Numerical approximation of a reaction-diffusion system with fast reversible reaction

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Abstract

We consider the finite volume approximation of a reaction-diffusion system with fast reversible reaction. We deduce 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 chemical kinetics factor. 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.

Key words: instantaneous reaction limit, mass-action kinetics, finite volume methods, convergence of approximate solutions, discrete a priori estimates, Kolmogorov’s theorem.

AMS subject classification: 35K45, 35K50, 35K55, 65M12, 65N12, 65N22, 80A30, 92E20.

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 timeframe of ordinary laboratory operations requires specialized instrumentation, techniques and ways of proceeding (see for example Espenson [4, Chapter 11]). This work tries to give an efficient, quick and cheap way for numerical investigations of such reactions.

In this article, we consider a reversible chemical reaction between mobile species \(A\) and \(B\), that takes place inside a bounded region \(\Omega \subset \mathbb{R}^d\) where \(d = 1, 2\) or \(3\). If the region is isolated and diffusion is modelled by Fick’s law, this leads to the reaction-diffusion system of partial differential equations

\[
\begin{align*}
\frac{\partial u}{\partial t} &= a \Delta u - \alpha k (r_A(u) - r_B(v)) \quad \text{in} \quad \Omega \times (0, T), \\
\frac{\partial v}{\partial t} &= b \Delta v + \beta k (r_A(u) - r_B(v)) \quad \text{in} \quad \Omega \times (0, T),
\end{align*}
\]

where \(T > 0\) and \(\Omega\) is a bounded set of \(\mathbb{R}^d\). An example of explicit expressions and values for \(\alpha, \beta, k, r_A, r_B, a, b\) is given in Section 6. We supplement the system (1) by the homogeneous Neumann boundary conditions

\[
\nabla u \cdot n = \nabla v \cdot n = 0 \quad \text{on} \quad \partial \Omega \times (0, T),
\]

and the initial conditions of the form

\[
u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x) \quad \text{in} \quad \Omega.
\]

In the sequel we call the system (1) together with the boundary conditions (2) and the initial conditions (3), Problem \(P^k\).

For a reversible reaction \(mA \rightleftharpoons nB\) 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 Erdi and Tóth [9] and Espenson [4].

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] study the limit to an instantaneous reaction. They exploit a natural Lyapunov functional and use compactness arguments to prove that

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

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

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

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

$$w_t = \Delta \phi(w) \quad \text{in} \quad \Omega \times (0, T)$$

$$\frac{\partial \phi(w)}{\partial n} = 0 \quad \text{on} \quad \partial \Omega \times (0, T)$$

$$w(x, 0) = w_0(x) := \frac{1}{\alpha}u_0(x) + \frac{1}{\beta}v_0(x) \quad \text{in} \quad \Omega,$$

with

$$\phi := \left(\frac{a}{\alpha} \text{id} + \frac{b}{\beta} \eta\right) \circ \left(\frac{1}{\alpha} \text{id} + \frac{1}{\beta} \eta\right)^{-1} \quad \text{on} \quad \mathbb{R}^+,$$

$$\eta = r_B^{-1} \circ r_A.$$

The identities in (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 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 $v$

$$u = \left(\frac{1}{\alpha} \text{id} + \frac{1}{\beta} \eta\right)^{-1}(w), \quad v = \eta \circ \left(\frac{1}{\alpha} \text{id} + \frac{1}{\beta} \eta\right)^{-1}(w).$$

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

1. Let $\Omega$ be an open, connected and bounded subset of $\mathbb{R}^d$, where $d = 1, 2$ or 3, with a smooth boundary $\partial \Omega$,
2. $u_0(x), \ v_0(x) \in L^\infty(\Omega)$ and there exist constants $U, V > 0$ such that $0 \leq u_0(x) \leq U$ and $0 \leq v_0(x) \leq V$ in $\Omega$,
3. $\alpha, \beta, \ a, \ b$ and $k$ are strictly positive real values (sometimes we use the notation $k\alpha = \hat{\alpha}$ and $k\beta = \hat{\beta}$),
4. Let $r_A(x), \ r_B(x) \in C^1(\mathbb{R})$ be strictly increasing functions, such that $r_A(0) = r_B(0) = 0$, and assume furthermore that $r_A(\mathbb{R}^+) \subset r_B(\mathbb{R}^+)$.

We recall from Bothe and Hilhorst [1, Section 2] that Problem $P^k$ has a unique classical solution $(u^k, v^k)$ on any 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 $u^k, \ v^k \in C^{2,1}(\Omega \times [0, T]) \cap C^{1,0}(\Omega \times [0, T])$ with $u^k, \ v^k \in C([0, T]; L^2(\Omega))$ (see also Ladyženskaja, Solonnikov and Ural’ceva [11]).

Next we present a notion of a weak solution of Problem $P^k$, 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 $P^k$ if and only if

1. $u^k, v^k \in L^2(0, T; H^1(\Omega))$ and $u^k_t, v^k_t \in L^2(0, T; (H^1(\Omega))^*)$;
2. Let $\Psi$ be the set of test functions, defined as

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

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

$$\int_\Omega u_0(x) \psi(x, 0) \, dx + \int_\Omega u^k(x, t) \psi_t(x, t) \, dx + \int_\Omega u^k(x, t) \Delta \psi(x, t) \, dx$$

$$- \hat{\alpha} \int_\Omega \psi(x, t) \left(r_A(u^k(x, t)) - r_B(v^k(x, t))\right) \, dx = 0 \quad (8)$$
\[ \int_{\Omega} v_0(x) \psi(x,0) \, dx + \int_{\Omega} v^k(x,t) \psi_1(x,t) \, dx + b \int_{\Omega} u^k(x,t) \Delta \psi(x,t) \, dx + \beta \int_{\Omega} \psi(x,t) \left( r_A(u^k(x,t)) - r_B(v^k(x,t)) \right) \, dx = 0. \] (9)

We remark that every essentially bounded weak solution of Problem $P^k$, in the sense of Definition 1.1, is also a classical solution.

This paper is organized as follows. In section 2 we define a finite volume discretisation and an approximate solution $(u^k_D, v^k_D)$ for Problem $P^k$. In section 3 we prove a discrete comparison principle which yields discrete $L^\infty$ estimates, and we show the existence and uniqueness of the approximate solution. Section 4 contains technical lemmas used further in the convergence proofs. The convergence of the approximate solution to the classical solution of Problem $P^k$ in the case of fixed $k$ is proved in section 5. In section 6 we use a suitable Lyapunov function and we obtain a discrete $L^2(0,T; H^1(\Omega))$ estimate, which does not depend on $k$. We then apply Kolmogorov’s theorem and deduce the convergence of the approximate solutions to the classical solution of Problem $P^k$. Afterwards we show that the approximate solution $(u^k_D, v^k_D)$ converges to $(u,v)$ defined in (7) as $k$ tends to $\infty$ and the size of the discretisation parameters tends to zero.

In Section 8 we present numerical results obtained with our finite volume scheme, for the reversible dimerisation of 2,2-dimethyl-3-benzodioxasilole (2,2-dimethyl-1,2,3-benzodioxasilole) which is a reaction of the type $2A \rightleftharpoons B$ (see Meyer, Klein and Weiss [12]). On the other hand we compute the approximate solution $(u^k_D, v^k_D)$ of the solution $(u^k, v^k)$ of Problem $P^k$ and on the other hand the numerical approximation $w_D$ of the solution $w$ of the problem (3) - (10), and we check that

\[ u^k_D \approx \left( \frac{1}{\alpha} \text{id} + \frac{1}{\beta} \eta \right)^{-1}(w_D) \quad \text{and} \quad v^k_D \approx \eta \circ \left( \frac{1}{\alpha} \text{id} + \frac{1}{\beta} \eta \right)^{-1}(w_D) \]

for $k$ large enough and size $(D)$ small enough.

**Remark 1.2.** In what follows we denote by $C$, $C_k$ and $C_\psi$ positive generic constants which may vary from line to line.

## 2 The finite volume scheme

The finite volume method has first been 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 Eymard, Gallouët and Herbin [6] and the references therein.

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

**Definition 2.1 (Admissible mesh of $\Omega$).** An admissible mesh $\mathcal{M}$ of $\Omega$ is given by a set of open, bounded subsets of $\Omega$ (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 $E \subset T^2$ the set of pairs $(K,L)$, such that the $d - 1$ Lebesgue measure of $\overline{K} \cap \overline{L}$ is strictly positive. For $(K,L) \in E$ 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 $N_K = \{ L \in T, (K,L) \in E \}$ and assume that $\partial K = \overline{K} \setminus K = (\overline{K} \cap \partial \Omega) \cup \bigcup_{L \in N_K} K|L$. 

\[ 3 \]
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

\[
d_{K|L} = d(x_K, x_L) \quad \text{and} \quad T_{K|L} = \frac{m_{K|L}}{d_{K|L}},
\]

where the last quantity is sometimes called the transmissibility across the edge \(K|L\).

Since Problem \(P^k\) 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 \(t^{(n)}\) with \(t^{(0)} = 0\) and \(t^{(N+1)} = T\). The time steps are defined by

\[
t^{(n)} = t^{(n+1)} - t^{(n)} \quad \text{for} \quad n \in \{0, \ldots, N\}.
\]

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 \(D\) of \(Q_T\) is defined as

\[
D = \left(\mathcal{M}, \mathcal{E}, (x_K)_{K \in \mathcal{E}}, (t^{(n)})_{n \in \{0, \ldots, N+1\}}\right),
\]

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

\[
\text{size} (D) = \max \left\{ \text{size} (\mathcal{M}), t^{(n)} : n \in \{0, \ldots, N\} \right\}.
\]

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 \(D\) be an admissible discretization of \(Q_T\) in the sense of Definition 2.3. We prescribe the approximate initial conditions

\[
u^{(0)}_K = \frac{1}{m_K} \int_K u_0(x) \, dx \quad \text{and} \quad v^{(0)}_K = \frac{1}{m_K} \int_K v_0(x) \, dx,
\]

where \(K \in \mathcal{M}\), and associate to Problem \(P^k\) the finite volume scheme

\[
m_K \left( u^{(n+1)}_K - u^{(n)}_K \right) - t^{(n)} a \sum_{L \in \mathcal{N}_K} T_{K|L} \left( u^{(n+1)}_L - u^{(n+1)}_K \right) + t^{(n)} b \sum_{L \in \mathcal{N}_K} T_{K|L} \left( v^{(n+1)}_L - v^{(n+1)}_K \right) - \alpha m_K \left( u^{(n+1)}_K - v^{(n+1)}_K \right) = 0,
\]

\[
m_K \left( v^{(n+1)}_K - v^{(n)}_K \right) - t^{(n)} b \sum_{L \in \mathcal{N}_K} T_{K|L} \left( v^{(n+1)}_L - v^{(n+1)}_K \right) + t^{(n)} b \sum_{L \in \mathcal{N}_K} T_{K|L} \left( v^{(n+1)}_K - v^{(n+1)}_L \right) - \beta m_K \left( u^{(n+1)}_K - v^{(n+1)}_K \right) = 0.
\]

Note that (11) is a nonlinear system of equations in the unknowns

\[
(u^{(n+1)}_K, v^{(n+1)}_K)_{K \in \mathcal{M}, n \in \{0, \ldots, N\}}.
\]

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

\[
u_D(x, t) = u^{(n+1)}_K \quad \text{and} \quad v_D(x, t) = v^{(n+1)}_K.
\]

In the next section, we will prove the existence and uniqueness of the solution of the discrete problem (11), together with the initial values (10).

### 3 The approximate solution

In this section we prove the existence and uniqueness of the solution of the system (11). Let us start with a discrete version of the comparison principle.
Proposition 3.1. (Discrete comparison principle) We suppose that the hypotheses \( \mathcal{H} \) are satisfied. Let \( \mathcal{D} \) be a discretization as in Definition 27. Let \( (u_{K}^{(0)}, v_{K}^{(0)})_{K \in \mathcal{M}} \) and \( (\bar{u}_{K}^{(0)}, \bar{v}_{K}^{(0)})_{K \in \mathcal{M}} \) be given sequences of real values such that

\[
u_{K}^{(0)} \leq \bar{u}_{K}^{(0)} \quad \text{and} \quad v_{K}^{(0)} \leq \bar{v}_{K}^{(0)},
\]

for all \( K \in \mathcal{M} \). If the sequences \( (u_{K}^{(n)}, v_{K}^{(n)})_{K \in \mathcal{M}, n \in \{0, \ldots, N\}} \) and \( (\bar{u}_{K}^{(n)}, \bar{v}_{K}^{(n)})_{K \in \mathcal{M}, n \in \{0, \ldots, N\}} \) satisfy the equations (11) with the initial values \( (u_{K}^{(0)}, v_{K}^{(0)})_{K \in \mathcal{M}} \) and \( (\bar{u}_{K}^{(0)}, \bar{v}_{K}^{(0)})_{K \in \mathcal{M}} \), respectively, then for \( K \in \mathcal{M} \) and \( n \in \{0, \ldots, N\} \)

\[
u_{K}^{(n+1)} \leq \bar{u}_{K}^{(n+1)} \quad \text{and} \quad v_{K}^{(n+1)} \leq \bar{v}_{K}^{(n+1)}.
\]

(13)

Proof. We set \( \tilde{u}_{K}^{(n)} = u_{K}^{(n)} - \bar{u}_{K}^{(n)} \) and \( \tilde{v}_{K}^{(n)} = v_{K}^{(n)} - \bar{v}_{K}^{(n)} \) for all \( K \in \mathcal{M} \) and \( n \in \{0, \ldots, N+1\} \) and define

\[
\tilde{A}_{K}^{(n+1)} = r_{A}(u_{K}^{(n+1)}) - r_{A}(\bar{u}_{K}^{(n+1)}),
\]

\[
\tilde{B}_{K}^{(n+1)} = r_{B}(v_{K}^{(n+1)}) - r_{B}(\bar{v}_{K}^{(n+1)}),
\]

whenever \( \bar{u}_{K}^{(n+1)} \neq 0 \) (else \( \tilde{A}_{K}^{(n+1)} = 0 \)) or \( \bar{v}_{K}^{(n+1)} \neq 0 \) (else \( \tilde{B}_{K}^{(n+1)} = 0 \)). Since the functions \( r_{A} \) and \( r_{B} \) are monotone increasing, it follows that \( \tilde{A}_{K}^{(n+1)} \) and \( \tilde{B}_{K}^{(n+1)} \) are nonnegative. We then have, by subtracting the discrete equation (11) for \( \bar{v}_{K}^{(n+1)} \) and for \( \tilde{u}_{K}^{(n+1)} \),

\[
m_{K} \left( 1 + t_{\delta}^{(n)} \right) \left( \tilde{A}_{K}^{(n+1)} + \frac{a}{m_{K}} \sum_{L \in \mathcal{N}_{K}} T_{K|L} \right) \tilde{u}_{K}^{(n+1)}
\]

\[
= m_{K} \tilde{u}_{K}^{(n)} + t_{\delta}^{(n)} a \sum_{L \in \mathcal{N}_{K}} T_{K|L} \tilde{u}_{L}^{(n+1)}
\]

\[
+ t_{\delta}^{(n)} m_{K} \tilde{A}_{K}^{(n+1)} \left( r_{B}(v_{K}^{(n+1)}) - r_{B}(\bar{v}_{K}^{(n+1)}) \right),
\]

(14)

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

\[
m_{K} \left( 1 + t_{\delta}^{(n)} \right) \left( \tilde{A}_{K}^{(n+1)} + \frac{a}{m_{K}} \sum_{L \in \mathcal{N}_{K}} T_{K|L} \right) \tilde{u}_{K}^{(n+1)}
\]

\[
\leq m_{K} \tilde{u}_{K}^{(n)} + t_{\delta}^{(n)} a \sum_{L \in \mathcal{N}_{K}} T_{K|L} \tilde{u}_{L}^{(n+1)} + t_{\delta}^{(n)} m_{K} \tilde{A}_{K}^{(n+1)} \left( r_{B}(v_{K}^{(n+1)}) - r_{B}(\bar{v}_{K}^{(n+1)}) \right),
\]

(15)

where \( K \in \mathcal{M} \) and \( n \in \{0, \ldots, N\} \). Next we multiply the inequality (13) by indicator of the set where \( \bar{v}_{K}^{(n+1)} \) is nonnegative. Since the right-hand-side of (13) is nonnegative as well, we obtain, acting similarly for both components,

\[
m_{K} \left( 1 + t_{\delta}^{(n)} \right) \left( \tilde{A}_{K}^{(n+1)} + \frac{b}{m_{K}} \sum_{L \in \mathcal{N}_{K}} T_{K|L} \right) \left( \tilde{v}_{K}^{(n+1)} \right)^{+}
\]

\[
\leq m_{K} \tilde{v}_{K}^{(n)} + t_{\delta}^{(n)} b \sum_{L \in \mathcal{N}_{K}} T_{K|L} \left( \tilde{v}_{L}^{(n+1)} \right)^{+} + t_{\delta}^{(n)} m_{K} \tilde{A}_{K}^{(n+1)} \left( r_{A}(v_{K}^{(n+1)}) - r_{A}(\bar{v}_{K}^{(n+1)}) \right)^{+},
\]

(16)

Since

\[
\tilde{A}_{K}^{(n+1)} \left( \tilde{v}_{K}^{(n+1)} \right)^{+} = \left( r_{A}(u_{K}^{(n+1)}) - r_{A}(\bar{u}_{K}^{(n+1)}) \right)^{+}
\]

\[
\tilde{B}_{K}^{(n+1)} \left( \tilde{v}_{K}^{(n+1)} \right)^{+} = \left( r_{B}(v_{K}^{(n+1)}) - r_{B}(\bar{v}_{K}^{(n+1)}) \right)^{+}
\]

we add the first equation of (16) divided by \( \tilde{A} \) and the second equation of (16) divided by \( \tilde{B} \), which yields

\[
m_{K} \left( \frac{1}{\tilde{A}} + t_{\delta}^{(n)} \frac{a}{m_{K} \tilde{A}} \sum_{L \in \mathcal{N}_{K}} T_{K|L} \right) \left( \tilde{u}_{K}^{(n+1)} \right)^{+} + m_{K} \left( \frac{1}{\tilde{B}} + t_{\delta}^{(n)} \frac{b}{m_{K} \tilde{B}} \sum_{L \in \mathcal{N}_{K}} T_{K|L} \right) \left( \tilde{v}_{K}^{(n+1)} \right)^{+}
\]

\[
\leq m_{K} \frac{1}{\tilde{A}} \left( \tilde{u}_{K}^{(n)} \right)^{+} + t_{\delta}^{(n)} \frac{a}{\tilde{A}} \sum_{L \in \mathcal{N}_{K}} T_{K|L} \left( \tilde{u}_{L}^{(n+1)} \right)^{+} + m_{K} \frac{1}{\tilde{B}} \left( \tilde{v}_{K}^{(n)} \right)^{+} + t_{\delta}^{(n)} \frac{b}{\tilde{B}} \sum_{L \in \mathcal{N}_{K}} T_{K|L} \left( \tilde{v}_{L}^{(n+1)} \right)^{+},
\]

(17)
for \( K \in \mathcal{M} \) and \( n \in \{0, \ldots, N\} \). Let us note that

\[
\sum_{K \in \mathcal{M}} \sum_{L \in \mathcal{N}_K} T_{K|L}(\hat{u}_K^{(n+1)})^+ = \sum_{L \in \mathcal{M}} \sum_{K \in \mathcal{N}_L} T_{L|K}(\hat{v}_L^{(n+1)})^+
\]

\[
= \sum_{L \in \mathcal{M}} \sum_{K \in \mathcal{N}_L} T_{K|L}(\hat{u}_L^{(n+1)})^+ = \sum_{K \in \mathcal{M}} \sum_{L \in \mathcal{N}_K} T_{K|L}(\hat{v}_L^{(n+1)})^+.
\]

Summing the inequalities (17) over \( K \in \mathcal{M} \), we get

\[
\sum_{K \in \mathcal{M}} \left[ m_K \left( \frac{1}{\alpha} (\hat{u}_K^{(n+1)})^+ + \frac{1}{\beta} (\hat{v}_K^{(n+1)})^+ \right) \right] \leq \sum_{K \in \mathcal{M}} \left[ m_K \left( \frac{1}{\alpha} (\hat{u}_K^{(n)})^+ + \frac{1}{\beta} (\hat{v}_K^{(n)})^+ \right) \right],
\]

which therefore leads, by induction, to

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

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

Corollary 3.2 (Discrete contraction in \( L^1 \) property). With the notation from Proposition 7, we have that

\[
\sum_{K \in \mathcal{M}} m_K \left( \frac{|u_K^{(n)} - u_K^{(n+1)}|}{\alpha} + \frac{|v_K^{(n)} - v_K^{(n+1)}|}{\beta} \right) \leq \sum_{K \in \mathcal{M}} m_K \left( \frac{|u_K^{(n)} - u_K^{(n)}|}{\alpha} + \frac{|v_K^{(n)} - v_K^{(n)}|}{\beta} \right)
\]

for \( n \in \{0, \ldots, N\} \). In other words, the discrete counterpart of the \( L^1(\Omega) \)-contraction property for solutions of (11) (see e.g. [11]) is preserved by the numerical scheme (11).

Proof The proof directly follows from the proof of Proposition 5.1. Let us consider the term \( \hat{u}_K \). We multiply the equation (13) by \( \text{sgn} (\hat{u}_K^{(n+1)}) \). Then, the inequality \( x \leq |x| \) yields

\[
m_K \left( 1 + t_\delta^{(n)} \left( \frac{\bar{A}_K^{(n+1)}}{\bar{A}_K^{(n+1)}} + \frac{1}{\bar{A}_K^{(n+1)}} \right) \right) |u_K^{(n+1)}| \leq m_K |\hat{u}_K^{(n)}| + t_\delta^{(n)} \frac{1}{m_K} \sum_{L \in \mathcal{N}_K} T_{K|L} |\hat{u}_L^{(n+1)}| + t_\delta^{(n)} m_K \bar{A}_K^{(n+1)} r_B(v_K^{(n+1)}) - r_B(\hat{v}_K^{(n+1)}).
\]

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

\[
\bar{A}_K^{(n+1)} |\hat{u}_K^{(n+1)}| = r_A(u_K^{(n+1)}) - r_A(\hat{u}_K^{(n+1)}),
\]

\[
\bar{B}_K^{(n+1)} |\hat{v}_K^{(n+1)}| = r_B(v_K^{(n+1)}) - r_B(\hat{v}_K^{(n+1)}),
\]

which enable us to obtain the counterpart of the inequalities in (17) which we sum over \( K \in \mathcal{M} \), as in the proof of Proposition 5.1. This yields the result.

We now are in a position to prove a discrete \( L^\infty \) estimate for the approximate solution.

Theorem 3.3. Let \( D = (\mathcal{M}, P, E, (t_\delta^{(n)})_{n \in \{0, \ldots, N+1\}}) \) be an admissible discretization of \( Q_T \) in the sense of Definition 2.6. We suppose that the hypotheses \( \mathcal{H} \) are satisfied. Let \( (u_K^{(0)}, v_K^{(0)})_{K \in \mathcal{M}} \) be given by (11) and \( (u_K^{(n+1)}, v_K^{(n+1)}) \) satisfy (11) for \( K \in \mathcal{M} \) and \( n \in \{0, \ldots, N\} \). Then

\[
0 \leq u_K^{(n+1)} \leq U + \frac{\alpha}{\beta} V \quad \text{and} \quad 0 \leq v_K^{(n+1)} \leq V + \frac{\beta}{\alpha} U,
\]

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

Proof From Proposition 5.1 we immediately obtain that \( u_K^{(n+1)} \) and \( v_K^{(n+1)} \) are nonnegative for \( K \in \mathcal{M} \) and \( n \in \{0, \ldots, N\} \). 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 \( (\bar{u}_n)_{n \in \{0, \ldots, N+1\}} \), \( (\bar{v}_n)_{n \in \{0, \ldots, N+1\}} \) (we postpone for a moment the proof that they exist) such that

\[
\bar{u}_0 = U, \quad \bar{v}_0 = V
\]
and
\[
\begin{align*}
\dot{u}^{(n+1)} - \bar{u}^{(n)} &= \alpha \delta t^{(n)} \left( r_B(\bar{u}^{(n+1)}) - r_A(\bar{u}^{(n+1)}) \right), \\
\dot{v}^{(n+1)} - \bar{v}^{(n)} &= \beta \delta t^{(n)} \left( r_A(\bar{u}^{(n+1)}) - r_B(\bar{v}^{(n+1)}) \right),
\end{align*}
\]  
(19)
for \( n \in \{0, \ldots, N\} \). We note that the sequences \((\bar{u}^{(n+1)})_{n \in \{0, \ldots, N\}}\) and \((\bar{v}^{(n+1)})_{n \in \{0, \ldots, N\}}\) satisfy (11) with the initial data \(U, V\). Therefore they satisfy the comparison principle from Proposition 3.1 which yields
\[
0 \leq \bar{u}^{(n+1)} \quad \text{and} \quad 0 \leq \bar{v}^{(n+1)} \quad \text{for all} \quad n \in \{0, \ldots, N\}.
\]  
(20)
Adding up the first equation of (19) divided by \( \alpha \) and the second one divided by \( \beta \), we obtain
\[
\frac{\bar{u}^{(n+1)}}{\alpha} + \frac{\bar{v}^{(n+1)}}{\beta} = \frac{\bar{u}^{(n)}}{\alpha} + \frac{\bar{v}^{(n)}}{\beta} = \ldots = \frac{U}{\alpha} + \frac{V}{\beta}.
\]
We deduce from the previous equation and from (20) that
\[
0 \leq \frac{\bar{u}^{(n+1)}}{\alpha} \leq U + \frac{\alpha}{\beta} V \quad \text{and} \quad 0 \leq \frac{\bar{v}^{(n+1)}}{\beta} \leq V + \frac{\beta}{\alpha} U,
\]  
(21)
for \( n \in \{0, \ldots, N\} \).

In order to prove the existence of the sequences \((\bar{u}^{(n)})_{n \in \{0, \ldots, N+1\}}\) and \((\bar{v}^{(n)})_{n \in \{0, \ldots, N+1\}}\) we use the topological degree theory in finite dimensional spaces. The reader can find basic definitions as well as further informations about this powerful theory in Deimling [3]. An example of the application of this tool to the analysis of finite volume schemes can be found in Eymard, Gallouët, Ghilani and Herbin [5].

With \( \mathcal{F}, \mathcal{G} : \mathbb{R}^2 \to \mathbb{R}^2 \) defined as
\[
\begin{align*}
\mathcal{F}(\bar{u}, \bar{v}) &= (\bar{u}(n), \bar{v}(n)), \\
\mathcal{G}(\bar{u}, \bar{v}) &= \left( \gamma \delta t^{(n-1)} \left( r_A(\bar{u}^{(n)}) - r_B(\bar{v}^{(n)}) \right), \\
&\quad - \gamma \delta t^{(n-1)} \left( r_A(\bar{u}^{(n)}) - r_B(\bar{v}^{(n)}) \right) \right),
\end{align*}
\]
we rewrite the system (19) in the form
\[
\mathcal{F}(\bar{u}^{(n+1)}, \bar{v}^{(n+1)}) + \mathcal{G}(\bar{u}^{(n+1)}, \bar{v}^{(n+1)}) = y := (\bar{u}^{(n)}, \bar{v}^{(n)}).
\]
Moreover we see that setting \( \mathcal{O} = B(0, r) \subset \mathbb{R}^2 \) a ball centered at \((0, 0)\) with a radius
\[
r > \sqrt{(U + \frac{\alpha}{\beta} V)^2 + (V + \frac{\beta}{\alpha} U)^2}
\]
we fulfill all the assumptions of Theorem 3.1, page 16].
For the continuous function \( \mathcal{H} : [0, 1] \times B(0, r) \to \mathbb{R}^2 \) given by
\[
\mathcal{H}(\lambda, \bar{u}^{(n+1)}, \bar{v}^{(n+1)}) = \mathcal{F}(\bar{u}^{(n+1)}, \bar{v}^{(n+1)}) + \lambda \mathcal{G}(\bar{u}^{(n+1)}, \bar{v}^{(n+1)}),
\]
we see that
\[
d(\mathcal{F} + \lambda \mathcal{G}, B, (\bar{u}^{(n)}, \bar{v}^{(n)})) = d(\mathcal{H}(\lambda), B, (\bar{u}^{(n)}, \bar{v}^{(n)}))
\]
for all \( \lambda \in [0, 1] \) and \((\bar{u}^{(n)}), (\bar{v}^{(n)})\) such that \( 0 \leq \bar{g}^{(n)} \leq U - \frac{\alpha}{\beta} V \) and \( 0 \leq \bar{v}^{(n)} \leq V - \frac{\beta}{\alpha} U \) for \( n \in \{0, \ldots, N\} \).

On the other hand we deduce from [3] Theorem 3.1, page 16 (d1) that
\[
d(\mathcal{H}(0), B, (\bar{u}^{(n)}, \bar{v}^{(n)})) = 1.
\]  
(22)
In view of [3] Theorem 3.1, page 16 (d3) and (d4), (22) implies that the equality
\[
\mathcal{F}(\bar{u}^{(n+1)}, \bar{v}^{(n+1)}) + \mathcal{G}(\bar{u}^{(n+1)}, \bar{v}^{(n+1)}) = (\bar{u}^{(n)}, \bar{v}^{(n)})
\]
has a solution or, in other words, that there exists a solution of (19). The uniqueness of this solution immediately follows from Proposition 3.1.
We can prove in the same way the existence and uniqueness of the solution of the system (11). Indeed, we rewrite (11) in the form

\[ \tilde{F}\left((u^{(n+1)}_K)_{K \in \mathcal{M}},(v^{(n+1)}_K)_{K \in \mathcal{M}}\right) + \tilde{G}\left((u^{(n)}_K)_{K \in \mathcal{M}},(v^{(n)}_K)_{K \in \mathcal{M}}\right) = \left((u^{(n)}_K)_{K \in \mathcal{M}},(v^{(n)}_K)_{K \in \mathcal{M}}\right), \]  

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

\[ \tilde{F}\left((u^{(n)}_K)_{K \in \mathcal{M}},(v^{(n)}_K)_{K \in \mathcal{M}}\right) = \left((u^{(n)}_K)_{K \in \mathcal{M}},(v^{(n)}_K)_{K \in \mathcal{M}}\right), \]

\[ \tilde{G}\left((u^{(n)}_K)_{K \in \mathcal{M}},(v^{(n)}_K)_{K \in \mathcal{M}}\right) = (W_1,W_2), \]

where

\[ W_1 = -\frac{\delta(n)}{m_K} \sum_{L \in N_K} T_{K|L}(u^{(n)}_L - u^{(n)}_K) + \delta(n-1) \hat{a}(r_A(u^{(n)}_K) - r_B(v^{(n)}_K)), \]

and where

\[ W_2 = -\frac{\delta(n)}{m_K} \sum_{L \in N_K} T_{K|L}(v^{(n)}_L - v^{(n)}_K) - \delta(n-1) \hat{b}(r_A(u^{(n)}_K) - r_B(v^{(n)}_K)). \]

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

\[ R > \sqrt{\Theta(U + \frac{\delta}{\alpha}V)^2 + \Theta(V + \frac{\delta}{\alpha}U)^2}. \]

Since \( \Theta > 1 \), we deduce from the discrete \( L^\infty(Q_T) \) estimate of Theorem 3.3 that the equation (23) does not have any solutions on \( \partial\tilde{\Omega} \). Applying again [3, Theorem 3.1, page 16] with \( \tilde{H}(\lambda) = \tilde{F} + \lambda\tilde{G} \) and \( \lambda \in [0,1] \) completes the proof of the following result.

**Theorem 3.4.** We suppose that the hypotheses \( \mathcal{H} \) are satisfied. Let \( \mathcal{D} \) be a discretization as in Definition 2.3. Let \((u_0^K,v_0^K)_{K \in \mathcal{M}} \) be given by (10). Then there exists one and only one sequence \((u^{(n+1)}_K,v^{(n+1)}_K)_{K \in \mathcal{M}}, n \in \{0,\ldots,N\}\), which satisfies (11), with the initial condition \((u^{(0)}_K,v^{(0)}_K)_{K \in \mathcal{M}}\). \( \blacksquare \)

### 4 Convergence proof with \( k \) fixed

We begin with the discrete version of \( L^2(Q_T) \) estimates of the gradient of the approximate solutions.

**Proposition 4.1.** We suppose that the hypotheses \( \mathcal{H} \) are satisfied. Let \( \mathcal{D} \) be a discretization as in Definition 2.3. Let (10) and (11) give the sequences \((u^{(0)}_K,v^{(0)}_K)_{K \in \mathcal{M}} \) and \((u^{(n+1)}_K,v^{(n+1)}_K)_{K \in \mathcal{M}}, n \in \{0,\ldots,N\}\), respectively. Then, there exists a constant \( C_k > 0 \), which does not depend on \( \mathcal{D} \), but which depend on all the data of the continuous Problem \( \mathcal{P}^k \) (namely, the constants \( \alpha, \beta, U, V \) including \( k \) and the functions \( r_A, r_B \)), such that

\[ \frac{1}{\delta} \sum_{K \in \mathcal{M}} m_K \left(u^{(n+1)}_K\right)^2 - \frac{1}{\delta} \sum_{K \in \mathcal{M}} m_K \left(u^{(0)}_K\right)^2 + \delta \sum_{n=0}^N \sum_{(K,L) \in \mathcal{E}} T_{K|L} \left(u^{(n+1)}_L - u^{(n+1)}_K\right)^2 \leq C_k \]

(24)

and

\[ \frac{1}{\delta} \sum_{K \in \mathcal{M}} m_K \left(v^{(n+1)}_K\right)^2 - \frac{1}{\delta} \sum_{K \in \mathcal{M}} m_K \left(v^{(0)}_K\right)^2 + \delta \sum_{n=0}^N \sum_{(K,L) \in \mathcal{E}} T_{K|L} \left(v^{(n+1)}_L - v^{(n+1)}_K\right)^2 \leq C_k \]

(25)

**Proof** For the sake of simplicity we only present the proof for the \( u \)-component. We multiply the first equation in the finite volume scheme (11) by \( u^{(n+1)}_K \) and sum the result over all \( K \in \mathcal{M} \) and over all \( n \in \{0,\ldots,N\} \) to obtain

\[ S_1 + S_2 + S_3 = 0, \]

(26)
where

\[ S_1 = \sum_{n=0}^{N} \sum_{K \in \mathcal{M}} m_K \left( (u_{K}^{(n+1)} - u_{K}^{(n)}) u_{K}^{(n+1)} \right), \]

\[ S_2 = -a \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K \in \mathcal{M}} \sum_{L \in \mathcal{N}_K} T_{K|L} \left( (u_{L}^{(n+1)} - u_{K}^{(n+1)}) u_{K}^{(n+1)} \right), \]

\[ S_3 = \alpha \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K \in \mathcal{M}} \left( r_A (u_{K}^{(n+1)}) - r_B (u_{K}^{(n+1)}) \right) u_{K}^{(n+1)}. \]

Since

\[ \left( u_{K}^{(n+1)} \right)^2 - u_{K}^{(n)} u_{K}^{(n+1)} = \frac{1}{2} \left( u_{K}^{(n+1)} \right)^2 - \frac{1}{2} \left( u_{K}^{(n)} \right)^2 + \frac{1}{2} \left( u_{K}^{(n+1)} - u_{K}^{(n)} \right)^2, \]

we deduce that

\[ S_1 = \frac{1}{2} \sum_{n=0}^{N} \sum_{K \in \mathcal{M}} m_K \left( \left( u_{K}^{(n+1)} \right)^2 - \left( u_{K}^{(n)} \right)^2 \right) + \frac{1}{2} \sum_{n=0}^{N} \sum_{K \in \mathcal{M}} m_K \left( u_{K}^{(n+1)} - u_{K}^{(n)} \right)^2 \geq \frac{1}{2} \sum_{n=0}^{N} \sum_{K \in \mathcal{M}} m_K \left( \left( u_{K}^{(n+1)} \right)^2 - \left( u_{K}^{(n)} \right)^2 \right), \tag{27} \]

All the terms in the sum on \( n \) on the right hand side of (27) simplify except for the first and the last ones. We have that

\[ S_1 \geq \frac{1}{2} \sum_{K \in \mathcal{M}} m_K \left( u_{K}^{(N+1)} \right)^2 - \frac{1}{2} \sum_{K \in \mathcal{M}} m_K \left( u_{K}^{(0)} \right)^2. \tag{28} \]

We can perform a discrete integration by parts to obtain

\[ S_2 = a \sum_{n=0}^{N} t_\delta^{(n)} \sum_{(K,L) \in \mathcal{E}} T_{K|L} \left( u_{L}^{(n+1)} - u_{K}^{(n+1)} \right)^2. \tag{29} \]

Finally we use the hypothesis \( \mathcal{H}4 \) and the inequalities in (12) to estimate the last term, namely

\[- S_3 \leq \tilde{\alpha} \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K \in \mathcal{M}} m_K \left( r_A (U + \frac{\alpha}{\beta} V) + r_B (V + \frac{\beta}{\alpha} U) \right) (U + \frac{\alpha}{\beta} V) \]

\[ \leq \alpha k C \sum_{n=0}^{N} t_\delta^{(n)} \sum_{K \in \mathcal{M}} m_K = \alpha k C |\Omega| T, \tag{30} \]

with some positive constant \( C \).

Identities (26) and (29) together with the inequalities (28) and (30) immediately give (24). Since the argument in the case of the \( r \)-component is similar, we omit the proof. \( \blacksquare \)

### 4.1 Space and time translates of approximate solutions

We now turn to the space 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 and the next subsection together with the technical Proposition \[7,2\] will imply the relative compactness of the sequence of approximate solutions.

**Proposition 4.2** (Space translates estimates). We assume that

1. \( \mathcal{D} = \left( \mathcal{M}, \mathcal{E}, (x_K)_{K \in \mathcal{M}}, \left( t_\delta^{(n)} \right)_{n \in \{0, \ldots, N+1\}} \right) \) is an admissible discretization of \( Q_T \) in the sense of Definition \[26\].
2. the hypotheses \( \mathcal{H} \) and assumptions \[26\] are satisfied,
3. the functions \( (u_{\mathcal{D}} \text{ and } v_{\mathcal{D}}) \) are derived from the scheme (10) – (11) and given by the formulas (12).
Then there exists a positive constant $C_k$, which does not depend on $D$, but depends on all the data of the continuous Problem $P^k$, including $k$, such that

$$
\int_0^T \int_{\Omega_k} (u_D(x+\xi,t) - u_D(x,t))^2 \, dx \, dt \leq C_k(|\xi| (2 \text{size}(D) + |\xi|),
$$

(31)

and

$$
\int_0^T \int_{\Omega_k} (v_D(x+\xi,t) - v_D(x,t))^2 \, dx \, dt \leq C_k(|\xi| (2 \text{size}(D) + |\xi|),
$$

(32)

for all $\xi \in \mathbb{R}^d$ and for $\Omega_k$ defined as in Proposition 7.2.

**Proof** Inequalities (31) and (32) follow from the estimates (24) and (25), respectively. We refer to [6, Lemma 3.3] for a details.

**Proposition 4.3** (Time translates estimates). Let the assumptions of Proposition 4.2 be satisfied. Then, there exists some constant $C_k > 0$, which does not depend on $D$, but which depend on all the data including $k$, such that

$$
\int_{\Omega \times (0, T - \tau)} (u_D(x,t+\tau) - u_D(x,t))^2 \, dx \, dt \leq C_k (\text{size}(D) + \tau)
$$

(33)

and

$$
\int_{\Omega \times (0, T - \tau)} (v_D(x,t+\tau) - v_D(x,t))^2 \, dx \, dt \leq C_k (\text{size}(D) + \tau),
$$

(34)

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

**Proof** In order to apply Lemma 24 (see appendix), we follow the same steps as in [8, Lemma 5.5]. The only difference appear in the nonlinear part of the equations. However, these can be easily estimated using the regularity properties of functions $r_A(\cdot)$ and $r_B(\cdot)$, as well as $L^\infty$ estimates 15 in Theorem 3.3.

### 4.2 Convergence proof

In this section, we state convergence results with $k$ fixed. This differs from next section where we will introduce additional hypotheses about the nonlinear reaction terms and obtain convergence results which permit us to pass to the limit as $k \to \infty$.

**Theorem 4.4.** We suppose that the hypotheses $H$ are satisfied. Let $(u_D, v_D)$ be the approximate solution defined by (10), (14) and (18). There exist a pair of functions $(u^k, v^k)$ and a sequence $(u_{D^m}, v_{D^m})_{m \in \mathbb{N}}$ of $(u_D, v_D)$ such that

$$
(u_{D^m}, v_{D^m})_{m \in \mathbb{N}} \text{ converges to } (u^k, v^k) \in (L^2(0, T; H^1(\Omega)))^2
$$

strongly in $L^2(Q_T)$ as $\text{size}(D_m)$ tends to zero. The function pair $(u^k, v^k)$ is a weak solution of Problem $P^k$ in the sense of Definition 7.7.

Since Problem $P^k$ is a uniformly parabolic system, $(u^k, v^k)$ must coincide with the unique classical solution of Problem $P^k$. This immediately yields the following result.

**Corollary 4.5.** The pair $(u_D, v_D)$ converges to the unique classical solution $(u^k, v^k)$ of Problem $P^k$ as $\text{size}(D)$ tends to zero.

**Proof of Theorem 4.4** In view of the estimates (31), (32) and Proposition 7.2 which is a consequence of the Fréchet–Kolmogorov Theorem 2 Theorem IV.25, page 72], we deduce the relative compactness of the set $(u_D)$ so that there exists a sequence of $(u_{D^m})_{m=1}^\infty$ and a function $U_k$, such that $u_{D^m} \rightharpoonup U_k$ strongly in $L^2(Q_T)$ and weakly in $L^2(0, T; H^1(\Omega))$, as $m \to \infty$.

The same conclusion holds for the $v$-component. Indeed, the inequalities (32) and (33) permit to apply the compactness result in Proposition 7.2 for the sequence $(v_{D^m})_{m=1}^\infty$. There exists a function $V_k$ such that $v_{D^m} \rightharpoonup V_k$ strongly in $L^2(Q_T)$ and weakly in $L^2(0, T; H^1(\Omega))$, as $m \to \infty$.

Next we show that $(U_k, V_k)$ is a weak solution of Problem $P^k$, in the sense of Definition 11. Since the proof for the $v$-component is similar, we only present here the detailed proof in case of the $u$-component. Let $\psi \in \Psi$, where $\Psi$ is the class of test functions from Definition 11. We multiply the first equation of 11 by $\psi(x_K, t(\alpha))$, where $\psi \in \Psi$. Then we sum over all $K \in M$ and $n \in \{0 \ldots N - 1\}$ to obtain

$$
T_{1m}^u - T_{2m}^u + T_{3m}^u = 0,
$$

10
where
\[
\begin{align*}
T_{1m}^u &= \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} m_K (u_K^{(n+1)} - u_K^{(n)}) \psi(x_K, t^{(n)}), \\
T_{2m}^u &= a \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \sum_{L \in \mathcal{N}_K} T_{KL} (u_L^{(n+1)} - u_K^{(n+1)}) \psi(x_K, t^{(n+1)}), \\
T_{3m}^u &= \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} m_K \hat{a} \left( r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}) \right) \psi(x_K, t^{(n)}).
\end{align*}
\]

The complete proof, that
\[
\lim_{m \to \infty} T_{1m}^u = - \int_\Omega u_0(x) \psi(x, 0) \, dx - \int_0^T \int_\Omega u_k(x, t) \psi(x, t) \, dx \, dt
\]
and
\[
\lim_{m \to \infty} T_{2m}^u = -a \int_0^T \int_\Omega u_k(x, t) \Delta \psi(x, t) \, dx \, dt,
\]
can by found in [8] Lemma 5.5). Let us focus on the proof that
\[
\lim_{m \to \infty} T_{3m}^u = ak \int_0^T \int_\Omega (r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k)) \psi(x, t) \, dx \, dt.
\]

We write
\[
\hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} m_K \left( r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}) \right) \psi(x_K, t^{(n)})
\]
\[
= \hat{a} \int_0^T \int_\Omega \psi(x, t) (r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k)) \, dx \, dt
\]
\[
= \hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_{t^{(n+1)}}^{t^{(n+1)}} \int_K \left( r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}) \right) \psi(x_K, t^{(n)}) \, dx \, dt
\]
\[
= \hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_{t^{(n+1)}}^{t^{(n+1)}} \int_K \psi(x, t) (r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k)) \, dx \, dt
\]
\[
= \hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_{t^{(n+1)}}^{t^{(n+1)}} \int_K \psi(x, t) (r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k)) \, dx \, dt.
\]

Thanks to the regularity of the function \( \psi \), the last sum above converges to zero. Moreover,
\[
\hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_{t^{(n+1)}}^{t^{(n+1)}} \int_K \left( r_A(u_K^{(n+1)}) - r_B(v_K^{(n+1)}) \right) \psi(x_K, t^{(n)}) \, dx \, dt
\]
\[
= \hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_{t^{(n+1)}}^{t^{(n+1)}} \int_K \psi(x, t) (r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k)) \, dx \, dt
\]
\[
= \hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_{t^{(n+1)}}^{t^{(n+1)}} \int_K \psi(x, t) (r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k)) \, dx \, dt
\]
\[
= \hat{a} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_{t^{(n+1)}}^{t^{(n+1)}} \int_K \psi(x, t) (r_A(\mathcal{U}_k) - r_B(\mathcal{V}_k)) \, dx \, dt.
\]

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
The first term of above product converges to zero, as \( m \to \infty \), since \( \psi(x,t) \) 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 \( n \in \{0, \ldots, N\} \). The last two terms in (35) are similar and we show how the proof goes with the first one. Indeed,

\[
\hat{\alpha} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} T_{K,L}(u^{(n+1)}_L - u^{(n+1)}_K)^2 + \sum_{(K,L) \in \mathcal{E}} T_{K,L}(v^{(n+1)}_L - v^{(n+1)}_K)^2 \leq C
\]

and

\[
k \sum_{n=0}^{N} \sum_{K \in \mathcal{M}} m_K (r_A(u_k^{(n+1)}) - r_B(v_k^{(n+1)}))^2 \leq C.
\]

The proof of (35) yields

\[
\hat{\alpha} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_K |\psi(x,t)| |r_A(u_k^{(n+1)}) - r_A(u_k)| \, dx \, dt
\]

The first term of the above product is bounded. The second one converges to zero since \( \hat{\alpha} \) 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 \( n \in \{0, \ldots, N\} \). The last two terms in (35) are similar and we show how the proof goes with the first one. Indeed,

\[
\hat{\alpha} \sum_{n=0}^{N-1} \sum_{K \in \mathcal{M}} \int_K |\psi(x,t)| |r_A(u_k^{(n+1)}) - r_A(u_k)| \, dx \, dt
\]

The \( L^\infty \) norm of the function \( r_A(x) \) is taken over the finite interval \([0, U + \frac{\hat{\alpha}}{\hat{\alpha}} V]\). Because \( r_A(x) \) is of class \( C^1(\mathcal{R}) \) the first term of the above product is bounded. The second one converges to zero since \( u_{D,m} \to u_k \) as \( m \to \infty \) in \( L^2(\mathcal{Q}_T) \).

The case that \( k \) tends to infinity

In order to prove the convergence of the finite volume scheme when size (\( D \)) tends to zero and \( k \) tends to infinity, we impose some additional conditions on the nonlinear terms \( r_A(x) \) and \( r_B(x) \). At first we prove a counterpart of Proposition 3.3.

**Proposition 5.1.** Let us assume hypotheses \( \mathcal{H} \). Moreover, we assume that the functions \( r_A(x), \ r_B(x) \) satisfy

\[
r_A \in C^1(\mathcal{R}), \quad r_A(s) > 0 \quad \text{on} \quad (0, +\infty),
\]

\[
r_A(0) = 0, \quad \text{and} \quad \lim_{s \to 0^+} \frac{sr_A'(s)}{r_A(s)} < \infty,
\]

where \( \kappa \in \{A, B\} \). Let \( \mathcal{D} = (\mathcal{M}, \mathcal{E}, (x_K)_{K \in \mathcal{T}}, (t_n)_{n \in \{0, \ldots, N+1\}}) \) be an admissible discretization of \( \mathcal{Q}_T \) in the sense of Definition 2.2, and the sequences \((u_0^0, v_0^0)_{K \in \mathcal{M}}\) and \((u_0^{n+1}, v_0^{n+1})_{K \in \mathcal{M}}, \ n \in \{0, \ldots, N\}\) are given by (10) and (11), respectively. Then, there exists some positive constant \( C \) which is independent of the discretization \( \mathcal{D} \) and of the reaction rate \( k \), such that

\[
\sum_{n=0}^{N} t_n^3 \left( \sum_{(K,L) \in \mathcal{E}} T_{K,L}(u_L^{(n+1)} - u_L^{(n+1)})^2 + \sum_{(K,L) \in \mathcal{E}} T_{K,L}(v_L^{(n+1)} - v_L^{(n+1)})^2 \right) \leq C
\]

and

\[
k \sum_{n=0}^{N} t_n^3 \sum_{K \in \mathcal{M}} m_K (r_A(u_k^{(n+1)}) - r_B(v_k^{(n+1)}))^2 \leq C.
\]
Remark 5.2. Observe that the condition (39) holds, for example, in the case that the rate functions $r_A(s)$ and $r_B(s)$ behave like $s^\gamma$, for some positive $\gamma$, whenever $s \to 0^+$.

Proof of Proposition 5.1. Let $(a, b) \in \mathbb{R}^+$ be such that $r_A(a) = r_B(b)$. We define two functions

$$V_A(s) = \frac{1}{\alpha} \left( s \ln \frac{r_A(s)}{r_A(a)} + \int_a^s \frac{\sigma r_A'(\sigma)}{r_A(\sigma)} \, d\sigma \right),$$

$$V_B(s) = \frac{1}{\beta} \left( s \ln \frac{r_B(s)}{r_B(b)} + \int_a^b \frac{\sigma r_B'(\sigma)}{r_B(\sigma)} \, d\sigma \right),$$

which are continuous on $\mathbb{R}^+$ because of hypotheses $\mathcal{H}$ and the assumptions (36). We can extend these functions to also be continuous at $s = 0$. To do so for the function $V_A(s)$ we check that the hypotheses (36) give the integrability of $\frac{\sigma r_A'(\sigma)}{r_A(\sigma)}$ on the interval $[0, a]$ and we pass to the limit

$$\lim_{s \to 0^+} V_A(s) \geq \frac{1}{\alpha} \int_0^a \frac{\sigma r_A'(\sigma)}{r_A(\sigma)} \, d\sigma - \lim_{s \to 0^+} \frac{s}{\alpha} \frac{r_A'(s)}{r_A(s)} < \infty,$$

where we have applied de l’Hospital theorem as formulated in [13, Theorem 2, p. 174].

For a given $\varepsilon \in (0, 1)$ and $n \in \{0, \ldots, N\}$ we consider

$$A^{(n+1)}(\varepsilon) = \sum_{K \in M} m_K \left( V_A(u_K^{(n+1)} + \varepsilon) - V_A(u_K^{(n)} + \varepsilon) \right).$$

Since $V_A'(s) = \frac{r_A'(s)}{\alpha r_A(s)} > 0$ for all $s \in \mathbb{R}^+$ we deduce that

$$V_A(u_K^{(n)} + \varepsilon) - V_A(u_K^{(n+1)} + \varepsilon) = (u_K^{(n)} - u_K^{(n+1)}) V_A'(u_K^{(n+1)} + \varepsilon) + \frac{1}{2} (u_K^{(n)} - u_K^{(n+1)})^2 V_A''(s) \geq (u_K^{(n)} - u_K^{(n+1)}) V_A'(u_K^{(n+1)} + \varepsilon).$$

As a consequence

$$A^{(n+1)}(\varepsilon) \leq \sum_{K \in M} m_K (u_K^{(n+1)} - u_K^{(n)}) V_A'(u_K^{(n+1)} + \varepsilon).$$

We substitute $m_K(u_K^{(n+1)} - u_K^{(n)})$ from the scheme (11), which yields

$$A^{(n+1)}(\varepsilon) \leq A_1^{(n+1)}(\varepsilon) + A_2^{(n+1)}(\varepsilon),$$

with

$$A_1^{(n+1)}(\varepsilon) = -\delta_\varepsilon (\frac{a}{4}) \sum_{(K,L) \in \mathcal{E}} T_{K|L} (u_L^{(n+1)} - u_K^{(n+1)}) \left( V_A'(u_K^{(n+1)} + \varepsilon) - V_A'(u_K^{(n+1)} + \varepsilon) \right)$$

and

$$A_2^{(n+1)}(\varepsilon) = -\delta_\varepsilon (\frac{a}{4}) \sum_{K \in M} m_K \left( V_A'(u_K^{(n+1)} + \varepsilon) - V_A'(u_K^{(n+1)} + \varepsilon) \right) \left( r_A(u_K^{(n+1)} + \varepsilon) - r_B(u_K^{(n+1)} + \varepsilon) \right).$$

Since there exists some constant $C > 0$ such that $V_A'(s) \geq C$ for all $s \in [0, U + \frac{1}{2} V]$ we can use the $L^\infty$ bound [13] and the mean value theorem to obtain

$$A_1^{(n+1)}(\varepsilon) \leq -\delta_\varepsilon (\frac{a}{4}) \sum_{(K,L) \in \mathcal{E}} T_{K|L} (u_L^{(n+1)} - u_K^{(n+1)})^2.$$ 

Following the same steps for the function

$$B^{(n+1)}(\varepsilon) = \sum_{K \in M} m_K \left( V_B(u_K^{(n+1)} + \varepsilon) - V_B(u_K^{(n)} + \varepsilon) \right),$$

we arrive at

$$A^{(n+1)}(\varepsilon) + B^{(n+1)}(\varepsilon) \leq -C^{(n+1)} - D^{(n+1)}(\varepsilon),$$

with

$$C^{(n+1)} = \delta_\varepsilon (\frac{a}{4}) \sum_{(K,L) \in \mathcal{E}} T_{K|L} (u_L^{(n+1)} - u_K^{(n+1)})^2 + \frac{a}{4} \sum_{(K,L) \in \mathcal{E}} T_{K|L} (u_K^{(n+1)} - u_K^{(n+1)})^2,$$

and

$$D^{(n+1)} = \alpha_\varepsilon (\frac{b}{4}) \sum_{(K,L) \in \mathcal{E}} T_{K|L} (u_L^{(n+1)} - u_K^{(n+1)})^2 + \frac{b}{4} \sum_{(K,L) \in \mathcal{E}} T_{K|L} (u_K^{(n+1)} - u_K^{(n+1)})^2,$$
Let $\alpha V$ where we used that $r$ exist in view of Theorem 3.3 and regularity of the functions The assumptions (36) and Lemma 7.3 in the appendix, imply that for all $\delta$ small enough, we have:

$$D^{(n+1)}(\varepsilon) = t_3^{(n)} k \sum_{K \in \mathcal{M}} m_K \left( r_A(u^{(n+1)}_K) - r_B(v^{(n+1)}_K) \right) \left( \ln r_A(u^{(n+1)}_K) + \varepsilon \right) - \ln r_B(v^{(n+1)}_K) + \varepsilon).$$

where we used that $\alpha V_A(s) = \ln \frac{r_A(s)}{r_A(a)}$ and that $\beta V_B(s) = \ln \frac{r_B(s)}{r_B(b)}$.

Let

$$D_1^{(n+1)}(\varepsilon) = t_3^{(n)} k \sum_{K \in \mathcal{M}} m_K \left( r_A(u^{(n+1)}_K) + \varepsilon \right) - \ln r_B(v^{(n+1)}_K) + \varepsilon).$$

Since the inequality

$$(c - d)(\ln c - \ln d) \geq \frac{(c - d)^2}{c + d}$$

holds for all $(c, d) \in (0, U + \frac{\Omega}{\beta} V + 1) \times (0, V + \frac{\beta}{\alpha} U + 1)$, then

$$D_1^{(n+1)}(\varepsilon) \geq t_3^{(n)} k \frac{C_b}{C_b} \sum_{K \in \mathcal{M}} m_K \left( r_A(u^{(n+1)}_K) + \varepsilon \right) - \ln r_B(v^{(n+1)}_K) + \varepsilon)^2,$$

where $C_b$ is an upper bound for $r_A(c) + r_B(d)$ with $(c, d) \in (0, U + \frac{\Omega}{\beta} V + 1) \times (0, V + \frac{\beta}{\alpha} U + 1)$. Such bounds exist in view of Theorem 3.3 and regularity of the functions $r_A(x)$ and $r_B(x)$. Let us define

$$E^{(n+1)}(\varepsilon) := t_3^{(n)} k \frac{C_b}{C_b} \sum_{K \in \mathcal{M}} m_K \left( r_A(u^{(n+1)}_K) + \varepsilon \right) - \ln r_B(v^{(n+1)}_K) + \varepsilon)^2.$$

The assumptions (36) and Lemma 7.3 in the appendix, imply that for all $K \in \mathcal{M}$ and $\varepsilon > 0$ small enough, there exist constants $C_1, C_2$ such that

$$|r_A(u^{(n+1)}_K) - r_A(u^{(n+1)}_K)| \leq C_1 \varepsilon, \quad |r_B(v^{(n+1)}_K) - r_B(v^{(n+1)}_K)| \leq C_2 \varepsilon,$$

and

$$|\ln r_A(u^{(n+1)}_K)| \leq C_2(|\ln \varepsilon| + 1), \quad |\ln r_B(v^{(n+1)}_K)| \leq C_2(|\ln \varepsilon| + 1).$$

Then

$$-D^{(n+1)} \leq C\varepsilon|K|(|\ln \varepsilon| + 1) - D^{(n+1)}(\varepsilon),$$

for some positive constant $C$. As a consequence

$$A^{(n+1)}(\varepsilon) + B^{(n+1)}(\varepsilon) \leq - C^{(n+1)} + D^{(n+1)}(\varepsilon)$$

$$- C^{(n+1)} - E^{(n+1)}(\varepsilon) + C\varepsilon|K|(|\ln \varepsilon| + 1).$$

Now it is possible to pass to the limit in (36). We obtain

$$A^{(n+1)}(0) + B^{(n+1)}(0) \leq - C^{(n+1)} - E^{(n+1)}(0).$$

which is

$$\sum_{K \in \mathcal{M}} m_K \left( V_A(u^{(n+1)}_K) - V_A(u^{(n)}_K) \right) + \sum_{K \in \mathcal{M}} m_K \left( V_B(v^{(n+1)}_K) - V_B(v^{(n)}_K) \right) + t_3^{(n)} \frac{C_a}{C_a} \sum_{(K,L) \in \mathcal{E}} T_{K,L}(u^{(n+1)}_L - u^{(n+1)}_K)^2 + t_3^{(n)} \frac{C_b}{C_b} \sum_{(K,L) \in \mathcal{E}} T_{K,L}(v^{(n+1)}_L - v^{(n+1)}_K)^2 + t_3^{(n)} \frac{C_b}{C_b} \sum_{K \in \mathcal{M}} m_K \left( r_A(u^{(n+1)}_K) - r_B(v^{(n+1)}_K) \right)^2 \leq 0.$$
Since $V_A(s)$ and $V_B(s)$ are nonnegative and continuous on $[0, +\infty)$, and since $u^{(n+1)}_K$, $v^{(n+1)}_K$ are nonnegative and bounded for all $K \in \mathcal{M}$ and $n \in \{0, \ldots, N\}$, this concludes the proof. ■

5.1 Space and time translates of the approximate solutions

Since we have already presented the general methods in section 4 we only give here some essential ideas, leaving out the details of the proofs.

We begin with a counterpart of Proposition 4.2.

Proposition 5.3 (Space translates estimates). Let us assume that

1. $\left(\mathcal{M}, \mathcal{E}, (x_K)_{K \in \mathcal{T}}, (t^{(n)})_{n \in \{0, \ldots, N+1\}}\right)$ is an admissible discretization of $Q_T$ in the sense of Definition 2.3,

2. hypotheses $\mathcal{H}$ and assumptions (36) are satisfied,

3. functions $(u_D$ and $v_D)$ are derived from the scheme (10)–(11) and given by the formulas (12).

Then there exists a positive constant $C$ which is independent of $D$ and $k$, such that

$$
\int_0^T \int_{\Omega} (u_D(x + \xi, t) - u_D(x, t))^2 \, dx \, dt \leq C |\xi| (2 \text{size}(D) + |\xi|),
$$

(40)

and

$$
\int_0^T \int_{\Omega} (v_D(x + \xi, t) - v_D(x, t))^2 \, dx \, dt \leq C |\xi| (2 \text{size}(D) + |\xi|),
$$

(41)

for all $\xi \in \mathbb{R}^d$ and for $\Omega_\xi$ defined as in Proposition 7.2.

Proof As it was in the proof of Proposition 4.2 we refer to [6]Lemma 3.3 for a complete proof. The only difference is to apply the result of Proposition 5.1 instead of that of Proposition 4.1. ■

Let us now prove an analogue of Proposition 4.3

Lemma 5.4 (Time translates estimate). Let the assumptions 1. 2. and 3. of Lemma 5.3 be satisfied. Set $w_D = \frac{1}{\alpha} u_D + \frac{1}{\beta} v_D$. Then there exists a positive constant $C$ which is independent of $D$ and $k$, such that

$$
\int_{\Omega \times (0,T-\tau)} (w_D(x,t+\tau) - w_D(x,t))^2 \, dx \, dt \leq C (\text{size}(D) + \tau),
$$

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

Proof The proof is similar to that of Proposition 4.3. We present below the essential steps of the argument.

We define

$$
A(t) := \int_{\Omega} (w_D(x, t + \tau) - w_D(x, t))^2 \, dx,
$$

which can be easily transformed into

$$
A(t) = \sum_{K \in \mathcal{M}} m_K (w^{(n(t+\tau)+1)}_K - w^{(n(t)+1)}_K)^2
$$

$$
= \sum_{K \in \mathcal{M}} \left( w^{(n(t+\tau)+1)}_K - w^{(n(t)+1)}_K \right) \sum_{n=n(t)+1}^{n(t+\tau)} m_K (w^{(n+1)}_K - w^{(n)}_K).
$$

Since

$$
w^{(n+1)}_K - w^{(n)}_K = \frac{1}{\alpha} (u^{(n+1)}_K - u^{(n)}_K) + \frac{1}{\beta} (v^{(n+1)}_K - v^{(n)}_K),
$$

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we can apply discrete integration by parts in the scheme (11) to obtain
\[
\mathcal{A}(t) = \frac{a}{\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^n \sum_{(K,L) \in \mathcal{E}} T_{K|L}(u_L^{(n+1)} - u_K^{(n+1)}) (w_K^{(n(t+\tau)+1)} - w_L^{(n(t+\tau)+1)})
\]
\[
+ \frac{a}{\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^n \sum_{(K,L) \in \mathcal{E}} T_{K|L}(w_L^{(n(t)+1)} - w_K^{(n(t)+1)}) (w_K^{(n(t+\tau)+1)} - w_L^{(n(t+\tau)+1)})
\]
\[
\frac{b}{\beta} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^n \sum_{(K,L) \in \mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)}) (w_K^{(n(t+\tau)+1)} - w_L^{(n(t+\tau)+1)})
\]
\[
+ \frac{b}{\beta} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^n \sum_{(K,L) \in \mathcal{E}} T_{K|L}(v_L^{(n+1)} - v_K^{(n+1)}) (w_K^{(n(t)+1)} - w_L^{(n(t)+1)}).
\]

Next we estimate the second term in the sum above, to obtain
\[
\frac{a}{\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^n \sum_{(K,L) \in \mathcal{E}} \sqrt{T_{K|L}} (u_L^{(n+1)} - u_K^{(n+1)}) \cdot \sqrt{T_{K|L}} (u_L^{(n(t)+1)} - u_K^{(n(t)+1)})
\]
\[
\leq \frac{a}{2\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^n \sum_{(K,L) \in \mathcal{E}} T_{K|L} (u_L^{(n+1)} - u_K^{(n+1)})^2
\]
\[
+ \frac{a}{2\alpha} \sum_{n=n(t)+1}^{n(t+\tau)} t_\delta^n \sum_{(K,L) \in \mathcal{E}} T_{K|L} (w_L^{(n(t)+1)} - w_K^{(n(t)+1)})^2
\]
where the first inequality follows from the relation \(\pm s_1 s_2 \leq \frac{1}{2} (s_1^2 + s_2^2)\) and the second one follows from the simple inequality \((s_1 + s_2)^2 \leq 2(s_1^2 + s_2^2)\). To conclude the proof we integrate above inequalities over \(\mathbb{R}\) with respect to the time variable \(t\). Next we apply Proposition 5.3 (for details see \([8, \text{Lemma 5.5}]\)).

Proposition 5.3 together with Proposition 5.4 immediately give the following corollary.

**Corollary 5.5.** Let the assumptions 1, 2, and 3 of Proposition 5.3 be satisfied. We set \(w_D = \frac{1}{\alpha} u_D + \frac{1}{\beta} v_D\). Then, there exists a constant \(C > 0\), which is independent of the discretization parameters \(D\) and of \(k\), such that
\[
\int_{\Omega_t \times (0,T)} (w_D(x + \xi, t) - w_D(x, t))^2 \, dx \, dt \leq C|\xi|(2\text{size}(D) + |\xi|),
\]
for all \(\xi \in \mathbb{R}^d\) and \(\Omega_t = \{x \in \mathbb{R}^d, |x + \xi| \subset \Omega\}\). Moreover
\[
\int_{\Omega_t \times (0,T-t)} (w_D(x, t + \tau) - w_D(x, t))^2 \, dx \, dt \leq C(\text{size}(D) + \tau),
\]
where \(\tau \in (0,T)\).

**5.2 The limit as size(D) tends to zero and k tends to infinity**

We state below the main convergence results of this paper, first only letting the size of the volume elements and the time steps tend to zero, and then also letting the kinetic rate tend to infinity.
Proof. To prove the result we use Corollary 5.5. The method of proof is similar to that of Theorem 4.4.

It is now possible to pass to the limit as $k \to +\infty$.

Theorem 5.7. Let $(u_D^k, v_D^k)$ be the sequence of approximate solutions of Problem $P^k$, defined by (10), (11) and (12). Then

$$u_D^k \to \eta \left( \frac{1}{\alpha} \right)^{-1} (w)$$

and

$$v_D^k \to \eta \circ \left( \frac{1}{\alpha} \right)^{-1} (w)$$

as size$(D) \to 0$ and $k$ tends to infinity, where $\eta = r_B^{-1} \circ r_A$ and where $w$ is the unique weak solution of the problem (5) - (6).

Proof. Let $w_D^k = \frac{1}{\alpha} u_D^k + \frac{1}{\beta} v_D^k$. The estimates from Corollary 5.5, which are uniform with respect to $k$, permit to apply Proposition 7.2. As a consequence we deduce the relative compactness in $L^2(Q_T)$ of the sequence $\{w_D^k\}$. Then there exist a function $w \in L^2(Q_T)$ and a subsequence $\{w_D^{k_i}\}^\infty_{i=1}$ such that $w_D^{k_i}$ converges to $w$ strongly in $L^2(Q_T)$ as $k_i$ tends to infinity and size$(D_m) \to 0$. Theorem 4.3 implies that $w$ is nonnegative and bounded in $Q_T$. The inequality (38), namely

$$k_i \left| \int_{\Omega} \left( r_A(u_{D_m}^{k_i}) - r_B(v_{D_m}^{k_i}) \right) \right|^2 \leq C$$

where the positive constant $C$ is independent of $k_i$ and size$(D_m)$, implies that

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

and consequently almost everywhere, as $k_i$ tends to infinity. Then

$$v_{D_m}^{k_i} = \eta(v_{D_m}^{k_i}) + e_{D_m}^{k_i},$$

where $\eta(s) = r_B^{-1}(r_A(s))$ and $e_{D_m}^{k_i}$ tends to zero almost everywhere as size$(D_m)$ tends to zero and $k_i$ tends to infinity. In view of the hypotheses $H4$ the function $\eta(s)$ is well defined on $[0, \infty)$. Moreover, $H(u_D^{k_i}) = w_D^{k_i} - \frac{1}{\beta} e_{D_m}^{k_i}$ to $w$ a.e. in $Q_T$, where $H(s) = \frac{1}{\alpha s} + \frac{1}{\beta} \eta(s)$. Hypotheses $H4$ ensures that the function $H(s)$ has the continuous inverse function. Then Lebesgue’s dominated convergence theorem implies that there exists a function pair $(\bar{u}, \bar{v}) \in (L^2(Q_T))^2$

$$u_D^{k_i} \to \bar{u} \quad \text{and} \quad v_D^{k_i} \to \bar{v} \quad \text{in} \quad L^2(Q_T)$$

(47)
as size($D_m$) tends to zero and $k_i$ tends to infinity.

Next we identify the limit pair ($\bar{u}$, $\bar{v}$). Let $\overline{\varpi}$ be the solution of the problem (1) and the functions $\overline{\varpi}$ and $\overline{\varpi}$ are defined as in (7), namely

$$\overline{\varpi} = \left(\frac{1}{\alpha} \text{id} + \frac{1}{\beta} \eta\right)^{-1}(\overline{\varpi}), \quad \eta = \eta \circ \left(\frac{1}{\alpha} \text{id} + \frac{1}{\beta} \eta\right)^{-1}(\overline{\varpi}).$$

Let $\varepsilon > 0$ be arbitrary. We have that

$$\|\overline{\varpi} - \bar{u}\|_{L^2(Q_T)} \leq \|\overline{\varpi} - u^k\|_{L^2(Q_T)} + \|u^k - u^k_{D_m}\|_{L^2(Q_T)} + \|u^k_{D_m} - \bar{u}\|_{L^2(Q_T)}.$$

From (17) we deduce that there exists $k_0$ and $\delta_0$ such that, for all $k_i \geq k_0$ and all size($D_m$) $\leq \delta_0$, the last term of the inequality above is less then $\varepsilon/3$. From Theorem 1 in [1] there exists some $\bar{k}_0$, such that for all $k_i > \bar{k}_0$, $\|\overline{\varpi} - u^k\|_{L^2(Q_T)} \leq \varepsilon/3$. Then, fixing $k_i = \max(k_0, \bar{k}_0)$, we can take size($D_m$) $\leq \delta_0$ small enough so that by Proposition 5.6 $\|u^k_i - u^k_{D_m}\|_{L^2(Q_T)} \leq \varepsilon/3$.

Since the argument for the $v$-component is similar, this completes the proof. ■

6 Numerical example

In this section we give an example of an application of the finite volume scheme (11) in one space dimension. For the numerical experiments we choose the reaction of the reversible dimerisation of $\alpha$-phenylenedioxylidemethylsilane (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 $\Lambda$-ring formation reaction and a monomolecular backreaction (for further details we refer to Meyer, Klein and Weiss [12]).

Since the reaction is of the type $\text{A} \rightleftharpoons \text{B}$, the reaction terms take the form

$$r_A(u) = k_1 u^2 \quad \text{and} \quad r_B(v) = k_2 v.$$ 

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 $T = 298 K$,

$$k_1 \approx 1,072 \cdot 10^{-4} L^2 mol^{-2} \quad \text{and} \quad k_2 \approx 2,363 \cdot 10^{-6} L^2 mol^{-2}$$

and diffusion coefficients

$$a \approx 1,579 \cdot 10^{-9} m^2 s^{-1} \quad \text{and} \quad b \approx 1,042 \cdot 10^{-9} m^2 s^{-1}.$$ 

In the 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 $10^5$. In fact, we can multiply the system (1) by $10^5$ and change the time scale as $t \to 10^5 t$. 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 shows the initial conditions $u_0(x)$ and $v_0(x)$, defined as

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

and

$$v_0(x) = \begin{cases} 
\frac{1}{2} \cos \left(\frac{2\pi}{0.07} x\right) & \text{for } x \in [0, 0.07], \\
0 & \text{for } x \in [0.07, 0.1]
\end{cases}$$

On Figures 3 and 5 we see the time evolution of the solution $(u^k, v^k)$ until the times $T_{\max}^1 = 10^5 [s]$ and $T_{\max}^2 = 10^{11} [s]$, respectively. Then we follow the evolution of the solution $w_\varpi$ of the nonlinear diffusion problem (6) for initial condition deduced from that used in the reaction–diffusion Problem $\mathcal{P}^k$. We have used a uniform mesh with $h = 0.002$ and initial time step $t_s = 10^{-8}$ to obtain the approximate solution $(u^k_{\varpi}, v^k_{\varpi})$ and $t_s = 10^{-6}$ to obtain the approximate solution $w_\varpi$ to the nonlinear diffusion problem.

We can use the approximate solution $w_\varpi$ and the formulas (11) to define functions $u^k_{\varpi}$ and $v^k_{\varpi}$. Indeed, let

$$u^w_{\varpi} = h(w_\varpi) \quad \text{and} \quad v^w_{\varpi} = g(h(w_\varpi)),$$
where
\[ h(y) = \frac{1}{2} \left( \sqrt{\frac{\alpha k_1}{\beta k_2}}^2 + \frac{4k_2}{3k_1} - \frac{\alpha k_2}{3k_1} \right) \] (50)
and
\[ g(h) = h \frac{a}{\alpha} + h^2 \frac{b k_1}{3 k_2}. \] (51)

Proceeding in the similar way as in the proof of Theorem 5.7, we write for the u-component that
\[ \left\| u_D^k - h(w_D) \right\|_{L^2(Q_T)} \lesssim \left\| u_D^k - u \right\|_{L^2(Q_T)} + \left\| u^k - h(w) \right\|_{L^2(Q_T)} + \left\| h(w) - h(w_D) \right\|_{L^2(Q_T)}. \] (52)

We simultaneously pass to the limit as size \( (D) \to 0 \) and \( k \to \infty \). From Theorem 5.7, we immediately deduce that the first term on the right hand side of (52) tends to zero. The same conclusion holds for the two other terms. Indeed, [1, Theorem 1, Sec. 3] implies that \( \left\| u^k - h(w) \right\|_{L^2(Q_T)} \) tends to zero as \( k \to \infty \). Moreover, [7, Theorem 5.1] yields that \( \left\| w - w_D \right\|_{L^2(Q_T)} \to 0 \) as size \( (D) \to 0 \) and since the function \( h \) is well defined and continuous, we conclude that for every small \( \varepsilon > 0 \) there exist \( D \) small enough and \( k \) large enough so that
\[ \left\| u_D^k - h(w_D) \right\|_{L^2(Q_T)} \lesssim \varepsilon. \]
We proceed in the same way to show that for every small \( \varepsilon > 0 \) there exist \( D \) small enough and \( k \) large enough so that
\[ \left\| v_D^k - g(h(w_D)) \right\|_{L^2(Q_T)} \lesssim \varepsilon. \]

The results from our numerical experiment agree with above analysis, since
\[ \max_{x \in \Omega} \left| u_D^k(x, T_{max}^1) - h(w_D)(x, T_{max}^1) \right|_\infty \simeq 4.74 \cdot 10^{-3}, \]
\[ \max_{x \in \Omega} \left| v_D^k(x, T_{max}^1) - g(h(w_D)(x, T_{max}^1)) \right|_\infty \simeq 4.032 \cdot 10^{-3}, \]
whereas
\[ \max_{x \in \Omega} \left| u_D^k(x, T_{max}^2) - h(w_D)(x, T_{max}^2) \right|_\infty \simeq 3.121 \cdot 10^{-14}, \]
\[ \max_{x \in \Omega} \left| v_D^k(x, T_{max}^2) - g(h(w_D)(x, T_{max}^2)) \right|_\infty \simeq 1.84 \cdot 10^{-13}. \]
In order to show the accuracy of our method in the fast reaction limit, let us increase the kinetics parameter $k$ in Problem $\mathcal{P}^k$ keeping all other data as previously. Let

$$\mathcal{J}_u^k = \max_{x \in \Omega} \left| u^k_D(x, T^2_{\text{max}}) - h(w_D)(x, T^2_{\text{max}}) \right|_{\infty}$$

and

$$\mathcal{J}_v^k = \max_{x \in \Omega} \left| v^k_D(x, T^2_{\text{max}}) - g(h(w_D))(x, T^2_{\text{max}}) \right|_{\infty}.$$ 

Table 1 below shows the numerical results.

| $k$  | $\mathcal{J}_u^k$       | $\mathcal{J}_v^k$       |
|------|------------------------|------------------------|
| $10^{-7}$ | 2.3498·10^{-2}  | 4.5272·10^{-2}  |
| $10^{-6}$ | 3.976·10^{-3}  | 1.988·10^{-3}  |
| $10^{-5}$ | 4.699·10^{-8}  | 2.3498·10^{-8}  |
| $10^{-4}$ | 9.3725·10^{-10} | 4.6862·10^{-10} |
| $10^{-3}$ | 2.498·10^{-16} | 9.992·10^{-16} |
| $10^{-2}$ | 1.7892·10^{-12} | 8.95·10^{-13} |
| $10^{-1}$ | 4.163·10^{-17} | 9.992·10^{-16} |
| $10^0$  | 3.121·10^{-17} | 1.84·10^{-16} |

Table 1: The accuracy of our method in the fast reaction limit, when the kinetics parameter $k$ in Problem $\mathcal{P}^k$ increases and all other data are unchanged.
Appendix

The proof of the following result can be found in [5 Lemma 5.3 and Lemma 5.4].

**Lemma 7.1.** Let \( \zeta(n) \in \mathbb{Z} \) be a strictly increasing sequence of real numbers such that \( \lim_{n \to -\infty} \zeta(n) = -\infty \) and \( \lim_{n \to \infty} \zeta(n) = \infty \). Moreover, let \( \zeta(n) := \zeta(n+1) - \zeta(n) \) be uniformly bounded. For all \( t \in \mathbb{R} \) we denote by \( n(t) \) an integer \( n \), such that \( t \in [\zeta(n), \zeta(n+1)) \). 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 \( \zeta \in \mathbb{R} \)

\[
\int_{\mathbb{R}} \left( \sum_{n=n(t)+1}^{n(t)+\tau} \zeta(n) a_{n+1} \right) dt = \tau \sum_{n \in \mathbb{Z}} \zeta(n) a_{n+1}.
\]

\[
\int_{\mathbb{R}} \left( \sum_{n=n(t)+1}^{n(t)+\tau} \zeta(n) a_{n+1} \right) dt \leq (\tau + \sum_{n \in \mathbb{Z}} \zeta(n) a_{n+1}).
\]

The following proposition is a direct corollary from Fréchet–Kolmogorov Theorem (see Brezis [2] Theorem IV.25, page 72).

**Proposition 7.2.** 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 \( w_n(x,t) : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R} \), such that

1. for all \( n \in \mathbb{N} \), \( w_n \in L^\infty(\mathcal{O}) \) and there exists a constant \( C_0 > 0 \) which does not depend on \( n \), such that \( \|w_n\|_{L^\infty(\mathcal{O})} \leq C_0 \),

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

\[
\int_{\mathcal{O}_{\xi,t}} (w_n(x + \xi, t + \tau) - w_n(x,t))^2 dxdt \leq C_1 |\xi| + C_2 \tau + \mu_n,
\]

for \( \xi \in \mathbb{R}^d \), \( \tau \in \mathbb{R} \), \( n \in \{0, \ldots, N\} \) and

\[
\mathcal{O}_{\xi,t} = \{(x,t) \in \mathbb{R}^{d+1} : \text{the interval } [(x,t),(x+\xi,t+\tau)] \text{ lies in } \mathcal{O}\}.
\]

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 \( w_n \rightarrow w \) in \( L^2(\mathcal{O}) \), as \( n \to \infty \).

**Lemma 7.3.** Let \( A > 0 \) and a function \( r(s) \) satisfying

\[
r \in C^1(\mathbb{R}), \quad r'(\cdot) > 0 \quad \text{on} \quad (0, +\infty), \quad r(0) = 0, \quad \text{and} \quad \limsup_{s \to 0^+} \frac{sr'(s)}{r(s)} < \infty \quad (55)
\]

be given.

Then there exists \( \varepsilon_0 > 0 \) only depending on \( r(s) \) and \( C > 0 \), depending only on \( r(s) \) and \( A \), such that for all \( \varepsilon \in (0, \varepsilon_0) \) and for all \( u \in [0, A] \) the inequality

\[
\ln r(u + \varepsilon) \leq C (|\ln \varepsilon| + 1)
\]

holds.

**Proof** Let \( \alpha = \limsup_{s \to 0^+} \frac{sr'(s)}{r(s)} + 1 \). There exists a constant \( \varepsilon_0 > 0 \), such that for all \( s \in (0, \varepsilon_0) \)

\[
\frac{r'(s)}{r(s)} \leq \frac{\alpha}{s}. \quad (56)
\]

Let \( \varepsilon \in (0, \varepsilon_0) \) and \( u \in [0, A] \). Then, either \( r(u + \varepsilon) \geq 1 \), which implies

\[\ln r(u + \varepsilon) \leq \ln r(A + \varepsilon_0)\]

or \( r(u + \varepsilon) \leq 1 \). In that case

\[\ln r(u + \varepsilon) \leq \ln r(\varepsilon),\]

holds. Integrating inequality \(56 \) over the interval \( [\varepsilon, \varepsilon_0] \), we obtain

\[
\ln r(\varepsilon) \leq \ln r(\varepsilon_0) + \alpha (|\ln \varepsilon_0| + |\ln \varepsilon|).
\]

Setting \( C = \max \{\alpha, \alpha|\ln \varepsilon_0| + |\ln r(\varepsilon_0)|, \ln (r(A + \varepsilon_0))\} \) we conclude the proof. \( \blacksquare \)
References

[1] D. Bothe and D. Hilhorst, A reaction-diffusion system with fast reversible reaction, *J. Math. Anal. Appl.*, 2003, 1, 268, 125–135.

[2] H. Brezis, Analyse fonctionnelle, Collection Mathematiques Appliquées pour la Maitrise, Masson, Paris, 1983.

[3] K. Deimling, Nonlinear functional analysis, Springer-Verlag, Berlin, 1985.

[4] J.H. Espenson, Chemical Kinetics and Reaction Mechanisms, Mc Graw-Hill, 1995.

[5] R. Eymard, T. Gallouët, M. Ghilani, and R. Herbin, Error estimate for the finite volume approximate of the solution to a nonlinear convective equation, *Theory Appl. Transp. Porous Media*, 1998, 11, 13–24.

[6] R. Eymard, T. Gallouet, and R. Herbin, Finite Volume Methods, Handbook of Numerical Analysis, VII, North-Holland, Amsterdam, 2000.

[7] R. Eymard, T. Gallouet, D. Hilhorst, and Y. Naït Slimane Finite volumes and nonlinear diffusion equations, *RAIRO Model. Math. Anal. Numer.*, 1998, 32, 6, 747761.

[8] R. Eymard, M. Gutnic, and D. Hilhorst, The finite volume method for Richards equation, *Comput. Geosci.*, 2000, 3, 3–4, 259294.

[9] P. Érdi and J. Tóth, Mathematical models of chemical reactions, *Nonlinear Science: Theory and Applications*, Princeton University Press, Princeton, NJ, 1989.

[10] G. B. Folland, Real analysis Pure and Applied Mathematics John Wiley & Sons Inc., New York Modern techniques and their applications, 1984.

[11] O. A. Ladyženskaja and V. A. Solonnikov and N. N. Ural’ceva, Linear and Quasilinear Equations of Parabolic Type, Translations of Mathematical Monographs, Vol. 23, American Mathematical Society, Providence, R.I., 1967.

[12] H. Meyer, J. Klein, and A. Weiss, Kinetische untersuchung reversiblen dimerisierung von o-phenylenedioxydimethylsilan, *J. Organometallic Chem.*, 1979, 117, 323328.

[13] S. M. Nikolsky, A course of mathematical analysis, Vol. 1, Mir Publishers, Moscow, Translated from the second Russian edition by V. M. Volosov, 1977