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Numerical Approximation of a Reaction-Diffusion System with Fast Reversible Reaction*****

Robert EYMARD* Danielle HILHORST**
Hideki MURAKAWA*** Michal OLECH****

(*Dedicated to Professor Roger Temam on the Occasion of his* 70*th Birthday*)

Abstract The authors consider the finite volume approximation of a reaction-diffusion system with fast reversible reaction. It is deduced from a priori estimates that the approximate solution converges to the weak solution of the reaction-diffusion problem and satisfies estimates which do not depend on the kinetic rate. It follows that the solution converges to the solution of a nonlinear diffusion problem, as the size of the volume elements and the time steps converge to zero while the kinetic rate tends to infinity.

Keywords Instantaneous reaction limit, Mass-action kinetics, Finite volume methods, Convergence of approximate solutions, Discrete a priori estimates, Kolmogorov's theorem

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1 Introduction

In this paper, we consider chemical systems with fast reactions where mean reaction times vary from approximately 10^{-14} second to 1 minute. In particular, reactions that involve bond making or breaking are not likely to occur in less than 10^{-13} second. Moreover, chemical systems almost always involve some elementary reaction steps that are reversible and fast.

The study of reactions with rates that are outside of the time frame of ordinary laboratory operations requires specialized instrumentation, techniques and ways of proceeding (see for example [5, Chapter 11]). The aim of this paper is to provide an efficient, quick and cheap way for the numerical investigation of such reactions.

In this article, we consider a reversible chemical reaction between mobile species $\mathcal{A}$ and $\mathcal{B}$, that takes place inside a bounded region $\Omega \subset \mathbb{R}^d$ where $d = 1, 2$ or 3. If the region is isolated

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*Université Paris-Est, 77454 Marne-la-Vallée Cedex 2, France. E-mail: Robert.Eymard@univ-mlv.fr
**Laboratoire de Mathématiques, CNRS and Université de Paris-Sud 11, 91405 Orsay Cédex, France. E-mail: Danielle.Hilhorst@math.u-psud.fr
***Graduate School of Science and Engineering for Research, University of Toyama, 3190 Gofuku, Toyama 930-8555, Japan. E-mail: murakawa@sci.u-toyama.ac.jp
****Instytut Matematyczny Uniwersytetu Wroclawskiego, pl. Grunwaldzki 2/4, 50-384 Wroclaw, Polska; Laboratoire de Mathématiques, CNRS Université de Paris-Sud, 91405 Orsay Cédex, France. E-mail: olech@math.uni.wroc.pl
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and diffusion is modelled by Fick's law, this leads to the reaction-diffusion system of partial differential equations

$$\begin{aligned} u_t &= a\Delta u - \alpha k(r_A(u) - r_B(v)), \quad \text{in } \Omega \times (0,T), \\ v_t &= b\Delta v + \beta k(r_A(u) - r_B(v)), \quad \text{in } \Omega \times (0,T), \end{aligned} \tag{1.1}$$

where $T > 0$ and Ω is a bounded set of $\mathbb{R}^d$. An example of explicit expressions and values for α, β, k, r_A, r_B, a, b is given in Section 6. We supplement the system (1.1) by the homogeneous Neumann boundary conditions

$$\nabla u \cdot \boldsymbol{n} = \nabla v \cdot \boldsymbol{n} = 0, \quad \text{on } \partial\Omega \times (0,T), \tag{1.2}$$

and the initial conditions

$$u(x,0) = u_0(x), \quad v(x,0) = v_0(x), \quad \text{in } \Omega. \tag{1.3}$$

In the sequel, system (1.1) together with the boundary conditions (1.2) and the initial conditions (1.3) is called Problem $\mathcal{P}^k$.

For a reversible reaction $m\mathcal{A} \rightleftharpoons n\mathcal{B}$ one has $\alpha = m,\ \beta = n$ and the rate functions are of the form $r_A(u) = u^m$ and $r_B(v) = v^n$. Further discussion about this motivation and some concrete examples can be found in [5, 9].

In practice, especially for ionic or radical reactions, changes due to reaction are often very fast compared to diffusive effects. This corresponds to a large rate constant k. Bothe and Hilhorst [1] studied the limit to an instantaneous reaction. They exploited a natural Lyapunov functional and use compactness arguments to prove that

$$u^k \to u \quad \text{and} \quad v^k \to v, \quad \text{in } L^2(\Omega \times (0,T))$$

as k tends to infinity, where (u^k, v^k) is the solution of Problem $\mathcal{P}^k$ and the limit (u,v) is determined by

$$r_A(u) = r_B(v) \quad \text{and} \quad \frac{u}{\alpha} + \frac{v}{\beta} = w, \tag{1.4}$$

where w is the unique weak solution of the nonlinear diffusion problem

$$\begin{aligned} & w_t = \Delta\phi(w), \quad \text{in } \Omega \times (0,T), \\ & \frac{\partial \phi(w)}{\partial \boldsymbol{n}} = 0, \quad \text{on } \partial\Omega \times (0,T), \\ & w(x,0) = w_0(x) := \frac{1}{\alpha} u_0(x) + \frac{1}{\beta} v_0(x), \quad \text{in } \Omega. \end{aligned} \tag{1.5}$$

Here,

$$\phi := \Big(\frac{a}{\alpha}\text{id} + \frac{b}{\beta}\eta\Big) \circ \Big(\frac{1}{\alpha}\text{id} + \frac{1}{\beta}\eta\Big)^{-1}, \quad \eta := r_B^{-1} \circ r_A.$$

The identities in (1.4) can be explained as follows: the first one states that the system is in chemical equilibrium, while the second one defines w as the quantity that is conserved under the chemical reaction. Given a function w, the system (1.4) can be uniquely solved for (u,v) if $r_A,\ r_B$ are strictly increasing with for instance $r_A(\mathbb{R}^+) \subset r_B(\mathbb{R}^+)$ so that $\eta = r_B^{-1} \circ r_A$

is well-defined and strictly increasing. Under these assumptions u is the unique solution of $\frac{1}{\alpha}u + \frac{1}{\beta}\eta(u) = w$, which gives the explicit representation of u and v

$$u = f(w) \quad \text{and} \quad v = g(w). \tag{1.6}$$

Here, $f := \left(\frac{1}{\alpha}\mathrm{id} + \frac{1}{\beta}\eta\right)^{-1}$ and $g := \eta \circ f$.

We assume the following hypotheses, which we denote by $\mathcal{H}$:

(1) *Let* Ω *be an open, connected and bounded subset of* $\mathbb{R}^d$*, where* $d = 1, 2$ *or* 3*, with a smooth boundary* $\partial\Omega$*,*

(2) $u_0,\ v_0 \in L^\infty(\Omega)$ *and there exist constants* $U,\ V > 0$ *such that* $0 \leqslant u_0(x) \leqslant U$ *and* $0 \leqslant v_0(x) \leqslant V$ *for all* $x \in \Omega$*,*

(3) α*,* β*,* a*,* b *and* k *are strictly positive real values,*

(4) *Let* $r_A,\ r_B : \mathbb{R} \to \mathbb{R}$ *be strictly increasing and locally Lipschitz functions, such that* $r_A(0) = r_B(0) = 0$*, and assume furthermore that* $r_A(\mathbb{R}^+) \subset r_B(\mathbb{R}^+)$*.*

It follows as in [1, Section 2] that Problem $\mathcal{P}^k$ has a unique classical solution (u^k, v^k) on every finite time interval $[0, T]$, for all nonnegative bounded initial data. By classical solution, we mean a function pair $(u^k,\ v^k)$ such that $u^k,\ v^k \in C^{2,1}(\Omega \times (0,T]) \cap C^{1,0}(\overline{\Omega} \times (0,T])$ with $u^k, v^k \in C([0,T];\ L^2(\Omega))$ (see also [11]).

Next we present a notion of a weak solution of Problem $\mathcal{P}^k$, which will be used in the Sections 4 and 5.

Definition 1.1 *We say that* (u^k, v^k) *is a weak solution to Problem* $\mathcal{P}^k$ *if and only if*
(1) $u^k, v^k \in L^2(0,T;H^1(\Omega))$;
(2) *Let* Ψ *be the set of test functions, defined as*

$$\Psi = \{\psi \in C^{2,1}(\overline{\Omega} \times [0,T]) : \nabla\psi \cdot \boldsymbol{n} = 0 \text{ on } \partial\Omega \times [0,T] \text{ and } \psi(T) = 0\}.$$

For a.e. $t \in (0,T)$ *and all* $\psi \in \Psi$*,*

$$\begin{aligned}
&\int_\Omega u_0(x)\psi(x,0)\mathrm{d}x + \int_\Omega u^k(x,t)\psi_t(x,t)\mathrm{d}x + a\int_\Omega u^k(x,t)\Delta\psi(x,t)\mathrm{d}x \\
&- \alpha k\int_\Omega \psi(x,t)(r_A(u^k(x,t)) - r_B(v^k(x,t)))\mathrm{d}x = 0, && (1.7)\\
&\int_\Omega v_0(x)\psi(x,0)\mathrm{d}x + \int_\Omega v^k(x,t)\psi_t(x,t)\mathrm{d}x + b\int_\Omega v^k(x,t)\Delta\psi(x,t)\mathrm{d}x \\
&+ \beta k\int_\Omega \psi(x,t)(r_A(u^k(x,t)) - r_B(v^k(x,t)))\mathrm{d}x = 0. && (1.8)
\end{aligned}$$

We remark that every essentially bounded weak solution of Problem $\mathcal{P}^k$, in the sense of Definition 1.1, is also a classical solution. The weak solution of the nonlinear diffusion equation (1.5) is similarly defined.

This paper is organized as follows. In Section 2, we define a finite volume discretisation and an approximate solution $(u^k_{\mathcal{D}}, v^k_{\mathcal{D}})$ for Problem $\mathcal{P}^k$. Section 3 contains a discrete comparison principle which yields discrete L^∞ estimates, and we show the existence and uniqueness of the approximate solution. We prove technical lemmas used further in the convergence proofs. Bothe and Hilhorst [1] used a Lyapunov functional to obtain $L^2(0,T;H^1(\Omega))$ estimates. However, we can drop every argument connected to the Lyapunov functional. Furthermore, we can weaken their assumptions. We obtain discrete $L^2(0,T;H^1(\Omega))$ estimates using suitable combinations of energy estimates. In Section 4, the convergence of the approximate solution to the classical solution of Problem $\mathcal{P}^k$ in the case of fixed k is proved. In Section 5, we show that the approximate solution $(u^k_{\mathcal{D}}, v^k_{\mathcal{D}})$ converges to (u,v) defined in (1.6) as k tends to infinity and the size of the discretisation parameters tends to zero. Afterwards, we examine the rate of convergence with respect to k. In Section 6, we present numerical results obtained with our finite volume scheme, for the reversible dimerisation of *o*-phenylenedioxydimethylsilane (2, 2-dimethyl-1, 2, 3-benzodioxasilole) which is a reaction of the type $2\mathcal{A} \rightleftharpoons \mathcal{B}$ (see [12]). We compute the approximate solution $(u^k_{\mathcal{D}}, v^k_{\mathcal{D}})$ of the solution (u^k, v^k) of Problem $\mathcal{P}^k$ and the numerical approximation $w_{\mathcal{D}}$ of the solution w of the problem (1.5). Moreover, we numerically check our convergence result.

Remark 1.1 In what follows, we denote by C and C_k positive generic constants which may vary from line to line.

2 The Finite Volume Scheme

The finite volume method was first developed by engineers in order to study complex, coupled physical problems where the conservation of quantities such as masses, energy or impulsion must be carefully respected by the approximate solution. Another advantage of this method is that a large variety of meshes can be used in the computations. The finite volume methods are particularly well suited for numerical investigations of conservations laws. They are one of the most popular methods among the engineers performing computations for industrial purposes: the modelling of flows in porous media, problems related to oil recovery, questions related to hydrology, such as the numerical approximation of a stationary incompressible Navier-Stokes equations.

For a comprehensive discussion about the finite volume method, we refer to [6] and the references therein.

Following [6], we define a finite volume discretization of Q_T.

Definition 2.1 (Admissible Mesh of Ω) *An admissible mesh $\mathcal{M}$ of Ω is given by a set of open, bounded subsets of Ω (control volumes) and a family of points (one per control volume), satisfying the following properties:*

(1) *The closure of the union of all the control volumes is $\overline{\Omega}$. We denote by m_K the measure of each volume element K and* $\text{size}(\mathcal{M}) = \max_{K\in\mathcal{M}} m_k$.

(2) *$K \cap L = \emptyset$ for any $(K,L) \in \mathcal{M}^2$, such that $K \neq L$. If $\overline{K} \cap \overline{L} \neq \emptyset$, then it is a subset of a hyperplane in $\mathbb{R}^d$. Let us denote by $\mathcal{E} \subset \mathcal{M}^2$ the set of pairs (K,L), such that $K \neq L$ and the $d-1$ Lebesgue measure of $\overline{K} \cap \overline{L}$ is strictly positive. For $(K,L) \in \mathcal{E}$, we write $K|L$ for the set $\overline{K} \cap \overline{L}$ and $m_{K|L}$ for the $d-1$ Lebesgue measure of $K|L$.*

(3) *For any $K \in \mathcal{M}$, we also define $\mathcal{N}_K = \{L \in \mathcal{M},\ (K,L) \in \mathcal{E}\}$ and assume that $\partial K = \overline{K} \backslash K = (\overline{K} \cap \partial\Omega) \cup \Big(\bigcup_{L\in\mathcal{N}_K} K|L \Big)$.*

(4) *There exists a family of points $(x_K)_{K\in\mathcal{M}}$, such that $x_K \in K$ and if $L \in \mathcal{N}_K$ then the straight line (x_K, x_L) is orthogonal to $K|L$. We set*

$$d_{K|L} = d(x_K, x_L) \quad \textit{and} \quad T_{K|L} = \frac{m_{K|L}}{d_{K|L}},$$

where the last quantity is sometimes called the transmissibility across the edge $K|L$.

Since Problem $\mathcal{P}^k$ is a time evolution problem, we also need to discretize the time interval $(0,T)$.

Definition 2.2 (Time Discretization) *A time discretization of the interval $(0,T)$ is given by an integer value N and by a strictly increasing sequence of real values $(t^{(n)})_{n\in\{0,\cdots,N+1\}}$ with $t^{(0)}=0$ and $t^{(N+1)}=T$. The time steps are defined by*

$$t_\delta^{(n)} = t^{(n+1)} - t^{(n)} \quad \text{for } n\in\{0,\cdots,N\}.$$

We may then define a discretization of the whole domain Q_T in the following way.

Definition 2.3 (Discretization of Q_T) *A finite volume discretization $\mathcal{D}$ of Q_T is defined as*

$$\mathcal{D} = (\mathcal{M}, \mathcal{E}, (x_K)_{K\in\mathcal{M}}, (t^{(n)})_{n\in\{0,\cdots,N+1\}}),$$

where $\mathcal{M}$, $\mathcal{E}$ and $(x_K)_{K\in\mathcal{M}}$ are given in Definition 2.1 and the sequence $(t^{(n)})_{n\in\{0,\cdots,N+1\}}$ is a time discretization of $(0,T)$ in the sense of Definition 2.2. One then sets

$$\operatorname{size}(\mathcal{D}) = \max\{\operatorname{size}(\mathcal{M}), t_\delta^{(n)} : n\in\{0,\cdots,N\}\}.$$

We present below the finite volume scheme which we use and define approximate solutions. We assume that the hypotheses $\mathcal{H}$ hold and suppose that $\mathcal{D}$ is an admissible discretization of Q_T in the sense of Definition 2.3. We prescribe the approximate initial conditions

$$u_K^{(0)} = \frac{1}{m_K}\int_K u_0(x)\mathrm{d}x \quad \text{and} \quad v_K^{(0)} = \frac{1}{m_K}\int_K v_0(x)\mathrm{d}x \tag{2.1}$$

for all $K\in\mathcal{M}$, and associate to Problem $\mathcal{P}^k$ the finite volume scheme

$$\begin{aligned}
&m_K(u_K^{(n+1)} - u_K^{(n)}) - t_\delta^{(n)} a \sum_{L\in\mathcal{N}_K} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})\\
&+t_\delta^{(n)} m_K \alpha k (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)})) = 0,\\
&m_K(v_K^{(n+1)} - v_K^{(n)}) - t_\delta^{(n)} b \sum_{L\in\mathcal{N}_K} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)})\\
&-t_\delta^{(n)} m_K \beta k (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)})) = 0.
\end{aligned} \tag{2.2}$$

Note that (2.2) is a nonlinear system of equations in the unknowns

$$(u_K^{(n+1)}, v_K^{(n+1)})_{K\in\mathcal{M},\ n\in\{0,\cdots,N\}}.$$

For $x\in\Omega$ and $t\in(0,T)$, let $K\in\mathcal{M}$ be such that $x\in K$ and $n\in\{0,\cdots,N\}$ be such that $t\in(t^{(n)},t^{(n+1)}]$. We can then define the approximate solutions

$$u_{\mathcal{D}}(x,t) = u_K^{(n+1)} \quad \text{and} \quad v_{\mathcal{D}}(x,t) = v_K^{(n+1)}. \tag{2.3}$$

In the next section, we prove the existence and uniqueness of the solution of the discrete problem (2.2), together with the initial values (2.1).

3 Existence and Uniqueness of the Approximate Solution and Some Basic Properties

In this section, we prove the existence and uniqueness of the solution of (2.2) and provide its basic properties.

3.1 The comparison principle and L^∞-estimate

Let us start with a discrete version of the comparison principle.

Lemma 3.1 (Discrete Comparison Principle) *We suppose that the hypotheses $\mathcal{H}$ are satisfied. Let $\mathcal{D}$ be a discretization as in Definition* 2.3. *Let $(u_K^{(0)}, v_K^{(0)})_{K\in\mathcal{M}}$ and $(\widetilde{u}_K^{(0)}, \widetilde{v}_K^{(0)})_{K\in\mathcal{M}}$ be given sequences of real values such that*

$$u_K^{(0)} \leqslant \widetilde{u}_K^{(0)} \quad \textit{and} \quad v_K^{(0)} \leqslant \widetilde{v}_K^{(0)}$$

for all $K \in \mathcal{M}$. If $(u_K^{(n+1)}, v_K^{(n+1)})_{K\in\mathcal{M},\ n\in\{0,\cdots,N\}}$ and $(\widetilde{u}_K^{(n+1)}, \widetilde{v}_K^{(n+1)})_{K\in\mathcal{M},\ n\in\{0,\cdots,N\}}$ satisfy equations (2.2) *with the initial values $(u_K^{(0)}, v_K^{(0)})_{K\in\mathcal{M}}$ and $(\widetilde{u}_K^{(0)}, \widetilde{v}_K^{(0)})_{K\in\mathcal{M}}$, respectively, then for $K \in \mathcal{M}$ and $n \in \{0, \cdots, N\}$,*

$$u_K^{(n+1)} \leqslant \widetilde{u}_K^{(n+1)} \quad \text{and} \quad v_K^{(n+1)} \leqslant \widetilde{v}_K^{(n+1)}. \tag{3.1}$$

Proof We set $\widehat{u}_K^{(n)} = u_K^{(n)} - \widetilde{u}_K^{(n)}$ and $\widehat{v}_K^{(n)} = v_K^{(n)} - \widetilde{v}_K^{(n)}$ for all $K \in \mathcal{M}$ and $n \in \{0, \cdots, N+1\}$ and define

$$\begin{aligned}
\widehat{A}_K^{(n+1)} &= (r_A(u_K^{(n+1)}) - r_A(\widetilde{u}_K^{(n+1)}))/\widehat{u}_K^{(n+1)},\\
\widehat{B}_K^{(n+1)} &= (r_B(v_K^{(n+1)}) - r_B(\widetilde{v}_K^{(n+1)}))/\widehat{v}_K^{(n+1)},
\end{aligned}$$

whenever $\widehat{u}_K^{(n+1)} \neq 0$ (else $\widehat{A}_K^{(n+1)} = 0$) or $\widehat{v}_K^{(n+1)} \neq 0$ (else $\widehat{B}_K^{(n+1)} = 0$). Since the functions r_A and r_B are monotone increasing, it follows that $\widehat{A}_K^{(n+1)}$ and $\widehat{B}_K^{(n+1)}$ are nonnegative. We then have, by subtracting the discrete equation (2.2) for $\widetilde{u}_K^{(n+1)}$ from that for ${u_K}^{(n+1)}$,

$$\begin{aligned}
&m_K\Big(1 + t_\delta^{(n)}\Big(\alpha k\widehat{A}_K^{(n+1)} + \frac{a}{m_K}\sum_{L\in\mathcal{N}_K} T_{K|L}\Big)\Big)\widehat{u}_K^{(n+1)}\\
&= m_K\widehat{u}_K^{(n)} + t_\delta^{(n)} a\sum_{L\in\mathcal{N}_K} T_{K|L}\widehat{u}_L^{(n+1)} + t_\delta^{(n)} m_K\alpha k(r_B(v_K^{(n+1)}) - r_B(\widetilde{v}_K^{(n+1)}))
\end{aligned}\tag{3.2}$$

for $K \in \mathcal{M}$ and $n \in \{0, \cdots, N\}$. Setting $s^+ = \max(s, 0)$ and using that $s \leqslant s^+$, $(s+t)^+ \leqslant s^+ + t^+$, we obtain

$$\begin{aligned}
&m_K\Big(1 + t_\delta^{(n)}\Big(\alpha k\widehat{A}_K^{(n+1)} + \frac{a}{m_K}\sum_{L\in\mathcal{N}_K} T_{K|L}\Big)\Big)\widehat{u}_K^{(n+1)}\\
&\leqslant m_K(\widehat{u}_K^{(n)})^+ + t_\delta^{(n)} a\sum_{L\in\mathcal{N}_K} T_{K|L}(\widehat{u}_L^{(n+1)})^+ + t_\delta^{(n)} m_K\alpha k(r_B(v_K^{(n+1)}) - r_B(\widetilde{v}_K^{(n+1)}))^+,
\end{aligned}\tag{3.3}$$

where $K \in \mathcal{M}$ and $n \in \{0, \cdots, N\}$. Next we multiply the inequality (3.3) by indicator of the set where $\widehat{u}_K^{(n+1)}$ is nonnegative. Since the right-hand side of (3.3) is nonnegative as well, we obtain, acting similarly for both components,

$$\begin{aligned}
&m_K\Big(1 + t_\delta^{(n)}\Big(\alpha k\widehat{A}_K^{(n+1)} + \frac{a}{m_K}\sum_{L\in\mathcal{N}_K} T_{K|L}\Big)\Big)(\widehat{u}_K^{(n+1)})^+\\
&\leqslant m_K(\widehat{u}_K^{(n)})^+ + t_\delta^{(n)} a\sum_{L\in\mathcal{N}_K} T_{K|L}(\widehat{u}_L^{(n+1)})^+ + t_\delta^{(n)} m_K\alpha k(r_B(v_K^{(n+1)}) - r_B(\widetilde{v}_K^{(n+1)}))^+,\\
&m_K\Big(1 + t_\delta^{(n)}\Big(\beta k\widehat{B}_K^{(n+1)} + \frac{b}{m_K}\sum_{L\in\mathcal{N}_K} T_{K|L}\Big)\Big)(\widehat{v}_K^{(n+1)})^+\\
&\leqslant m_K(\widehat{v}_K^{(n)})^+ + t_\delta^{(n)} b\sum_{L\in\mathcal{N}_K} T_{K|L}(\widehat{v}_L^{(n+1)})^+ + t_\delta^{(n)} m_K\beta k(r_A(u_K^{(n+1)}) - r_A(\widetilde{u}_K^{(n+1)}))^+.
\end{aligned}\tag{3.4}$$

Since

$$\widehat{A}_K^{(n+1)}(\widehat{u}_K^{(n+1)})^+ = (r_A(u_K^{(n+1)}) - r_A(\widetilde{u}_K^{(n+1)}))^+,$$
$$\widehat{B}_K^{(n+1)}(\widehat{v}_K^{(n+1)})^+ = (r_B(v_K^{(n+1)}) - r_B(\widetilde{v}_K^{(n+1)}))^+,$$

we add the first equation of (3.4) divided by α and the second equation of (3.4) divided by β, which yields

$$\begin{aligned} & m_K\Big(\frac{1}{\alpha} + t_\delta^{(n)}\frac{a}{m_K\alpha}\sum_{L\in\mathcal{N}_K} T_{K|L}\Big)(\widehat{u}_K^{(n+1)})^+ + \ m_K\Big(\frac{1}{\beta} + t_\delta^{(n)}\frac{b}{m_K\beta}\sum_{L\in\mathcal{N}_K} T_{K|L}\Big)(\widehat{v}_K^{(n+1)})^+ \\ \leqslant\ & m_K\frac{1}{\alpha}(\widehat{u}_K^{(n)})^+ + t_\delta^{(n)}\frac{a}{\alpha}\sum_{L\in\mathcal{N}_K} T_{K|L}(\widehat{u}_L^{(n+1)})^+ + \ m_K\frac{1}{\beta}(\widehat{v}_K^{(n)})^+ \\ & + t_\delta^{(n)}\frac{b}{\beta}\sum_{L\in\mathcal{N}_K} T_{K|L}(\widehat{v}_L^{(n+1)})^+ \end{aligned} \tag{3.5}$$

for $K\in\mathcal{M}$ and $n\in\{0,\cdots,N\}$. Let us note that

$$\begin{aligned} \sum_{K\in\mathcal{M}}\sum_{L\in\mathcal{N}_K} T_{K|L}(\widehat{u}_K^{(n+1)})^+ &= \sum_{L\in\mathcal{M}}\sum_{K\in\mathcal{N}_L} T_{L|K}(\widehat{u}_L^{(n+1)})^+ = \sum_{L\in\mathcal{M}}\sum_{K\in\mathcal{N}_L} T_{K|L}(\widehat{u}_L^{(n+1)})^+ \\ &= \sum_{K\in\mathcal{M}}\sum_{L\in\mathcal{N}_K} T_{K|L}(\widehat{u}_L^{(n+1)})^+. \end{aligned}$$

Summing the inequalities (3.5) over $K\in\mathcal{M}$, we obtain

$$\sum_{K\in\mathcal{M}}\Big[m_K\Big(\frac{1}{\alpha}(\widehat{u}_K^{(n+1)})^+ + \frac{1}{\beta}(\widehat{v}_K^{(n+1)})^+\Big)\Big] \leqslant \sum_{K\in\mathcal{M}}\Big[m_K\Big(\frac{1}{\alpha}(\widehat{u}_K^{(n)})^+ + \frac{1}{\beta}(\widehat{v}_K^{(n)})^+\Big)\Big],$$

which, by induction, leads to

$$\sum_{K\in\mathcal{M}}\Big[m_K\Big(\frac{1}{\alpha}(\widehat{u}_K^{(n+1)})^+ + \frac{1}{\beta}(\widehat{v}_K^{(n+1)})^+\Big)\Big] = 0,$$

where $n\in\{0,\cdots,N\}$. It implies that $(\widehat{u}_K^{(n+1)})^+ = (\widehat{v}_K^{(n+1)})^+ = 0$, which completes the proof.

Corollary 3.1 (Uniqueness) *The discrete system* (2.1), (2.2) *possesses at most one solution.*

Corollary 3.2 (Discrete Contraction in L^1 Property) *With the notation from Lemma* 3.1*, we have*

$$\sum_{K\in\mathcal{M}} m_K\Big(\frac{|u_K^{(n+1)} - \widetilde{u}_K^{(n+1)}|}{\alpha} + \frac{|v_K^{(n+1)} - \widetilde{v}_K^{(n+1)}|}{\beta}\Big) \leqslant \sum_{K\in\mathcal{M}} m_K\Big(\frac{|u_K^{(n)} - \widetilde{u}_K^{(n)}|}{\alpha} + \frac{|v_K^{(n)} - \widetilde{v}_K^{(n)}|}{\beta}\Big)$$

for $n\in\{0,\cdots,N\}$. This represents the discrete counterpart of the $L^1(\Omega)$-contraction property for solutions of (1.1), (1.2) *which is proved in* [3].

Proof The proof directly follows as in the proof of Lemma 3.1. Let us consider the term $\widehat{u}_K$. We multiply the equation (3.2) by $\operatorname{sgn}(\widehat{u}_K^{(n+1)})$. Then, the inequality $x\leqslant|x|$ yields

$$m_K\Big(1 + t_\delta^{(n)}\Big(\alpha k\widehat{A}_K^{(n+1)} + a\sum_{L\in\mathcal{N}_K} T_{K|L}\Big)\Big)|\widehat{u}_K^{(n+1)}|$$

$$\leqslant m_K|\widehat{u}_K^{(n)}| + t_\delta^{(n)}\frac{a}{m_K}\sum_{L\in\mathcal{N}_K} T_{K|L}|\widehat{u}_L^{(n+1)}| + t_\delta^{(n)} m_K \alpha k |r_B(v_K^{(n+1)}) - r_B(\widetilde{v}_K^{(n+1)})|.$$

We proceed in the same way for $\widehat{v}_K^{(n+1)}$ and remark that

$$\widehat{A}_K^{(n+1)}|\widehat{u}_K^{(n+1)}| = |r_A(u_K^{(n+1)}) - r_A(\widetilde{u}_K^{(n+1)})|,$$
$$\widehat{B}_K^{(n+1)}|\widehat{v}_K^{(n+1)}| = |r_B(v_K^{(n+1)}) - r_B(\widetilde{v}_K^{(n+1)})|,$$

which enable us to obtain the counterpart of the inequalities in (3.5) which we sum over $K \in \mathcal{M}$, as in the proof of Lemma 3.1. This yields the result.

We now are in a position to prove a discrete L^∞ estimate for the approximate solution.

Theorem 3.1 *Let $\mathcal{D} = (\mathcal{M}, \mathcal{E}, \mathcal{P}, (t^{(n)})_{n\in\{0,\cdots,N+1\}})$ be an admissible discretization of Q_T in the sense of Definition 2.3. We suppose that the hypotheses $\mathcal{H}$ are satisfied. Let $(u_K^{(0)}, v_K^{(0)})_{K\in\mathcal{M}}$ be given by (2.1) and $(u_K^{(n+1)}, v_K^{(n+1)})$ satisfy (2.2) for $K \in \mathcal{M}$ and $n \in \{0,\cdots,N\}$. Then*

$$0 \leqslant u_K^{(n+1)} \leqslant U + \frac{\alpha}{\beta}V \quad \text{and} \quad 0 \leqslant v_K^{(n+1)} \leqslant V + \frac{\beta}{\alpha}U \tag{3.6}$$

for all $K \in \mathcal{M}$ and $n \in \{0,\cdots,N\}$, where U and V are the positive constants from the hypothesis $\mathcal{H}(2)$.

Proof From Lemma 3.1 we immediately obtain that $u_K^{(n+1)}$ and $v_K^{(n+1)}$ are nonnegative for $K \in \mathcal{M}$ and $n \in \{0,\cdots,N\}$. In order to find a discrete upper solution, we consider approximate solutions of the corresponding system of ordinary differential equations. More precisely, we consider sequences $(\overline{u}^{(n)})_{n\in\{0,\cdots,N+1\}}$, $(\overline{v}^{(n)})_{n\in\{0,\cdots,N+1\}}$ (we postpone for a moment the proof that they exist) such that

$$\overline{u}^{(0)} = U, \quad \overline{v}^{(0)} = V$$

and

$$\begin{aligned} \overline{u}^{(n+1)} - \overline{u}^{(n)} &= \alpha k\, t_\delta^{(n)}(r_B(\overline{v}^{(n+1)}) - r_A(\overline{u}^{(n+1)})), \\ \overline{v}^{(n+1)} - \overline{v}^{(n)} &= \beta k\, t_\delta^{(n)}(r_A(\overline{u}^{(n+1)}) - r_B(\overline{v}^{(n+1)})) \end{aligned} \tag{3.7}$$

for $n \in \{0,\cdots,N\}$. We note that the sequences $(\overline{u}^{(n+1)})_{n\in\{0,\cdots,N\}}$, $(\overline{v}^{(n+1)})_{n\in\{0,\cdots,N\}}$ satisfy (2.2) with the initial data U, V. Therefore, they satisfy the comparison principle from Lemma 3.1 which yields

$$0 \leqslant \overline{u}^{(n+1)} \quad \text{and} \quad 0 \leqslant \overline{v}^{(n+1)} \quad \text{for all } n \in \{0,\cdots,N\}. \tag{3.8}$$

Adding up the first equation of (3.7) divided by α and the second one divided by β, we obtain

$$\frac{\overline{u}^{(n+1)}}{\alpha} + \frac{\overline{v}^{(n+1)}}{\beta} = \frac{\overline{u}^{(n)}}{\alpha} + \frac{\overline{v}^{(n)}}{\beta} = \cdots = \frac{U}{\alpha} + \frac{V}{\beta}.$$

We deduce from the previous equation and from (3.8) that

$$0 \leqslant \overline{u}^{(n+1)} \leqslant U + \frac{\alpha}{\beta}V \quad \text{and} \quad 0 \leqslant \overline{v}^{(n+1)} \leqslant V + \frac{\beta}{\alpha}U \tag{3.9}$$

for $n \in \{0,\cdots,N\}$.

3.2 Existence of the approximate solution

In order to prove the existence of the solution of the system (2.1), (2.2), we make use of the topological degree theory in finite dimensional spaces. The proof of existence of the solution of the system (3.7) is similar. The reader can find basic definitions as well as further information in [4]. An example of the application of this tool to the analysis of a finite volume scheme can be found for instance in [8]. We rewrite (2.2) in the form

$$\begin{aligned}&\mathcal{F}((u_K^{(n+1)})_{K\in\mathcal{M}},(v_K^{(n+1)})_{K\in\mathcal{M}})+\mathcal{G}((u_K^{(n+1)})_{K\in\mathcal{M}},(v_K^{(n+1)})_{K\in\mathcal{M}})\\&=((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}}),\end{aligned}\tag{3.10}$$

where $\mathcal{F},\mathcal{G}:\mathbb{R}^{2\Theta}\to\mathbb{R}^{2\Theta}$, with Θ the number of control volumes for the discretization $\mathcal{D}$, are continuous functions given by

$$\begin{aligned}&\mathcal{F}((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}})=((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}}),\\&\mathcal{G}((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}})=(\mathcal{W}_1,\mathcal{W}_2),\end{aligned}$$

where

$$\mathcal{W}_1=-\frac{t_\delta^{(n-1)}a}{m_K}\sum_{L\in\mathcal{N}_K}T_{K|L}(u_L^{(n)}-u_K^{(n)})+t_\delta^{(n-1)}\alpha k(r_A(u_K^{(n)})-r_B(v_K^{(n)})),$$

and

$$\mathcal{W}_2=-\frac{t_\delta^{(n-1)}b}{m_K}\sum_{L\in\mathcal{N}_K}T_{K|L}(v_L^{(n)}-v_K^{(n)})-t_\delta^{(n-1)}\beta k(r_A(u_K^{(n)})-r_B(v_K^{(n)})).$$

We set $\mathcal{O}=B(0,R)\subset\mathbb{R}^{2\Theta}$ a ball centered at zero with a radius

$$R>\sqrt{\Theta\Big(U+\frac{\alpha}{\beta}V\Big)^2+\Theta\Big(V+\frac{\beta}{\alpha}U\Big)^2}.$$

Since $\Theta>1$, we deduce from the discrete $L^\infty(Q_T)$ estimate of Theorem 3.1 that system (3.10) does not have any solutions on $\partial\mathcal{O}$. Similarly, one can show that for all $\lambda\in[0,1]$ the system

$$\begin{aligned}&\mathcal{F}((u_K^{(n+1)})_{K\in\mathcal{M}},(v_K^{(n+1)})_{K\in\mathcal{M}})+\lambda\mathcal{G}((u_K^{(n+1)})_{K\in\mathcal{M}},(v_K^{(n+1)})_{K\in\mathcal{M}})\\&=((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}})\end{aligned}\tag{3.11}$$

does not possess any solution on the boundary of $\mathcal{O}$. Therefore, it follows from [4, Theorem 3.1, p. 16] (d3) that

$$d(\mathcal{F}+\lambda\mathcal{G},\mathcal{O},((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}}))=d(\mathcal{F},\mathcal{O},((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}}))\tag{3.12}$$

for all $\lambda\in[0,1]$. On the other hand we deduce from [4, Theorem 3.1, p. 16] (d1) that

$$d(\mathcal{F},\mathcal{O},((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}}))=1,\tag{3.13}$$

so that

$$d(\mathcal{F}+\mathcal{G},\mathcal{O},((u_K^{(n)})_{K\in\mathcal{M}},(v_K^{(n)})_{K\in\mathcal{M}}))=1.$$

Also using [4, Theorem 3.1, p. 16] (d4), we conclude that there exists a solution of (3.10).

Theorem 3.2 *We suppose that the hypotheses $\mathcal{H}$ are satisfied. Let $\mathcal{D}$ be a discretization as in Definition* 2.3*. Let $(u_K^{(0)}, v_K^{(0)})_{K\in\mathcal{M}}$ be given by* (2.1)*. Then there exists one and only one sequence*

$$(u_K^{(n+1)}, v_K^{(n+1)})_{K\in\mathcal{M},\ n\in\{0,\cdots,N\}},$$

which satisfies (2.2)*, with the initial condition $(u_K^{(0)}, v_K^{(0)})_{K\in\mathcal{M}}$.*

3.3 Estimates of the gradient and some relationship between $u_\mathcal{D}$ and $v_\mathcal{D}$

We prove the following estimates.

Lemma 3.2 *We suppose that the hypotheses $\mathcal{H}$ are satisfied. Let $\mathcal{D}$ be a discretization as in Definition* 2.3*. Let* (2.1) *and* (2.2) *give $(u_K^{(0)}, v_K^{(0)})_{K\in\mathcal{M}}$ and $(u_K^{(n+1)}, v_K^{(n+1)})_{K\in\mathcal{M},\ n\in\{0,\cdots,N\}}$, respectively. Then, there exists a constant $C>0$, which does not depend on the discretization $\mathcal{D}$ and on the reaction rate k such that*

$$\sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})^2 + \sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)})^2 \leqslant C, \quad (3.14)$$

$$\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))^2 \leqslant \frac{C}{k}. \quad (3.15)$$

The bounds (3.14) constitute a discrete version of $L^2(Q_T)$ gradient estimates.

Bothe and Hilhorst [1] imposed some additional assumptions on the nonlinear terms r_A and r_B to prove the continuous version of this lemma. However, our idea of proof can simplify their argument. A similar idea can be found in [13].

Proof We multiply the first equation in the finite volume scheme (2.2) by $\eta(u_K^{(n+1)})$ and sum the result over all $K\in\mathcal{M}$ and over all $n\in\{0,\cdots,N\}$ to obtain

$$\mathcal{S}_1 + \mathcal{S}_2 + \mathcal{S}_3 = 0, \quad (3.16)$$

where

$$\mathcal{S}_1 = \sum_{n=0}^{N} \sum_{K\in\mathcal{M}} m_K (u_K^{(n+1)} - u_K^{(n)}) \eta(u_K^{(n+1)}),$$

$$\mathcal{S}_2 = -a \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} \sum_{L\in\mathcal{N}_K} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)}) \eta(u_K^{(n+1)}),$$

$$\mathcal{S}_3 = k\alpha \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)})) \eta(u_K^{(n+1)}).$$

Let us define $\Phi_\eta(s) = \int_0^s \eta(r)\mathrm{d}r$ for all $s\in\mathbb{R}$. Since Φ_η is non-negative and convex, we can estimate $\mathcal{S}_1$ as follows:

$$\begin{aligned}\mathcal{S}_1 &\geqslant \sum_{n=0}^{N} \sum_{K\in\mathcal{M}} m_K (\Phi_\eta(u_K^{(n+1)}) - \Phi_\eta(u_K^{(n)})) \\ &= \sum_{K\in\mathcal{M}} m_K \Phi_\eta(u_K^{(N+1)}) - \sum_{K\in\mathcal{M}} m_K \Phi_\eta(u_K^{(0)}) \geqslant -\sum_{K\in\mathcal{M}} m_K \Phi_\eta(u_K^{(0)}).\end{aligned}$$

We can perform a discrete integration by parts to obtain

$$\mathcal{S}_2 = a\sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})(\eta(u_L^{(n+1)}) - \eta(u_K^{(n+1)})). \tag{3.17}$$

This is positive because η is an increasing function. Therefore, we obtain

$$\mathcal{S}_3 \leqslant \sum_{K\in\mathcal{M}} m_K \Phi_\eta(u_K^{(0)}). \tag{3.18}$$

We multiply the second equation in (2.2) by $v_K^{(n+1)}$ and sum the result over all $K \in \mathcal{M}$ and over all $n \in \{0, \cdots, N\}$. Noting that

$$(v_K^{(n+1)})^2 - v_K^{(n)} v_K^{(n+1)} = \frac{1}{2}(v_K^{(n+1)})^2 - \frac{1}{2}(v_K^{(n)})^2 + \frac{1}{2}(v_K^{(n+1)} - v_K^{(n)})^2,$$

a similar argument as above gives us the following relation:

$$\begin{aligned}
& b\sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)})^2 \\
& - k\beta \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))v_K^{(n+1)} \\
\leqslant{} & \frac{1}{2}\sum_{K\in\mathcal{M}} m_K (v_K^{(0)})^2.
\end{aligned} \tag{3.19}$$

Summing up (3.18) and (3.19) weighted by $\frac{1}{\alpha}$ and $\frac{1}{\beta}$, respectively, we have

$$\begin{aligned}
& \frac{b}{\beta}\sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)})^2 \\
& + k\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))(\eta(u_K^{(n+1)}) - v_K^{(n+1)}) \\
\leqslant{} & \frac{1}{\alpha}\sum_{K\in\mathcal{M}} m_K \Phi_\eta(u_K^{(0)}) + \frac{1}{2\beta}\sum_{K\in\mathcal{M}} m_K (v_K^{(0)})^2.
\end{aligned} \tag{3.20}$$

The right-hand side is bounded due to the Hypotheses $\mathcal{H}$. Since r_B is Lipschitz continuous on the finite interval $\left[0, U + \frac{\alpha}{\beta}V\right]$, we denote by L_B the local Lipschitz constant. Then, it follows from (3.20) that

$$\begin{aligned}
& k\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))^2 \\
={} & k\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))(r_B(\eta(u_K^{(n+1)})) - r_B(v_K^{(n+1)})) \\
\leqslant{} & L_B k\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))(\eta(u_K^{(n+1)}) - v_K^{(n+1)}) \leqslant C
\end{aligned}$$

for some positive constant C, which implies (3.15).

Adding up the first equation of (2.2) divided by α and the second one divided by β yields

$$m_K(w_K^{(n+1)} - w_K^{(n)}) - t_\delta^{(n)} \sum_{L \in \mathcal{N}_K} T_{K|L}\Big(\frac{a}{\alpha}(u_L^{(n+1)} - u_K^{(n+1)}) + \frac{b}{\beta}(v_L^{(n+1)} - v_K^{(n+1)})\Big) = 0. \quad (3.21)$$

Here, $w_K^{(n)} := \frac{1}{\alpha}u_K^{(n)} + \frac{1}{\beta}v_K^{(n)}$. Multiply it by $w_K^{(n+1)}$, sum over all $K \in \mathcal{M}$ and $n \in \{0, \cdots, N-1\}$ and apply discrete integration by parts to obtain

$$\begin{aligned}
&\frac{1}{2}\sum_{K \in \mathcal{M}} m_K(w_K^{(N+1)})^2 - \frac{1}{2}\sum_{K \in \mathcal{M}} m_K(w_K^{(0)})^2 \\
&\leqslant -\sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L) \in \mathcal{E}} T_{K|L}\Big(\frac{a}{\alpha^2}(u_L^{(n+1)} - u_K^{(n+1)})^2 \\
&\quad - \frac{a+b}{\alpha\beta}(u_L^{(n+1)} - u_K^{(n+1)})(v_L^{(n+1)} - v_K^{(n+1)}) - \frac{b}{\beta^2}(v_L^{(n+1)} - v_K^{(n+1)})^2\Big).
\end{aligned}$$

It follows from the elementary relation

$$\frac{a+b}{\alpha\beta} \leqslant \frac{a}{2\alpha^2} + \frac{(a+b)^2}{2a\beta^2} \quad (3.22)$$

for all $s_1, s_2 \in \mathbb{R}$ that

$$\begin{aligned}
&\frac{1}{2}\sum_{K \in \mathcal{M}} m_K(w_K^{(N+1)})^2 + \frac{a}{2\alpha^2}\sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L) \in \mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})^2 \\
&\leqslant \frac{1}{2}\sum_{K \in \mathcal{M}} m_K(w_K^{(0)})^2 + \Big|\frac{(a+b)^2}{2a\beta^2} - \frac{b}{\beta^2}\Big|\sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L) \in \mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)})^2,
\end{aligned}$$

which is bounded because of (3.20) and the Hypotheses $\mathcal{H}$. This completes the proof of Lemma 3.2.

If r_B^{-1} is locally Lipschitz continuous, we can obtain further relationship between $u_\mathcal{D}$ and $v_\mathcal{D}$, that leads to the error estimates given in Section 5.

Lemma 3.3 *In addition to the assumptions of Lemma* 3.2*, suppose that there exists a positive constant* l_B *such that*

$$l_B|s_1 - s_2| \leqslant |r_B(s_1) - r_B(s_2)| \quad \textit{for all } s_1,\ s_2 \in \Big[0, \max\Big\{\eta\Big(U + \frac{\alpha}{\beta}V\Big), V + \frac{\beta}{\alpha}U\Big\}\Big]. \quad (3.23)$$

Then, there exists a positive constant C *independent of* $\mathcal{D}$ *and* k *such that*

$$\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K \in \mathcal{M}} m_K(\eta(u_K^{(n+1)}) - v_K^{(n+1)})^2 \leqslant \frac{C}{k}.$$

Proof We deduce from (3.20) that

$$\begin{aligned}
&k\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K \in \mathcal{M}} m_K(\eta(u_K^{(n+1)}) - v_K^{(n+1)})^2 \\
&\leqslant \frac{k}{l_B}\sum_{n=0}^{N} t_\delta^{(n)} \sum_{K \in \mathcal{M}} m_K(r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))(\eta(u_K^{(n+1)}) - v_K^{(n+1)}) \leqslant C
\end{aligned}$$

for some positive constant C. This concludes the proof.

3.4 Space and Time Translates of Approximate Solutions

We now turn to the space and time translates estimates. We use here methods which have been presented for example by Eymard, Gutnic and Hilhorst [8] and by Eymard, Gallouët, Hilhorst and Slimane [7]. The results of the current subsection together with the technical Lemma A.2 will imply the relative compactness of the sequence of approximate solutions.

Lemma 3.4 *We assume that*

(1) $\mathcal{D} = (\mathcal{M}, \mathcal{E}, (x_K)_{K\in\mathcal{M}}, (t^{(n)})_{n\in\{0,\cdots,N+1\}})$ *is an admissible discretization of* Q_T *in the sense of Definition* 2.3*,*

(2) *the hypotheses* $\mathcal{H}$ *are satisfied,*

(3) *the functions* $u_\mathcal{D}$ *and* $v_\mathcal{D}$ *are derived from the scheme* (2.1)–(2.2) *and given by the formulas* (2.3)*.*

Then there exists a positive constant C*, which does not depend on* $\mathcal{D}$ *and* k *such that*

$$\int_0^T\int_{\Omega_\xi}(u_\mathcal{D}(x+\xi,t)-u_\mathcal{D}(x,t))^2\mathrm{d}x\mathrm{d}t \leqslant C|\xi|(2\,\mathrm{size}\,(\mathcal{D})+|\xi|), \tag{3.24}$$

$$\int_0^T\int_{\Omega_\xi}(v_\mathcal{D}(x+\xi,t)-v_\mathcal{D}(x,t))^2\mathrm{d}x\mathrm{d}t \leqslant C|\xi|(2\,\mathrm{size}\,(\mathcal{D}))+|\xi|) \tag{3.25}$$

for all $\xi\in\mathbb{R}^d$ *and for* Ω_ξ *defined as in Lemma* A.2*.*

Proof Inequalities (3.24) and (3.25) follow from the estimates (3.14). We refer to [6, Lemma 3.3] for more details.

Lemma 3.5 *Let the assumptions of Lemma* 3.4 *be satisfied. Then, there exists some constant* $C_k>0$*, which does not depend on* $\mathcal{D}$*, but which depends on all the data including* k*, such that*

$$\int_{\Omega\times(0,T-\tau)}(u_\mathcal{D}(x,t+\tau)-u_\mathcal{D}(x,t))^2\mathrm{d}x\mathrm{d}t \leqslant C_k(\mathrm{size}\,(\mathcal{D})+\tau), \tag{3.26}$$

$$\int_{\Omega\times(0,T-\tau)}(v_\mathcal{D}(x,t+\tau)-v_\mathcal{D}(x,t))^2\mathrm{d}x\mathrm{d}t \leqslant C_k(\mathrm{size}\,(\mathcal{D})+\tau) \tag{3.27}$$

for all $\tau\in(0,T)$*.*

Proof In order to apply Lemma A.1 (see Appendix), we follow the same steps as in [8, Lemma 5.5]. The only difference appears in the nonlinear part of the equations. However, these can be easily estimated using the regularity properties of functions r_A and r_B, as well as L^∞ estimates (3.6) in Theorem 3.1.

Lemma 3.6 *Let the assumptions of Lemma* 3.4 *hold. Set* $w_\mathcal{D}=\frac{1}{\alpha}u_\mathcal{D}+\frac{1}{\beta}v_\mathcal{D}$*. Then, there exists a constant* $C>0$*, which is independent of the discretization parameters* $\mathcal{D}$ *and of* k*, such that*

$$\int_{\Omega_\xi\times(0,T)}(w_\mathcal{D}(x+\xi,t)-w_\mathcal{D}(x,t))^2\mathrm{d}x\mathrm{d}t \leqslant C|\xi|(2\mathrm{size}\,(\mathcal{D})+|\xi|) \tag{3.28}$$

for all $\xi\in\mathbb{R}^d$ *and* $\Omega_\xi=\{x\in\mathbb{R}^d,[x,x+\xi]\subset\Omega\}$*. Moreover*

$$\int_{\Omega\times(0,T-\tau)}(w_\mathcal{D}(x,t+\tau)-w_\mathcal{D}(x,t))^2\mathrm{d}x\mathrm{d}t \leqslant C(\mathrm{size}\,(\mathcal{D})+\tau) \tag{3.29}$$

for all $\tau \in (0, T)$.

Proof The space translate estimate (3.28) immediately follows from Lemma 3.4. The proof of (3.29) is similar to that of Lemma 3.5. We present below the essential steps of the argument. We define

$$\mathcal{A}(t) := \int_\Omega (w_\mathcal{D}(x, t+\tau) - w_\mathcal{D}(x,t))^2 \mathrm{d}x,$$

which can be easily transformed into

$$\begin{aligned}\mathcal{A}(t) &= \sum_{K\in\mathcal{M}} m_K (w_K^{(n(t+\tau)+1)} - w_K^{(n(t)+1)})^2 \\ &= \sum_{k\in\mathcal{M}} \Big((w_K^{(n(t+\tau)+1)} - w_K^{(n(t)+1)}) \sum_{n=n(t)+1}^{n(t+\tau)} m_K (w_K^{(n+1)} - w_K^{(n)}) \Big).\end{aligned}$$

Since

$$w_K^{(n+1)} - w_K^{(n)} = \frac{1}{\alpha}(u_K^{(n+1)} - u_K^{(n)}) + \frac{1}{\beta}(v_K^{(n+1)} - v_K^{(n)}),$$

we can apply discrete integration by parts in the scheme (2.2) to obtain

$$\begin{aligned}\mathcal{A}(t) = &\frac{a}{\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})(w_K^{(n(t+\tau)+1)} - w_L^{(n(t+\tau)+1)}) \\ &+ \frac{a}{\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})(w_L^{(n(t)+1)} - w_K^{(n(t)+1)}) \\ &+ \frac{b}{\beta} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)})(w_K^{(n(t+\tau)+1)} - w_L^{(n(t+\tau)+1)}) \\ &+ \frac{b}{\beta} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)})(w_L^{(n(t)+1)} - w_K^{(n(t)+1)}).\end{aligned}$$

Next we estimate the second term in the sum above, to obtain

$$\begin{aligned}&\frac{a}{\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} \sqrt{T_{K|L}}\,(u_L^{(n+1)} - u_K^{(n+1)}) \cdot \sqrt{T_{K|L}}\,(w_L^{(n(t)+1)} - w_K^{(n(t)+1)}) \\ \leqslant &\frac{a}{2\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})^2 \\ &+ \frac{a}{2\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(w_L^{(n(t)+1)} - w_K^{(n(t)+1)})^2 \\ \leqslant &\frac{a}{2\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)})^2 \\ &+ \frac{a}{\alpha^3} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(u_L^{(n(t)+1)} - u_K^{(n(t)+1)})^2\end{aligned}$$

$$+\frac{a}{\alpha\beta^2}\sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \sum_{(K,L)\in\mathcal{E}} T_{K|L}(v_L^{(n(t)+1)} - v_K^{(n(t)+1)})^2,$$

where the first inequality follows from the relation $s_1 s_2 \leqslant \frac{1}{2}(s_1^2 + s_2^2)$ for all $s_1, s_2 \in \mathbb{R}$ and the second one follows from the simple inequality $(s_1 + s_2)^2 \leqslant 2(s_1^2 + s_2^2)$ for all $s_1, s_2 \in \mathbb{R}$. To conclude the proof we integrate above inequalities over $\mathbb{R}$ with respect to the time variable t. Finally we apply Lemma A.1 (for details see [8, Lemma 5.5]).

4 Convergence Proof with k Fixed

In this section, we state convergence results with k fixed. This differs from next section where we will obtain convergence results which permit us to pass to the limit as k tends to infinity.

Theorem 4.1 *We suppose that the hypotheses $\mathcal{H}$ are satisfied. Let $(u_\mathcal{D}, v_\mathcal{D})$ be the approximate solution defined by* (2.1), (2.2) *and* (2.3) *and $(u^k, v^k) \in L^2(0,T;\ H^1(\Omega))^2$ be the unique classical solution of Problem $\mathcal{P}^k$. Then the sequence $(u_\mathcal{D}, v_\mathcal{D})$ converges strongly in $L^2(Q_T)^2$ to $(u^k,\ v^k)$ as $\mathrm{size}\,(\mathcal{D})$ tends to zero. Hence, the sequence $w_\mathcal{D} = \frac{1}{\alpha}u_\mathcal{D} + \frac{1}{\beta}v_\mathcal{D}$ converges strongly in $L^2(Q_T)$ to the function $w^k = \frac{1}{\alpha}u^k + \frac{1}{\beta}v^k$ as $\mathrm{size}\,(\mathcal{D})$ tends to zero. Moreover, there exist positive constants C_1 which do not depend on k, such that*

$$\begin{aligned}&\int_{\Omega_\xi\times(0,T)} (u^k(x+\xi,t) - u^k(x,t))^2 \mathrm{d}x\mathrm{d}t\\ &+\int_{\Omega_\xi\times(0,T)} (v^k(x+\xi,t) - v^k(x,t))^2 \mathrm{d}x\mathrm{d}t \leqslant C_1|\xi|^2,\end{aligned}\tag{4.1}$$

$$\int_{\Omega_\xi\times(0,T)} (w^k(x+\xi,t) - w^k(x,t))^2 \mathrm{d}x\mathrm{d}t \leqslant C_1|\xi|^2,\tag{4.2}$$

$$\int_{\Omega\times(0,T-\tau)} (w^k(x,t+\tau) - w^k(x,t))^2 \mathrm{d}x\mathrm{d}t \leqslant C_1\tau,\tag{4.3}$$

$$\|r_A(u^k) - r_B(v^k)\|_{L^2(Q_T)} \leqslant C_1 k^{-\frac{1}{2}},\tag{4.4}$$

where $\tau \in (0,T)$, $\xi \in \mathbb{R}^d$ and $\Omega_\xi = \{x \in \mathbb{R}^d, [x, x+\xi] \subset \Omega\}$.

In addition to the above, if there exists a positive constant l_B satisfying (3.23)*, then*

$$\|\eta(u^k) - v^k\|_{L^2(Q_T)} \leqslant C_2 k^{-\frac{1}{2}}\tag{4.5}$$

holds for some positive constant C_2 independent of k.

Proof In view of the estimates (3.24), (3.26) and Proposition A.2 which is a consequence of the Fréchet-Kolmogorov Theorem [2, Theorem IV.25, p. 72], we deduce the relative compactness of the set $(u_\mathcal{D})$ so that there exists a sequence of $(u_{\mathcal{D}_m})_{m=1}^\infty$ and a function $\mathcal{U}_k$, such that $u_{\mathcal{D}_m}$ converges to $\mathcal{U}_k$ strongly in $L^2(Q_T)$ as m tends to infinity.

The same conclusion holds for the v-component. Indeed, the inequalities (3.25) and (3.27) permit to apply the compactness result in Lemma A.2 for the sequence $(v_{\mathcal{D}_m})_{m=1}^\infty$. There exists a function $\mathcal{V}_k$ such that $v_{\mathcal{D}_m}$ converges to $\mathcal{V}_k$ strongly in $L^2(Q_T)$ as m tends to infinity. We use [6, Theorem 3.10] to get $\mathcal{U}_k, \mathcal{V}_k \in L^2(0,T;H^1(\Omega))$.

Next we show that $(\mathcal{U}_k,\, \mathcal{V}_k)$ is a weak solution of Problem $\mathcal{P}^k$, in the sense of Definition 1.1. Let $\psi \in \Psi$, where Ψ is the class of test functions from Definition 1.1. We multiply the first equation of (2.2) by $\psi(x_K, t^{(n)})$. Then we sum over all $K \in \mathcal{M}$ and $n \in \{0, \cdots, N-1\}$ to obtain

$$\mathcal{T}^u_{1m} - \mathcal{T}^u_{2m} + \mathcal{T}^u_{3m} = 0,$$

where

$$\begin{aligned}
\mathcal{T}^u_{1m} &= \sum_{n=0}^{N-1} \sum_{K\in\mathcal{M}} m_K (u_K^{(n+1)} - u_K^{(n)}) \psi(x_K, t^{(n)}),\\
\mathcal{T}^u_{2m} &= a \sum_{n=0}^{N-1} t_\delta^{(n)} \sum_{K\in\mathcal{M}} \sum_{L\in\mathcal{N}_K} T_{K|L} (u_L^{(n+1)} - u_K^{(n+1)}) \psi(x_K, t^{(n)}),\\
\mathcal{T}^u_{3m} &= \sum_{n=0}^{N-1} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K \alpha k (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)})) \psi(x_K, t^{(n)}).
\end{aligned}$$

The complete proof, that

$$\lim_{m\to\infty} \mathcal{T}^u_{1m} = -\int_\Omega u_0(x)\psi(x,0)\mathrm{d}x - \int_0^T \int_\Omega \mathcal{U}_k(x,t)\psi_t(x,t)\mathrm{d}x\mathrm{d}t$$

and

$$\lim_{m\to\infty} \mathcal{T}^u_{2m} = -a \int_0^T \int_\Omega \mathcal{U}_k(x,t)\Delta\psi(x,t)\mathrm{d}x\mathrm{d}t,$$

can be found in [8, Lemma 5.5]. Let us focus on the proof that

$$\lim_{m\to\infty} \mathcal{T}^u_{3m} = \alpha k \int_0^T \int_\Omega (r_A(\mathcal{U}_k(x,t)) - r_B(\mathcal{V}_k(x,t)))\psi(x,t)\mathrm{d}x\mathrm{d}t. \tag{4.6}$$

We write

$$\begin{aligned}
&\sum_{n=0}^{N-1} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)})) \psi(x_K, t^{(n)})\\
&\quad - \int_0^T \int_\Omega \psi(r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k))\mathrm{d}x\mathrm{d}t\\
&= \sum_{n=0}^{N-1} \sum_{K\in\mathcal{M}} \int_{t^{(n)}}^{t^{(n+1)}} \int_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)})) \psi(x_K, t^{(n)})\mathrm{d}x\mathrm{d}t\\
&\quad - \sum_{n=0}^{N-1} \sum_{K\in\mathcal{M}} \int_{t^{(n)}}^{t^{(n+1)}} \int_K \psi(r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k))\mathrm{d}x\mathrm{d}t\\
&\quad - \sum_{K\in\mathcal{M}} \int_{t^{(N)}}^{t^{(N+1)}} \int_K \psi(r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k))\mathrm{d}x\mathrm{d}t.
\end{aligned}$$

Thanks to the regularity of the function ψ, the last sum above converges to zero. Moreover,

$$\sum_{n=0}^{N-1} \sum_{K\in\mathcal{M}} \int_{t^{(n)}}^{t^{(n+1)}} \int_K (r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)})) \psi(x_K, t^{(n)})\mathrm{d}x\mathrm{d}t$$

$$
\begin{aligned}
&-\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K \psi(r_A(\mathcal{U}_k)-r_B(\mathcal{V}_k))\mathrm{d}x\mathrm{d}t\\
=&\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K (\psi(x_K,t^{(n)})-\psi(x,t))(r_A(u_K^{(n+1)})-r_B(v_K^{(n+1)})\mathrm{d}x\mathrm{d}t\\
&+\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K \psi(r_A(u_K^{(n+1)})-r_A(\mathcal{U}_k))\mathrm{d}x\mathrm{d}t\\
&-\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K \psi(r_B(v_K^{(n+1)})-r_B(\mathcal{V}_k))\mathrm{d}x\mathrm{d}t. \qquad (4.7)
\end{aligned}
$$

Next we show that the three terms above tend to zero as $m\to\infty$. First we take their absolute value and apply the triangle inequality. The Cauchy-Schwarz inequality applied to the first sum of the right-hand side of (4.7) yields

$$
\begin{aligned}
&\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K |\psi(x_K,t^{(n)})-\psi(x,t)||r_A(u_K^{(n+1)})-r_B(v_K^{(n+1)})|\mathrm{d}x\mathrm{d}t\\
\leqslant&\Big(\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K (\psi(x_K,t^{(n)})-\psi(x,t))^2\mathrm{d}x\mathrm{d}t\Big)^{\frac{1}{2}}\\
&\times\Big(\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K (r_A(u_K^{(n+1)})-r_B(v_K^{(n+1)})^2\mathrm{d}x\mathrm{d}t\Big)^{\frac{1}{2}}.
\end{aligned}
$$

The first term of above product converges to zero, as $m\to\infty$, since ψ is smooth enough. The second term is bounded. Indeed, it is sufficient to remark that $r_A(u_K^{(n+1)})$, $r_B(v_K^{(n+1)})$ are bounded for all $K\in\mathcal{M}$ and $n\in\{0,\cdots,N\}$. The last two terms in (4.7) are similar, and we show how the proof goes with the first one. Indeed, let L_A be the local Lipschitz constant of r_A valid over the finite interval $[0,U+\frac{\alpha}{\beta}V]$. Then we have

$$
\begin{aligned}
&\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K |\psi||r_A(u_K^{(n+1)})-r_A(\mathcal{U}_k)|\mathrm{d}x\mathrm{d}t\\
\leqslant& L_A\|\psi\|_{L^\infty(Q_T)}\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K |u_{\mathcal{D}_m}-\mathcal{U}_k|\mathrm{d}x\mathrm{d}t\\
\leqslant& L_A(T\mathrm{meas}(\Omega))^{\frac{1}{2}}\|\psi\|_{L^\infty(Q_T)}\Big(\sum_{n=0}^{N-1}\sum_{K\in\mathcal{M}}\int_{t^{(n)}}^{t^{(n+1)}}\int_K |u_{\mathcal{D}_m}-\mathcal{U}_k|^2\mathrm{d}x\mathrm{d}t\Big)^{\frac{1}{2}},
\end{aligned}
$$

which converges to zero since $u_{\mathcal{D}_m}\to\mathcal{U}_k$ as $m\to\infty$ in $L^2(Q_T)$. Therefore, we obtain (4.6).

In a similar fashion, we deduce from the second equation of (2.2) that

$$
\begin{aligned}
&\int_\Omega v_0(x)\psi(x,0)\mathrm{d}x+\int_0^T\int_\Omega \mathcal{V}_k(x,t)\psi_t(x,t)\mathrm{d}x\mathrm{d}t+b\int_0^T\int_\Omega \mathcal{V}_k(x,t)\Delta\psi(x,t)\mathrm{d}x\mathrm{d}t\\
&+\beta k\int_0^T\int_\Omega (r_A(\mathcal{U}_k(x,t))-r_B(\mathcal{V}_k(x,t)))\psi(x,t)\mathrm{d}x\mathrm{d}t=0
\end{aligned}
$$

for all $\psi\in\Psi$. Hence, $(\mathcal{U}_k,\ \mathcal{V}_k)$ is a weak solution of Problem $\mathcal{P}^k$. Since Problem $\mathcal{P}^k$ is a uniformly parabolic system, (u^k,v^k) must coincide with the classical solution of Problem $\mathcal{P}^k$.

Because the solution is unique, the original sequence $(u_{\mathcal{D}}, v_{\mathcal{D}})$ converges the solution of Problem $\mathcal{P}^k$. The assertions (4.1)–(4.5) follow immediately from Lemmas 3.2–3.4 and 3.6.

5 The Case That k Tends to Infinity

In this section, we investigate the convergence of the finite volume scheme when size$(\mathcal{D})$ tends to zero and k tends to infinity.

5.1 The limit as size($\mathcal{D}$) tends to zero and k tends to infinity

We state the main convergence results of this paper.

It is now possible to pass to the limit as k tends to infinity.

Theorem 5.1 *Let* $(u_{\mathcal{D}}^k,\ v_{\mathcal{D}}^k)$ *be the sequence of approximate solutions of Problem* $\mathcal{P}^k$*, defined by* (2.1)*,* (2.2) *and* (2.3)*. Then*

$$u_{\mathcal{D}}^k \to f(w) \quad \textit{and} \quad v_{\mathcal{D}}^k \to g(w)$$

strongly in $L^2(Q_T)$ *as* size$(\mathcal{D})$ *tends to zero and* k *tends to infinity, where* f *and* g *are defined in Section* 1 *and where* w *is the unique weak solution of the problem* (1.5)*.*

Proof We follow the same procedure as in [1]. Let $w_{\mathcal{D}}^k = \frac{1}{\alpha}u_{\mathcal{D}}^k + \frac{1}{\beta}v_{\mathcal{D}}^k$. The estimates from Lemma 3.6, which are uniform with respect to k, permit to apply Lemma A.2. As a consequence we deduce the relative compactness in $L^2(Q_T)$ of the sequence $\{w_{\mathcal{D}}^k\}$. Then, there exist a function $w \in L^2(Q_T)$ and a subsequence $\{w_{\mathcal{D}_m}^{k_i}\}$ such that $w_{\mathcal{D}_m}^{k_i}$ converges to w strongly in $L^2(Q_T)$ and a.e. in Q_T as k_i tends to infinity and size$(\mathcal{D}_m)$ tends to zero. Theorem 3.1 implies that w is nonnegative and bounded in Q_T. The inequality (3.15), namely

$$k_i\|r_A(u_{\mathcal{D}_m}^{k_i}) - r_B(v_{\mathcal{D}_m}^{k_i})\|_{L^2(Q_T)}^2 \leqslant C$$

where the positive constant C is independent of k_i and size$(\mathcal{D}_m)$, implies that

$$r_A(u_{\mathcal{D}_m}^{k_i}) - r_B(v_{\mathcal{D}_m}^{k_i}) \to 0, \quad \text{in } L^2(Q_T),$$

and consequently almost everywhere, as size$(\mathcal{D}_m)$ tends to zero and k_i tends to infinity. Then

$$v_{\mathcal{D}_m}^{k_i} = \eta(u_{\mathcal{D}_m}^{k_i}) + e_{\mathcal{D}_m}^{k_i},$$

where $e_{\mathcal{D}_m}^{k_i}$ tends to zero almost everywhere as size$(\mathcal{D}_m)$ tends to zero and k_i tends to infinity. In view of the hypotheses $\mathcal{H}(4)$ the function η is well defined on $[0, \infty)$. Moreover,

$$f^{-1}(u_{\mathcal{D}_m}^{k_i}) = w_{\mathcal{D}_m}^{k_i} - \frac{1}{\beta}e_{\mathcal{D}_m}^{k_i} \to w, \quad \text{a.e. in } Q_T.$$

Hypotheses $\mathcal{H}(4)$ ensures that the function f is continuous. Then Lebesgue's dominated convergence theorem implies

$$u_{\mathcal{D}_m}^{k_i} \to f(w) \quad \text{and} \quad v_{\mathcal{D}_m}^{k_i} \to g(w)$$

strongly in $L^2(Q_T)$ as size$(\mathcal{D}_m)$ tends to zero and k_i tends to infinity. Lemma 3.4 and [6, Theorem 3.10] imply $f(w), g(w) \in L^2(0, T; H^1(\Omega))$.

Next we identify the limit function w. Let $\psi \in \Psi$, where Ψ is the class of test functions from Definition 1.1. We multiply (3.21) by $\psi(x_K, t^{(n)})$ and sum over all $K \in \mathcal{M}$ and $n \in \{0, \cdots, N-1\}$. Then, letting $\operatorname{size}(\mathcal{D}_m) \to 0$ and $k_i \to \infty$ yields

$$
\begin{aligned}
&-\int_\Omega w_0(x)\psi(x,0)\mathrm{d}x - \int_0^T\int_\Omega w(x,t)\psi_t(x,t)\mathrm{d}x\mathrm{d}t \\
&+\int_0^T\int_\Omega \Big(\frac{a}{\alpha}f(w(x,t)) + \frac{b}{\beta}g(w(x,t))\Big)\Delta\psi(x,t)\mathrm{d}x\mathrm{d}t = 0.
\end{aligned}
$$

Obviously, $\frac{a}{\alpha}f(w) + \frac{b}{\beta}g(w) = \phi(w)$. Therefore, w is the weak solution of (1.5). Since the weak solution of (1.5) is unique, the original sequences $\{u^k_{\mathcal{D}}\}$ and $\{v^k_{\mathcal{D}}\}$ converge to $f(w)$ and $g(w)$, respectively. Thus, the proof is complete.

5.2 The rate of convergence with respect to k

We can obtain the convergence rates with respect to k under additional conditions on r_B.

Theorem 5.2 *We assume that the hypotheses $\mathcal{H}$ hold and moreover that there exists a positive constant satisfying* (3.23)*. Let $(u^k,\ v^k)$ be the weak solution of Problem $\mathcal{P}^k$ and w be that of* (1.5)*. Then, there exists a positive constant C independent of k such that*

$$
\begin{aligned}
&\Big\|w - \Big(\frac{1}{\alpha}u^k + \frac{1}{\beta}v^k\Big)\Big\|_{L^2(Q_T)} + \|f(w) - u^k\|_{L^2(Q_T)} + \|g(w) - v^k\|_{L^2(Q_T)} \\
&+\Big\|\int_0^t \Big(\phi(w) - \Big(\frac{a}{\alpha}u^k + \frac{b}{\beta}v^k\Big)\Big)\Big\|_{L^\infty(0,T;H^1(\Omega))} \leqslant Ck^{-\frac{1}{2}}.
\end{aligned}
$$

Proof We define errors as follows:

$$
e_u := f(w) - u^k, \quad e_v := g(w) - v^k, \quad e_w := \frac{1}{\alpha}e_u + \frac{1}{\beta}e_v, \quad e_\phi := \phi(w) - \Big(\frac{a}{\alpha}u^k + \frac{b}{\beta}v^k\Big).
$$

Since $\phi(w), u^k, v^k \in L^2(0,T;H^1(\Omega))$ and $C^{2,1}(\overline{\Omega}\times[0,T])$ is dense in $H^1(Q_T)$, we deduce from the weak formulations of (1.5) and (1.1) that

$$
-\int_0^T\int_\Omega e_w\psi_t\mathrm{d}x\mathrm{d}t + \int_0^T\int_\Omega \nabla e_\phi\cdot\nabla\psi\mathrm{d}x\mathrm{d}t = 0
$$

for all functions $\psi \in H^1(Q_T)$ with $\psi(\,\cdot\,,T) = 0$. For fixed $t_0 \in (0,T]$, take

$$
\psi(x,t) = \begin{cases} \displaystyle\int_t^{t_0} e_\phi(x,s)\mathrm{d}s, & \text{if } 0 \le t < t_0,\ \text{a.e. } x \in \Omega, \\ 0, & \text{otherwise,} \end{cases}
$$

to get

$$
\int_0^{t_0}\int_\Omega e_w(x,t)e_\phi(x,t)\mathrm{d}x\mathrm{d}t + \int_0^{t_0}\int_\Omega \nabla e_\phi(x,t)\cdot\nabla\int_t^{t_0} e_\phi(x,s)\mathrm{d}s\mathrm{d}x\mathrm{d}t = 0.
$$

Therefore, we easily obtain

$$
\begin{aligned}
&\frac{a}{\alpha^2}\|e_u\|^2_{L^2(\Omega\times(0,t_0))} + \frac{b}{\beta^2}\|e_v\|^2_{L^2(\Omega\times(0,t_0))} + \frac{a+b}{\alpha\beta}\int_0^{t_0}\int_\Omega (f(w)-u^k)(\eta(f(w)) - \eta(u^k))\mathrm{d}x\mathrm{d}t \\
&+\frac{1}{2}\Big\|\nabla\int_0^{t_0} e_\phi\Big\|^2_{L^2(\Omega)} = -\frac{a+b}{\alpha\beta}\int_0^{t_0}\int_\Omega e_u(\eta(u^k) - v^k)\mathrm{d}x\mathrm{d}t. \qquad (5.1)
\end{aligned}
$$

The third term of left-hand side is positive because η is an increasing function. The right-hand side can be estimated by means of the elementary relation (3.22) as follows:

$$\Big|\frac{a+b}{\alpha\beta}\int_0^{t_0}\int_\Omega e_u(\eta(u^k)-v^k)\mathrm{d}x\mathrm{d}t\Big| \leqslant \frac{a}{2\alpha^2}\|e_u\|^2_{L^2(\Omega\times(0,t_0))}+\frac{(a+b)^2}{2a\beta^2}\|\eta(u^k)-v^k\|^2_{L^2(\Omega\times(0,t_0))}.$$

The first term can be absorbed into the left-hand side of (5.1). The estimate (4.5) and the definition of e_w imply the desired estimates.

6 Numerical Example

In this section, we give an example of an application of the finite volume scheme (2.2) in one space dimension. For the numerical experiments we choose the reaction of the reversible dimerisation of *o*-phenylenedioxydimethylsilane $(2,2$-dimethyl-$1,2,3$-benzodioxasilole) which has been studied by ^{1}H NMR spectroscopy. The kinetics of this reaction can be described quantitatively by a bimolecular lO-ring formation reaction and a monomolecular backreaction (for further details we refer to [12]). Since the reaction is of the type $2\mathcal{A} \rightleftharpoons \mathcal{B}$, the reaction terms take the form

$$r_A(u)=k_1u^2 \quad \text{and} \quad r_B(v)=k_2v.$$

Moreover $\alpha=2$ and $\beta=1$. For this particular process benzene was chosen as a solvent. Then it was possible to estimate rate constants for both reactions at the temperature $T=298K$,

$$k_1\approx 1.072\cdot 10^{-4}\,\mathrm{L}^2\mathrm{mol}^{-2} \quad \text{and} \quad k_2\approx 2.363\cdot 10^{-6}\,\mathrm{L}^2\mathrm{mol}^{-2}$$

and diffusion coefficients

$$a\approx 1.579\cdot 10^{-9}\,\mathrm{m}^2\mathrm{s}^{-1} \quad \text{and} \quad b\approx 1.042\cdot 10^{-9}\,\mathrm{m}^2\mathrm{s}^{-1}.$$

In the first experiment we set $k=1$ for the chemical kinetics factor. We remark that it is equivalent to the situation when coefficients $a,\ b,\ k_1$ and k_2 are of order 1 and k is of order 10^4. In fact, we can multiply the system (1.1) by 10^9 and change the time scale as $t\mapsto 10^9t$. However the above reasoning is formally correct and shows in an explicit way the order of the kinetics factor k; in our example we decided to keep constants in the form given by the spectroscopic analysis.

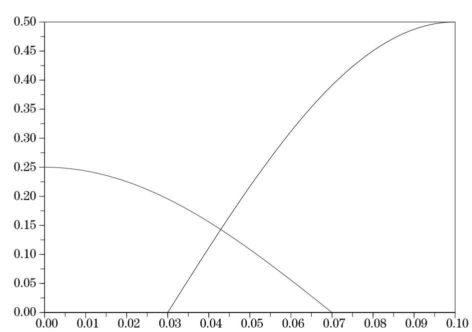


Figure 1 Initial data defined in (6.1) and (6.2).

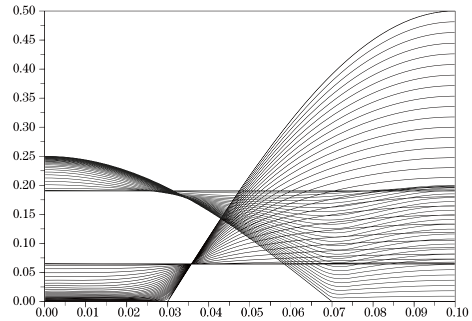


Figure 2 Numerical solutions $u_{\mathcal{D}}^k$ and $v_{\mathcal{D}}^k$.

Figure 1 shows the initial conditions u_0 and v_0 defined as

$$u_0(x) = \begin{cases} 0 & \text{for } x \in [0, 0.03], \\ \dfrac{1}{2}\sin\left(\dfrac{50\pi}{7}(x - 0.03)\right) & \text{for } x \in [0.03, 0.1] \end{cases} \tag{6.1}$$

and

$$v_0(x) = \begin{cases} \dfrac{1}{4}\cos\left(\dfrac{50\pi}{7}x\right) & \text{for } x \in [0, 0.07], \\ 0 & \text{for } x \in [0.07, 0.1]. \end{cases} \tag{6.2}$$

We used a uniform mesh with mesh size $h = 0.00025$ and initial time step size $t_\delta^{(0)} = 0.1$. The time step sizes are determined by

$$t_\delta^{(n+1)} = \frac{\gamma \ t_\delta^{(n)}}{\max\limits_{x \in \Omega}\{|u_{\mathcal{D}}^k(x, t^{(n+1)}) - u_{\mathcal{D}}^k(x, t^{(n+1)})|, |v_{\mathcal{D}}^k(x, t^{(n+1)}) - v_{\mathcal{D}}^k(x, t^{(n+1)})|\}}, \tag{6.3}$$

while $t^{(n)} < T$. If n satisfies $t^{(n)} < T \leqslant t^{(n+1)}$, then we put $N = n$ and define $t_\delta^{(N)} := T - t^{(N)}$. Here, $\gamma = 0.02$. We carried out a numerical simulation until the time $T = 10^{11}$ [s]. Figure 2 shows the time evolution of the numerical solution $(u_{\mathcal{D}}^k, v_{\mathcal{D}}^k)$. The number of time steps was $N = 34$. We can obtain numerical solutions efficiently until very large final times.

Next, we deal with the case that the kinetics parameter k is sufficiently large, namely $k = 10^{10}$. The numerical solution is regarded as an approximate solution of the nonlinear diffusion problem (1.5) according to Theorem 5.1. Let us define $w_0 = \frac{1}{\alpha}u_0 + \frac{1}{\beta}v_0$, where u_0 and v_0 are given by (6.1) and (6.2). We carried out numerical simulation using initial data $\overline{u}_0 = f(w_0)$ and $\overline{v}_0 = g(w_0)$, the same mesh size and initial time step size as above and $\gamma = 0.002$ in (6.3). Here, the functions f and g are defined in Section 1. The numerical solution

$$w_{\mathcal{D}}^k = \frac{1}{\alpha}u_{\mathcal{D}}^k + \frac{1}{\beta}v_{\mathcal{D}}^k$$

is drawn in Figure 4. The number of time steps was $N = 29$.

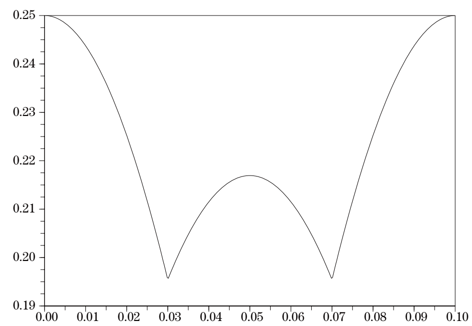


Figure 3 Initial datum w_0.

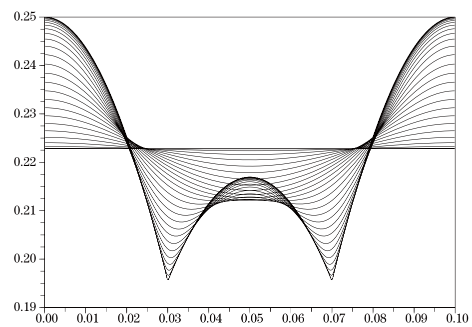


Figure 4 Numerical solutions $w_{\mathcal{D}}^k$.

We examine the sensitivity of the numerical results to the choice of k with $h = 0.00025$ and $t_\delta^{(n)} = \delta = 10$ fixed and the initial data u_0, v_0 above until $T = 10^4$. Numerical results at times $t = 0, 10\delta, 20\delta, \cdots, T - 10\delta, T$ for various choices of k are shown in Figure 5. We can observe that the larger k, the more rapidly the numerical solutions converge to w-shape, that is, they approach the chemical equiliblium. Then they are slowly evolving according to the nonlinear diffusion.

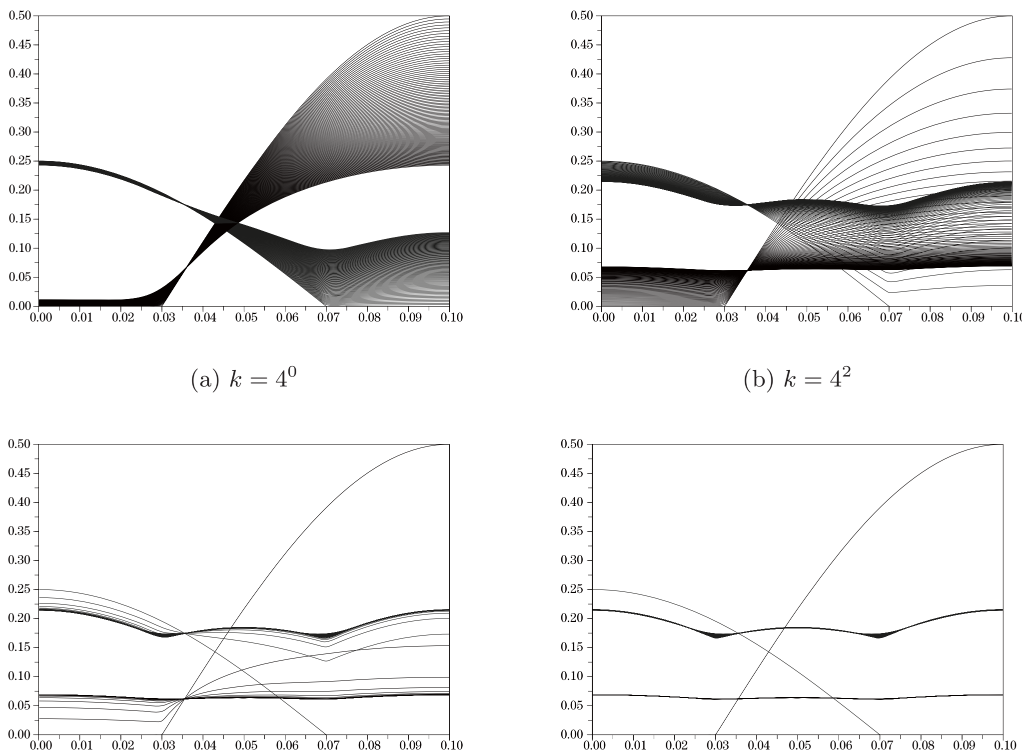
The rates of convergence with respect to k are examined. We regard the numerical solution $w_{\mathcal{D}}^k$ with $k = 10^{10}$ and initial data $\overline{u}_0$, $\overline{v}_0$ above as an "exact" solution, denoted by w, of (1.5). Numerical solutions are compared with the 'exact' solution. We calculate the difference between $r_A(u_{\mathcal{D}}^k)$ and $r_B(v_{\mathcal{D}}^k)$, and the errors, that is,

$$E_r := \Big(\frac{1}{T\text{meas}(\Omega)} \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K(r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}))^2\Big)^{\frac{1}{2}} \frac{1}{k_2},$$

$$E_u := \Big(\frac{1}{T\text{meas}(\Omega)} \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K(f(w(x_K, t^{(n)})) - u_K^{(n+1)})^2\Big)^{\frac{1}{2}},$$

$$E_v := \Big(\frac{1}{T\text{meas}(\Omega)} \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K\in\mathcal{M}} m_K(g(w(x_K, t^{(n)})) - v_K^{(n+1)})^2\Big)^{\frac{1}{2}}.$$

Table 1 sums up the computational results. We observe that the convergence rates for E_r, E_u and E_v are of order $-\frac{1}{2}$. They agree with our theoretical results (4.4) and Theorem 5.2.



(a) $k = 4^0$ (b) $k = 4^2$

(c) $k = 4^4$ (d) $k = 4^6$

Figure 5 Numerical solutions $u^k_{\mathcal{D}}$ and $v^k_{\mathcal{D}}$ for various choices of the parameter k.

Table 1 Errors for Various Choices of k

k	E_r	E_u	E_v
4^0	3.150861	0.170829	0.085569
4^1	1.684189	0.102105	0.051139
4^2	0.842005	0.052032	0.026037
4^3	0.414095	0.025948	0.012977
4^4	0.195023	0.012807	0.006404
4^5	0.082297	0.006132	0.003066
4^6	0.029367	0.002728	0.001364

7 Appendix

The proof of the following result can be found in [8, Lemmas 5.3 and 5.4].

Lemma A.1 *We denote by* $(t^{(n)})_{n\in\mathbb{Z}}$ *a strictly increasing sequence of real numbers such that* $\lim\limits_{n\to-\infty} t^{(n)} = -\infty$ *and* $\lim\limits_{n\to\infty} t^{(n)} = \infty$*. Moreover, let* $t_\delta^{(n)} := t^{(n+1)} - t^{(n)}$ *be uniformly bounded. For all* $t \in \mathbb{R}$ *we denote by* $n(t)$ *an integer* n*, such that* $t \in [t^{(n)}, t^{(n+1)})$*. Let* $(a^{(n)})_{n\in\mathbb{Z}}$ *be a family of nonnegative real values such that* $a^{(n)} \neq 0$ *for finitely many* $n \in \mathbb{Z}$*. Then, for all*

$\tau \in (0, +\infty)$ *and* $\zeta \in \mathbb{R}$,

$$\int_{\mathbb{R}} \sum_{n=n(t)+1}^{n(t+\tau)} (t_\delta^{(n)} a^{(n+1)}) \mathrm{d}t = \tau \sum_{n \in \mathbb{Z}} (t_\delta^{(n)} a^{(n+1)}), \tag{A.1}$$

$$\int_{\mathbb{R}} \Big(\sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^{(n)} \Big) a^{(n(t+\zeta)+1)} \mathrm{d}t \leqslant (\tau + \max_{n \in \mathbb{Z}} t_\delta^{(n)}) \sum_{n \in \mathbb{Z}} (t_\delta^{(n)} a^{(n+1)}). \tag{A.2}$$

The following lemma is a direct corollary from Fréchet-Kolmogorov Theorem (see [2, Theorem IV.25, p. 72]).

Lemma A.2 *Let* $\mathcal{O}$ *be a bounded and open subset of* $\mathbb{R}^{d+1}$, $d = 1, 2$ *or* 3. *Let* $(w_n)_{n \in \mathbb{N}}$ *be a sequence of functions* $w_n(x,t) : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$, *such that*

(1) *for all* $n \in \mathbb{N}$, $w_n \in L^\infty(\mathcal{O})$ *and there exists a constant* $C_b > 0$ *which does not depend on* n, *such that* $\|w_n\|_{L^\infty(\mathcal{O})} \leqslant C_b$,

(2) *there exist positive constants* C_1, C_2 *and a sequence of nonnegative real values* $(\mu_n)_{n \in \mathbb{N}}$, *such that* $\lim_{n \to \infty} \mu_n = 0$ *and* $\int_{\mathcal{O}_{\xi,\tau}} (w_n(x+\xi, t+\tau) - w_n(x,t))^2 \mathrm{d}x\mathrm{d}t \leqslant C_1|\xi| + C_2\tau + \mu_n$ *for* $\xi \in \mathbb{R}^d$, $\tau \in \mathbb{R}$, $n \in \{0, \cdots, N\}$ *and* $\mathcal{O}_{\xi,\tau} = \{(x,t) \in \mathbb{R}^{d+1}$: *the interval* $[(x,t), (x+\xi, t+\tau)]$ *lies in* $\mathcal{O}\}$. *Then there exists a subsequence of* $(w_n)_{n \in \mathbb{N}}$, *denoted again by* $(w_n)_{n \in \mathbb{N}}$ *and a function* $w \in L^\infty(\mathcal{O})$ *such that* $w_n \to w$ *in* $L^2(\mathcal{O})$, *as* $n \to \infty$.

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