_0'(x)\bigr]\bigr)_x, \\ k_v(x) &= D_2 v_0''(x) - \bigl(v_0(x)\bigl[D_1' u_0'(x) + D_2' v_0'(x)\bigr]\bigr)_x, \end{aligned}$$

converges to the solution (u, v, w) *of* (1.1), (1.2) *in the Sobolev space* $W^{1,\infty}$. *If*

$$\sum_{k=0}^{\infty} K_k t^{k/2} \le \varepsilon_0, \quad \text{where } K_k = K_{k-1} \frac{C}{1 - 2CT^{1/2}} \int_0^1 \frac{\theta^{k-1}}{\sqrt{1-\theta}}\, d\theta,$$

then $0 \le u^{(k)}(t,x) \le 1$ *and* $0 \le v^{(k)}(t,x) \le 1$, $k = 0, 1, \ldots$.

Proof We have

$$u_t^{(0)}(t,x) = k_u(x), \qquad u_x^{(0)}(t,x) = u_0'(x) + tk_u'(x), \qquad u_{xx}^{(0)}(t,x) = u_0''(x) + tk_u''(x).$$

Hence

$$\begin{aligned} k_u(x) &= D_1 u_0''(x) - u_0'(x)\bigl[D_1' u_0'(x) + D_2' v_0'(x)\bigr] - u_0(x)\bigl[D_1' u_0''(x) + D_2' v_0''(x)\bigr] \\ &= D_1\bigl(u_{xx}^{(0)}(t,x) - tk_u''(x)\bigr) \\ &\quad - \bigl(u_x^{(0)}(t,x) - tk_u'(x)\bigr)\bigl[D_1' u_x^{(0)} + D_2' v_x^{(0)} - t\bigl(D_1' k_u'(x) + D_2' k_v'(x)\bigr)\bigr] \\ &\quad - \bigl(u^{(0)}(t,x) - tk_u(x)\bigr)\bigl[D_1' u_{xx}^{(0)} + D_2' v_{xx}^{(0)} - t\bigl(D_1' k_u''(x) + D_2' k_v''(x)\bigr)\bigr]. \end{aligned}$$

Thus we get

$$\begin{aligned} \Delta u_t^{(0)}(t,x) &= u_t^{(1)}(t,x) - u_t^{(0)}(t,x) \\ &= D_1 u_{xx}^{(1)}(t,x) - u_x^{(0)}(t,x)\bigl[D_1' u_x^{(1)}(t,x) + D_2' v_x^{(1)}(t,x)\bigr] \\ &\quad - u^{(0)}(t,x)\bigl[D_1' u_{xx}^{(1)}(t,x) + D_2' v_{xx}^{(1)}(t,x)\bigr] - k_u(x) \\ &= D_1 \Delta u_{xx}^{(0)}(t,x) - \bigl(u^{(0)}(t,x)\bigl[D_1' \Delta u_x^{(0)}(t,x) + D_2' \Delta v_x^{(0)}(t,x)\bigr]\bigr)_x \\ &\quad + tR_1(x) + t^2 R_2(x), \end{aligned}$$

where

$$\begin{aligned} R_1(x) &:= D_1 k_u''(x) - u_x^{(0)}(t,x)\bigl(D_1' k_u'(x) + D_2' k_v'(x)\bigr) - k_u'(x)\bigl[D_1' u_x^{(0)}(t,x) + D_2' v_x^{(0)}(t,x)\bigr] \\ &\quad - u^{(0)}(t,x)\bigl(D_1' k_u''(x) + D_2' k_v''(x)\bigr) - k_u(x)\bigl[D_1' u_{xx}^{(0)}(t,x) + D_2' v_{xx}^{(0)}(t,x)\bigr], \\ R_2(x) &:= k_u'(x)\bigl(D_1' k_u'(x) + D_2' k_v'(x)\bigr) + k_u(x)\bigl(D_1' k_u''(x) + D_2' k_v''(x)\bigr). \end{aligned}$$

For $0 \le t \le T$ we have

$$\|R\|_{L^\infty} = \left\| tR_1 + t^2 R_2 \right\|_{L^\infty} \le T\left(\|R_1\|_{L^\infty} + T\|R_2\|_{L^\infty}\right) =: K_0.$$

Thus

$$\left\| \left(\Delta u^{(0)}, \Delta v^{(0)}\right)(t,\cdot) \right\|_{W^{1,\infty}} \le \int_0^t \frac{C}{\sqrt{t-s}} \left[\left\| \left(\Delta u^{(0)}, \Delta v^{(0)}\right)(s,\cdot)\right\|_{W^{1,\infty}} + K_0 \right] ds.$$

Applying Lemma A.1 we have

$$\left\| \left(\Delta u^{(0)}, \Delta v^{(0)}\right)(t,\cdot) \right\|_{W^{1,\infty}} \le K_1 t^{1/2}$$

and by induction $\|(\Delta u^{(k)}, \Delta v^{(k)})(t,\cdot)\|_{W^{1,\infty}} \le K_{k+1} t^{\frac{k+1}{2}}$ for $k = 1, 2, \ldots$. Hence

$$K_{k+1} = K_k \frac{C}{1 - 2CT^{1/2}} \int_0^1 \frac{\theta^k}{\sqrt{1-\theta}}\, d\theta. \qquad \square$$

Remark 3.4 The functions $k_u, k_v \in \mathcal{X}$ can be slightly perturbed near the lateral boundary in order to fulfill the Neumann boundary condition.

4 Convergence of the Newton method

As in the previous section denote

$$\Delta u^{(k)} = u^{(k+1)} - u^{(k)}, \qquad \Delta v^{(k)} = v^{(k+1)} - v^{(k)}, \qquad \Delta w^{(k)} = w^{(k+1)} - w^{(k)}.$$

We assume that $(u^{(0)}, v^{(0)}, w^{(0)}) = (u_0, v_0, w_0)$ at $t = 0$ and formulate the Newton method for (1.1)-(1.3):

$$\begin{aligned}
u_t^{(k+1)} &= D_1 u_{xx}^{(k+1)} - \left(u^{(k)}\left[D_1' u_x^{(k)} + D_2' v_x^{(k)}\right]\right)_x \\
&\quad - \left(\Delta u^{(k)}\left[D_1' u_x^{(k)} + D_2' v_x^{(k)}\right]\right)_x - \left(u^{(k)}\left[D_1' \Delta u_x^{(k)} + D_2' \Delta v_x^{(k)}\right]\right)_x, \\
v_t^{(k+1)} &= D_2 v_{xx}^{(k+1)} - \left(v^{(k)}\left[D_1' u_x^{(k)} + D_2' v_x^{(k)}\right]\right)_x \\
&\quad - \left(\Delta v^{(k)}\left[D_1' u_x^{(k)} + D_2' v_x^{(k)}\right]\right)_x - \left(v^{(k)}\left[D_1' \Delta u_x^{(k)} + D_2' \Delta v_x^{(k)}\right]\right)_x, \\
w_t^{(k+1)} &= D_3 w_{xx}^{(k+1)} - \left(w^{(k)}\left[D_1' u_x^{(k)} + D_2' v_x^{(k)}\right]\right)_x \\
&\quad - \left(\Delta w^{(k)}\left[D_1' u_x^{(k)} + D_2' v_x^{(k)}\right]\right)_x - \left(w^{(k)}\left[D_1' \Delta u_x^{(k)} + D_2' \Delta v_x^{(k)}\right]\right)_x,
\end{aligned} \tag{4.1}$$

with the initial condition (3.2) and the Neumann boundary condition.

Lemma 4.1 *Assume* $u_0, v_0, w_0 \in \mathcal{X}$, $(u^{(0)}, v^{(0)}, w^{(0)}) = (u_0, v_0, w_0)$ *at* $t = 0$ *and* $u^{(0)} + v^{(0)} + w^{(0)} = 1$. *If* $(u^{(k)}, v^{(k)}, w^{(k)})$ *fulfills* (4.1) *with* (3.2) *and the Neumann boundary condition, then* $u^{(k)} + v^{(k)} + w^{(k)} = 1$.

Proof We show $u^{(k)} + v^{(k)} + w^{(k)} = 1 \Rightarrow u^{(k+1)} + v^{(k+1)} + w^{(k+1)} = 1$. The only solution to the differential equation

$$\begin{aligned} &u_t^{(k+1)} + v_t^{(k+1)} + w_t^{(k+1)} \\ &\quad = -\big(u_x^{(k+1)} + v_x^{(k+1)} + w_x^{(k+1)}\big)\big[D_1 u_x^{(k)} + D_2 v_x^{(k)} + D_3 w_x^{(k)}\big] \\ &\qquad - \big(u^{(k+1)} + v^{(k+1)} + w^{(k+1)} - 1\big)\big[D_1 u_{xx}^{(k)} + D_2 v_{xx}^{(k)} + D_3 w_{xx}^{(k)}\big] \end{aligned}$$

is $u^{(k+1)} + v^{(k+1)} + w^{(k+1)} \equiv 1$. □

The following theorem establishes the convergence of the Newton method.

Theorem 4.2 *Suppose* $(u_0, v_0, w_0) \in \mathcal{X}$ *and* $(u^{(0)}, v^{(0)}, w^{(0)}) = (u_0, v_0, w_0)$ *at* $t = 0$. *If* $u_x^{(k)}$, $v_x^{(k)}$, $w_x^{(k)}$ *are* C^2 *and*

$$0 \le u^{(k)} \le 1, \qquad 0 \le v^{(k)} \le 1, \qquad 0 \le w^{(k)} \le 1 \quad \text{for } k = 1, 2, \dots,$$

then the sequence $(u^{(k)}, v^{(k)}, w^{(k)})$ *defined by* (4.1), (3.2) *converges to the solution* (u, v, w) *of* (1.1)-(1.3) *with respect to the norms in the Sobolev space* $W^{1,\infty}$.

Proof We have the following differential equations:

$$\begin{aligned} \Delta u_t^{(k+1)} &= D_1 \Delta u_{xx}^{(k+1)} - \big(\Delta u^{(k)}\big[D_1' \Delta u_x^{(k)} + D_2' \Delta v_x^{(k)}\big]\big)_x \\ &\quad - \big(\Delta u^{(k+1)}\big[D_1' u_x^{(k+1)} + D_2' v_x^{(k+1)}\big]\big)_x - \big(u^{(k+1)}\big[D_1' \Delta u_x^{(k+1)} + D_2' \Delta v_x^{(k+1)}\big]\big)_x, \\ \Delta v_t^{(k+1)} &= D_2 \Delta v_{xx}^{(k+1)} - \big(\Delta v^{(k)}\big[D_1' \Delta u_x^{(k)} + D_2' \Delta v_x^{(k)}\big]\big)_x \\ &\quad - \big(\Delta v^{(k+1)}\big[D_1' u_x^{(k+1)} + D_2' v_x^{(k+1)}\big]\big)_x - \big(v^{(k+1)}\big[D_1' \Delta u_x^{(k+1)} + D_2' \Delta v_x^{(k+1)}\big]\big)_x, \\ \Delta w_t^{(k+1)} &= D_3 \Delta w_{xx}^{(k+1)} - \big(\Delta w^{(k)}\big[D_1' \Delta u_x^{(k)} + D_2' \Delta v_x^{(k)}\big]\big)_x \\ &\quad - \big(\Delta w^{(k+1)}\big[D_1' u_x^{(k+1)} + D_2' v_x^{(k+1)}\big]\big)_x - \big(w^{(k+1)}\big[D_1' \Delta u_x^{(k+1)} + D_2' \Delta v_x^{(k+1)}\big]\big)_x. \end{aligned}$$

By the Green functions $G^{1,k}$, $G^{2,k}$:

$$\begin{aligned} \Delta u^{(k+1)}(t,x) = {} & \int_0^t \int_{-L}^L G^{1,k}(t,s,x,y)\big(\Delta u^{(k)}(s,y)\big[D_1' \Delta u_y^{(k)}(s,y) + D_2' \Delta v_y^{(k)}(s,y)\big]\big)_y \,dy\,ds \\ & + \int_0^t \int_{-L}^L G^{1,k}(t,s,x,y)\Delta u_y^{(k+1)}(s,y)\big[D_1' u_y^{(k+1)}(s,y) + D_2' v_y^{(k+1)}(s,y)\big]\,dy\,ds \\ & + \int_0^t \int_{-L}^L G^{1,k}(t,s,x,y)\Delta u^{(k+1)}(s,y)\big[D_1' u_{yy}^{(k+1)}(s,y) + D_2' v_{yy}^{(k+1)}(s,y)\big]\,dy\,ds \\ & + \int_0^t \int_{-L}^L G^{1,k}(t,s,x,y)u_y^{(k+1)}(s,y)\big[D_1' \Delta u_y^{(k+1)}(s,y) + D_2' \Delta v_y^{(k+1)}(s,y)\big]\,dy\,ds. \end{aligned}$$

Using the integration by parts we get

$$\begin{aligned} &\int_0^t \int_{-L}^L G^{1,k}(t,s,x,y)\big(\Delta u^{(k)}(s,y)\big[D_1' \Delta u_y^{(k)}(s,y) + D_2' \Delta v_y^{(k)}(s,y)\big]\big)_y \,dy\,ds \\ &\quad = -\int_0^t \int_{-L}^L G_y^{1,k}(t,s,x,y)\Delta u^{(k)}(s,y)\big[D_1' \Delta u_y^{(k)}(s,y) + D_2' \Delta v_y^{(k)}(s,y)\big]\,dy\,ds. \end{aligned}$$

From the following property:

$$\int_{-L}^{L} \left| G_y^{i,k}(t,s,x,y) \right| dy \leq \frac{C}{\sqrt{t-s}},$$

estimates like (3.5), (3.6), and $xy \leq \frac{1}{2}(x^2 + y^2)$ we obtain

$$\left\| \Delta u^{(k+1)}(t,\cdot) \right\|_{L^\infty} \leq \int_0^t \frac{C_2}{2\sqrt{t-s}} Q^{1,k}(s)\, ds,$$

where

$$\begin{aligned} Q^{1,k}(s) = {} & \left\| \Delta u^{(k)}(s,\cdot) \right\|_{L^\infty}^2 + \left\| \Delta u_y^{(k)}(s,\cdot) \right\|_{L^\infty}^2 + \left\| \Delta v_y^{(k)}(s,\cdot) \right\|_{L^\infty}^2 + \left\| \Delta u_y^{(k+1)}(s,\cdot) \right\|_{L^\infty} \\ & + \left\| \Delta u^{(k+1)}(s,\cdot) \right\|_{L^\infty} ds + \left\| \Delta u_y^{(k+1)}(s,\cdot) \right\|_{L^\infty} + \left\| \Delta v_y^{(k+1)}(s,\cdot) \right\|_{L^\infty}. \end{aligned}$$

Similarly

$$\left\| \Delta v^{(k+1)}(t,\cdot) \right\|_{L^\infty} \leq \int_0^t \frac{C_2}{2\sqrt{t-s}} Q^{2,k}(s)\, ds,$$

where

$$\begin{aligned} Q^{2,k}(s) = {} & \left\| \Delta v^{(k)}(s,\cdot) \right\|_{L^\infty}^2 + \left\| \Delta u_y^{(k)}(s,\cdot) \right\|_{L^\infty}^2 + \left\| \Delta v_y^{(k)}(s,\cdot) \right\|_{L^\infty}^2 + \left\| \Delta v_y^{(k+1)}(s,\cdot) \right\|_{L^\infty} \\ & + \left\| \Delta v^{(k+1)}(s,\cdot) \right\|_{L^\infty} + \left\| \Delta u_y^{(k+1)}(s,\cdot) \right\|_{L^\infty} + \left\| \Delta v_y^{(k+1)}(s,\cdot) \right\|_{L^\infty}. \end{aligned}$$

We have

$$\begin{aligned} & \Delta u_x^{(k+1)}(t,x) \\ & \quad = \int_0^t \int_{-L}^{L} G_x^{1,k}(t,s,x,y) \left(\Delta u^{(k)}(s,y) \left[D_1' \Delta u_y^{(k)}(s,y) + D_2' \Delta v_y^{(k)}(s,y) \right] \right)_y dy\, ds \\ & \quad\quad + \int_0^t \int_{-L}^{L} G_x^{1,k}(t,s,x,y) \Delta u_y^{(k+1)}(s,y) \left[D_1' u_y^{(k+1)}(s,y) + D_2' v_y^{(k+1)}(s,y) \right] dy\, ds \\ & \quad\quad + \int_0^t \int_{-L}^{L} G_x^{1,k}(t,s,x,y) \Delta u^{(k+1)}(s,y) \left[D_1' u_{yy}^{(k+1)}(s,y) + D_2' v_{yy}^{(k+1)}(s,y) \right] dy\, ds \\ & \quad\quad + \int_0^t \int_{-L}^{L} G_x^{1,k}(t,s,x,y) u_y^{(k+1)}(s,y) \left[D_1' \Delta u_y^{(k+1)}(s,y) + D_2' \Delta v_y^{(k+1)}(s,y) \right] dy\, ds. \end{aligned}$$

By integration by parts:

$$\begin{aligned} & \int_0^t \int_{-L}^{L} G_x^{1,k}(t,s,x,y) \left(\Delta u^{(k)}(s,y) \left[D_1' \Delta u_y^{(k)}(s,y) + D_2' \Delta v_y^{(k)}(s,y) \right] \right)_y dy\, ds \\ & \quad = - \int_0^t \int_{-L}^{L} G_{xy}^{1,k}(t,s,x,y) \Delta u^{(k)}(s,y) \left[D_1' \Delta u_y^{(k)}(s,y) + D_2' \Delta v_y^{(k)}(s,y) \right] dy\, ds. \end{aligned}$$

Since $\Delta u^{(k)}(s,y)$, $\Delta u_y^{(k)}(s,y)$, $\Delta v_y^{(k)}(s,y)$ satisfy the Lipschitz condition, we have the estimates (see [12])

$$\begin{aligned}&\int_{-L}^{L}\left|G_{xy}^{i,k}(t,s,x,y)\Delta u^{(k)}(s,y)\Delta u_y^{(k)}(s,y)\right|dy\\&\quad\le\int_0^t\frac{C_3}{(t-s)^{3/4}}\left\|\Delta u^{(k)}(s,\cdot)\right\|_{L^\infty}\left\|\Delta u_y^{(k)}(s,\cdot)\right\|_{L^\infty}ds\end{aligned}$$

and

$$\begin{aligned}&\int_{-L}^{L}\left|G_{xy}^{i,k}(t,s,x,y)\Delta u^{(k)}(s,y)\Delta v_y^{(k)}(s,y)\right|dy\\&\quad\le\int_0^t\frac{C_3}{(t-s)^{3/4}}\left\|\Delta u^{(k)}(s,\cdot)\right\|_{L^\infty}\left\|\Delta v_y^{(k)}(s,\cdot)\right\|_{L^\infty}ds.\end{aligned}\tag{4.2}$$

Hence

$$\begin{aligned}&\left\|\Delta u_x^{(k+1)}(t,\cdot)\right\|_{L^\infty}\\&\quad\le\int_0^t\frac{C_4}{(t-s)^{3/4}}\left(\left\|\Delta u^{(k)}(s,\cdot)\right\|_{L^\infty}^2+\left\|\Delta u_y^{(k)}(s,\cdot)\right\|_{L^\infty}^2+\left\|\Delta v_y^{(k)}(s,\cdot)\right\|_{L^\infty}^2\right)ds\\&\qquad+\int_0^t\frac{C_5}{\sqrt{t-s}}\left(\left\|\Delta u_y^{(k+1)}(s,\cdot)\right\|_{L^\infty}+\left\|\Delta u^{(k+1)}(s,\cdot)\right\|_{L^\infty}+\left\|\Delta u_y^{(k+1)}(s,\cdot)\right\|_{L^\infty}\right.\\&\qquad\left.+\left\|\Delta v_y^{(k+1)}(s,\cdot)\right\|_{L^\infty}\right)ds.\end{aligned}$$

Similarly

$$\begin{aligned}&\left\|\Delta v_x^{(k+1)}(t,\cdot)\right\|_{L^\infty}\\&\quad\le\int_0^t\frac{C_4}{(t-s)^{3/4}}\left(\left\|\Delta v^{(k)}(s,\cdot)\right\|_{L^\infty}^2+\left\|\Delta u_y^{(k)}(s,\cdot)\right\|_{L^\infty}^2+\left\|\Delta v_y^{(k)}(s,\cdot)\right\|_{L^\infty}^2\right)ds\\&\qquad+\int_0^t\frac{C_5}{\sqrt{t-s}}\left(\left\|\Delta v_y^{(k+1)}(s,\cdot)\right\|_{L^\infty}+\left\|\Delta v^{(k+1)}(s,\cdot)\right\|_{L^\infty}+\left\|\Delta u_y^{(k+1)}(s,\cdot)\right\|_{L^\infty}\right.\\&\qquad\left.+\left\|\Delta v_y^{(k+1)}(s,\cdot)\right\|_{L^\infty}\right)ds.\end{aligned}$$

We have

$$\begin{aligned}\left\|\left(\Delta u^{(k+1)},\Delta v^{(k+1)}\right)(t,\cdot)\right\|_{W^{1,\infty}}\le{}&\int_0^t\frac{C_4}{(t-s)^{3/4}}\left\|\left(\Delta u^{(k)},\Delta v^{(k)}\right)(s,\cdot)\right\|_{W^{1,\infty}}^2ds\\&+\int_0^t\frac{C_5}{\sqrt{t-s}}\left\|\left(\Delta u^{(k+1)},\Delta v^{(k+1)}\right)(s,\cdot)\right\|_{W^{1,\infty}}ds.\end{aligned}$$

We apply Lemma A.1:

$$K_{k+1}t^{r_{k+1}}\left(1-2C_5T^{1/2}\right)\ge C_4K_kt^{2r_{k+1}+3/4}\int_0^1\frac{\theta^{2r_k}}{(1-\theta)^{3/4}}\,d\theta,$$

where

$$r_k=\frac{3}{4}\left(2^k-1\right)\approx 2^k\quad\text{and}\quad K_k\approx A^{2^k}.$$

□

We give sufficient conditions for the successive approximations to remain in $\mathcal{X}$.

Proposition 4.3 *Assume that* $u_0, v_0 \in C^4$, $0 < \varepsilon_0 \le u_0(x) \le 1 - \varepsilon_0 < 1$, $0 < \varepsilon_0 \le v_0(x) \le 1 - \varepsilon_0 < 1$ *and the sequence* $(u^{(k)}, v^{(k)}, w^{(k)})$ *defined by* (4.1) *with the first element given by*

$$u^{(0)}(t,x) = u_0(x) + tk_u(x) \quad \text{and} \quad v^{(0)}(t,x) = v_0(x) + tk_v(x),$$

where $k_u, k_v \in \mathcal{X}$ *are of the form*

$$k_u(x) = D_1 u_0''(x) - \big(u_0(x)\big[D_1' u_0'(x) + D_2' v_0'(x)\big]\big)_x,$$
$$k_v(x) = D_2 v_0''(x) - \big(v_0(x)\big[D_1' u_0'(x) + D_2' v_0'(x)\big]\big)_x,$$

converges to the solution (u, v, w) *of* (1.1), (1.2) *in the Sobolev space* $W^{1,\infty}$. *If*

$$\sum_{k=0}^{\infty} \tilde{K}_k t^{\frac{3k}{4}} \le \varepsilon_0, \quad \tilde{K}_k := \tilde{K}_{k-1} \frac{\tilde{C}}{1 - 2CT^{1/2}} \int_0^1 \frac{\theta^{k-1}}{(1-\theta)^{3/4}}\, d\theta,$$

then $0 \le u^{(k)}(t,x) \le 1$ *and* $0 \le v^{(k)}(t,x) \le 1$, $k = 0, 1, \ldots$.

Proof We have

$$\begin{aligned}
\Delta u_t^{(0)}(t,x) &= u_t^{(1)}(t,x) - u_t^{(0)}(t,x) \\
&= D_1 u_{xx}^{(1)} - \big(u^{(0)}\big[D_1' u_x^{(0)} + D_2' v_x^{(0)}\big]\big)_x \\
&\quad - \big(\Delta u^{(0)}\big[D_1' u_x^{(0)} + D_2' v_x^{(0)}\big]\big)_x - \big(u^{(0)}\big[D_1' \Delta u_x^{(0)} + D_2' \Delta v_x^{(0)}\big]\big)_x - k_u(x) \\
&= D_1 \Delta u_{xx}^{(0)} - \big(\Delta u^{(0)}\big[D_1' u_x^{(0)} + D_2' v_x^{(0)}\big]\big)_x - \big(u^{(0)}\big[D_1' \Delta u_x^{(0)} + D_2' \Delta v_x^{(0)}\big]\big)_x \\
&\quad + tR_1(x) + t^2 R_2(x),
\end{aligned}$$

where $R_1(x)$ and $R_2(x)$ are of the same form as in the proof of Proposition 3.3. Since

$$\big\|tR_1 + t^2 R_2\big\|_{L^\infty} \le T\big(\|R_1\|_{L^\infty} + T\|R_2\|_{L^\infty}\big) =: \tilde{K}_0$$

we have

$$\begin{aligned}
&\big\|\big(\Delta u^{(0)}, \Delta v^{(0)}\big)(t,\cdot)\big\|_{W^{1,\infty}} \\
&\quad \le \int_0^t \frac{C}{\sqrt{t-s}} \big\|\big(\Delta u^{(0)}, \Delta v^{(0)}\big)(s,\cdot)\big\|_{W^{1,\infty}}\, ds + \int_0^t \frac{\tilde{C}}{(t-s)^{3/4}} \tilde{K}_0\, ds.
\end{aligned}$$

Applying Lemma A.1 we get

$$\big\|\big(\Delta u^{(0)}, \Delta v^{(0)}\big)(t,\cdot)\big\|_{W^{1,\infty}} \le \tilde{K}_1 t^{3/4}$$

and by induction $\|(\Delta u^{(k)}, \Delta v^{(k)})(t,\cdot)\|_{W^{1,\infty}} \le \tilde{K}_{k+1} t^{\frac{3(k+1)}{4}}$ for $k = 1, 2, \ldots$. Hence

$$\tilde{K}_{k+1} := \tilde{K}_k \frac{\tilde{C}}{1 - 2CT^{1/2}} \int_0^1 \frac{\theta^k}{(1-\theta)^{3/4}}\, d\theta.$$

□

5 Conclusions

Assume that $(u^{(0)}, v^{(0)}, w^{(0)})$ coincides with (u_0, v_0, w_0) at $t = 0$ and consider the following iterative scheme for (1.1)-(1.3):

$$u_t^{(k+1)} = D_1 u_{xx}^{(k+1)} - \big(u^{(k+1)}\big[D_1 u_x^{(k)} + D_2 v_x^{(k)} + D_3 w_x^{(k)}\big]\big)_x,$$
$$v_t^{(k+1)} = D_2 v_{xx}^{(k+1)} - \big(v^{(k+1)}\big[D_1 u_x^{(k)} + D_2 v_x^{(k)} + D_3 w_x^{(k)}\big]\big)_x,$$
$$w_t^{(k+1)} = D_3 w_{xx}^{(k+1)} - \big(w^{(k+1)}\big[D_1 u_x^{(k)} + D_2 v_x^{(k)} + D_3 w_x^{(k)}\big]\big)_x$$

with the initial condition

$$u^{(k+1)}(0,x) = u_0(x), \qquad v^{(k+1)}(0,x) = v_0(x), \qquad w^{(k+1)}(0,x) = w_0(x)$$

for $x \in [-L, L]$ and the Neumann boundary condition. Denote

$$\Delta u^{(k)} = u^{(k+1)} - u^{(k)}, \qquad \Delta v^{(k)} = v^{(k+1)} - v^{(k)}, \qquad \Delta w^{(k)} = w^{(k+1)} - w^{(k)}.$$

Convergence problems occur in L^2 and the Sobolev norm $W^{1,\infty}$. Our attempt to obtain the following relation for the increments $\Delta u^{(k)}$, $\Delta v^{(k)}$, $\Delta w^{(k)}$:

$$\frac{d}{dt} A_{k+1}(t) \le C\big[A_{k+1}(t) + A_k(t)\big], \qquad A_k(t) = \int_{-L}^{L} \big[\big(\Delta u^{(k)}\big)^2 + \big(\Delta v^{(k)}\big)^2 + \big(\Delta w^{(k)}\big)^2\big]\,dx$$

was unsuccessful as it is difficult to estimate the following component:

$$\int_{-L}^{L} \Delta u^{(k+1)} \big(u^{(k+1)}\big[D_1 \Delta u_x^{(k)} + D_2 \Delta v_x^{(k)} + D_3 \Delta w_x^{(k)}\big]\big)_x \,dx.$$

This example of iterations shows that strongly coupled systems cause serious problems with their approximation. We think that the ternary system and suitable approximations to it will be somehow expressed in an abstract way, based on a Conti-Opial type theorem, like in [13].

In order to illustrate fast convergence of Newton's iterations we provide numerical examples with $D_1 = 1$, $D_2 = 0.5$, $D_3 = 0.2$, and u_0, v_0 being sample piecewise polynomial functions taking values in $[0.2, 0.8]$. We check the differences $u^{k+1} - u^k$ and $v^{k+1} - v^k$ for $k = 0, 1, 2, 3, 4$. Our computer programs are performed by implicit finite difference methods with steps $h_0 = h_1 = 0.01$; see Table 1 (direct iterations), Table 2 (Newton's iterations).

Appendix

Lemma A.1 *Assume that*

$$z(t) \le \int_0^t \frac{C}{\sqrt{t-s}} z(s)\,ds + \int_0^t \frac{\tilde{C}}{(t-s)^\alpha} p(s)\,ds \quad \textit{and} \quad p(s) \le K s^m.$$

Then $z(t) \le \tilde{K} t^{m+\alpha}$ *for* $t \in [0, T]$, *where* $\frac{1}{2} \le \alpha < 1$ *and* $1 - 2CT^{1/2} > 0$.

Table 1 Maximal differences between successive approximations $u^{(k)}$ by direct iterations (3.1) with $D_1 = 1$, $D_2 = 0.5$, $D_3 = 0.2$, $h = 0.01$, $h_0 = 0.01$

t	$\lvert u^{(1)} - u^{(0)}\rvert$	$\lvert u^{(2)} - u^{(1)}\rvert$	$\lvert u^{(3)} - u^{(2)}\rvert$	$\lvert u^{(4)} - u^{(3)}\rvert$	$\lvert u^{(5)} - u^{(4)}\rvert$
0.00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
0.05	1.023328e–01	3.742852e–03	1.383520e–04	7.409068e–06	3.256123e–07
0.10	1.476173e–01	6.990620e–03	2.908263e–04	1.835346e–05	1.004908e–06
0.15	1.783626e–01	9.324930e–03	4.031573e–04	2.746097e–05	1.675459e–06
0.20	2.028066e–01	1.096861e–02	4.788241e–04	3.397007e–05	2.215127e–06
0.25	2.239067e–01	1.206830e–02	5.253484e–04	3.806322e–05	2.601687e–06
0.30	2.425240e–01	1.273201e–02	5.499511e–04	4.011546e–05	2.844953e–06
0.35	2.593736e–01	1.304597e–02	5.585483e–04	4.051817e–05	2.967818e–06
0.40	2.745434e–01	1.307759e–02	5.556250e–04	3.970391e–05	2.985870e–06

Table 2 Maximal differences between successive approximations $u^{(k)}$ by Newton's method (4.1) with $D_1 = 1$, $D_2 = 0.5$, $D_3 = 0.2$, $h = 0.01$, $h_0 = 0.01$

t	$\lvert u^{(1)} - u^{(0)}\rvert$	$\lvert u^{(2)} - u^{(1)}\rvert$	$\lvert u^{(3)} - u^{(2)}\rvert$	$\lvert u^{(4)} - u^{(3)}\rvert$	$\lvert u^{(5)} - u^{(4)}\rvert$
0.00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00
0.05	9.970638e–02	1.703717e–03	6.949251e–07	1.628697e–13	8.038015e–14
0.10	1.430019e–01	3.927916e–03	4.076982e–06	4.423240e–12	5.245804e–14
0.15	1.723550e–01	5.877059e–03	9.749392e–06	2.192441e–11	3.896883e–14
0.20	1.956575e–01	7.536084e–03	1.659814e–05	1.148864e–10	3.987088e–14
0.25	2.155355e–01	8.989691e–03	2.404146e–05	4.279036e–10	3.957945e–14
0.30	2.332049e–01	1.029947e–02	3.161596e–05	1.167791e–09	3.042011e–14
0.35	2.489078e–01	1.153614e–02	4.250313e–05	2.625514e–09	1.676437e–14
0.40	2.631780e–01	1.269348e–02	5.972126e–05	5.163286e–09	2.378098e–13

Proof We have

$$
\begin{aligned}
z(t) &\le \int_0^t \frac{C}{\sqrt{t-s}} z(s)\,ds + \int_0^t \frac{\tilde{C}}{(t-s)^\alpha} K s^m\,ds \\
&\le \int_0^t \frac{C}{\sqrt{t-s}} \tilde{K} t^{m+\alpha}\,ds + \int_0^t \frac{\tilde{C}}{(t-s)^\alpha} K s^m\,ds
\end{aligned}
$$

for $0 \le t \le T$ and $\frac{1}{2} \le \alpha < 1$. We claim that

$$
\begin{aligned}
&2\tilde{K} C t^{m+\alpha} T^{1/2} + \tilde{C} K t^{m+\alpha} \int_0^1 \frac{\theta^m}{(1-\theta)^\alpha}\,d\theta \le \tilde{K} t^{m+\alpha}, \\
&\tilde{K} t^{m+\alpha} \bigl(1 - 2CT^{1/2}\bigr) \ge \tilde{C} K t^{m+\alpha} \int_0^1 \frac{\theta^m}{(1-\theta)^\alpha}\,d\theta.
\end{aligned}
$$

It suffices to take

$$
\tilde{K} := K \frac{\tilde{C}}{1 - 2CT^{1/2}} \int_0^1 \frac{\theta^m}{(1-\theta)^\alpha}\,d\theta. \tag{A.1}
$$

□

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
All authors contributed equally to the writing of this paper. All authors read and approved the final manuscript.

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