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A free boundary problem in a singular limit of a three-component reaction-diffusion system

By

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Abstract

We consider a three-component reaction-diffusion system with a reaction rate parameter, and investigate its singular limit as the reaction rate tends to infinity. The limit problem is described by a nonlinear cross-diffusion system. The system is regarded as a weak form of a free boundary problem which possesses three types of free boundaries. Triple junction points appear at the intersection of the three interfaces. Furthermore, the dynamics is governed by a system of equations in each region separated by the free boundaries. A linear numerical scheme for capturing the interfaces is introduced and numerical simulations are carried out to demonstrate our theoretical results.

§ 1. Introduction

We are interested in asymptotic behavior of solutions of reaction-diffusion systems. Especially, we are studying a kind of singular limit problems, which is called fast reaction limit. In this paper, we deal with fast reaction limit of the following three-component

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reaction-diffusion system:

$$
(\mathrm{RD})^k \qquad \begin{cases} \dfrac{\partial u}{\partial t} = d_1 \Delta u + f_1(u,v,w) - kuvw & \text{in} \quad Q, \\ \dfrac{\partial v}{\partial t} = d_2 \Delta v + f_2(u,v,w) - kuvw & \text{in} \quad Q, \\ \dfrac{\partial w}{\partial t} = d_3 \Delta w + f_3(u,v,w) - kuvw & \text{in} \quad Q, \\ \dfrac{\partial u}{\partial \nu} = \dfrac{\partial v}{\partial \nu} = \dfrac{\partial w}{\partial \nu} = 0 & \text{on} \quad \partial\Omega \times (0,T), \\ u(\cdot,0) = u_0^k,\ v(\cdot,0) = v_0^k,\ w(\cdot,0) = w_0^k & \text{in} \quad \Omega, \end{cases}
$$

where $\Omega \subset \mathbb{R}^N$ ($N \in \mathbb{N}$) is a bounded domain with smooth boundary $\partial\Omega$, d_1, d_2, d_3, k and T are positive numbers, ν is the unit outward normal vector to the boundary $\partial\Omega$, f_i are given functions and u_0^k, v_0^k and w_0^k are non-negative initial functions.

We consider a fast reaction limit of $(\mathrm{RD})^k$, that is, the behavior of solutions when the reaction rate k tends to infinity. Before we analyze it, we examine several problems in the literature, and then, focus on a certain kind of sets which play important roles in presuming the limit problems. In the following section, we introduce it and give our motivation. We obtained the following two main results theoretically. The fast reaction limit of $(\mathrm{RD})^k$ is described by a system of nonlinear diffusion equations. The system is regarded as a weak form of a free boundary problem which allows appearance of triple junction points. These results are presented in Section 3. In Section 4, a linear numerical scheme for capturing the free boundaries is proposed and numerical simulations are given to illustrate our results.

§ 2. Fast reaction limit and reaction limit set

The singular limit analysis for reaction-diffusion systems has been developed in the last decades, particularly, in the studies of fast reaction limit and reaction-diffusion system approximation. One of the aims of fast reaction limit analysis is to understand the behaviors of solutions of reaction-diffusion systems when a reaction speed is very fast. Meanwhile, the object of reaction-diffusion system approximation is to approximate nonlinear problems, especially nonlinear diffusion problems, by semilinear reaction-diffusion systems. Although these problems are in a different position, the way of analysis is similar. Both of them are investigations of relationship between reaction-diffusion interaction and nonlinear diffusion.

A typical example of such problems is the fast reaction limit of the two-component

Lotka-Volterra competition diffusion system in population ecology.

$$
(\mathrm{LV})^k \qquad \begin{cases} u_t = d_1\Delta u + \lambda u(1-u) - kuv & \text{in} \quad Q := \Omega \times (0,T), \\ v_t = d_2\Delta v + \mu v(1-v) - kuv & \text{in} \quad Q \\ \dfrac{\partial u}{\partial \nu} = \dfrac{\partial v}{\partial \nu} = 0 & \text{on} \quad \partial\Omega \times (0,T), \\ u(\cdot,0) = u_0^k, \ v(\cdot,0) = v_0^k & \text{in} \quad \Omega, \end{cases}
$$

where λ and μ are positive constants. The solution pair (u^k, v^k) represents densities of two competing species, and the positive parameter k is an interspecific competition rate. Dancer, Hilhorst, Mimura and Peletier [3] have considered how do the solutions behave when the interspecific competition rates are very large. They have studied in the case where k tends to infinity. They have shown that the limiting system can be described by the following nonlinear diffusion equation.

$$
(2.1) \qquad \begin{cases} \dfrac{\partial z}{\partial t} = \Delta\phi(z) + F(z) & \text{in} \quad Q, \\ \dfrac{\partial \phi(z)}{\partial \nu} = 0 & \text{on} \quad \partial\Omega \times (0,T), \\ z(\cdot,0) = z_0 & \text{in} \quad \Omega. \end{cases}
$$

Here,

$$
\phi(z) = \begin{cases} d_2 z & \text{if } z > 0, \\ d_1 z & \text{otherwise,} \end{cases} \qquad F(z) = \begin{cases} \mu z(1-z) & \text{if } z > 0, \\ \lambda z(1+z) & \text{otherwise,} \end{cases}
$$

and $z_0 := \lim_{k\to\infty}(v_0^k - u_0^k)$. Let z be a weak solution of (2.1). Then u^k converges to $z^- := \max\{-z, 0\}$ and v^k does to $z^+ := \max\{z, 0\}$ as k tends to infinity. The equation (2.1) is known as a weak form of the two-phase Stefan problem without latent heat. Thus they showed that the two species are spatially segregated as k tends to infinity and that the interface between two habitats is governed by a Stefan-type free boundary problem.

The fast reaction limit of the two-component Lotka-Volterra system is well studied (e.g., [9] and references therein). We are interested in the fast reaction limit of three-component Lotka-Volterra system.

$$
(2.2) \qquad \begin{cases} u_t = d_1\Delta u + \mu_1 u(1-u) - k(v+w)u & \text{in} \quad Q, \\ v_t = d_2\Delta v + \mu_2 v(1-v) - k(w+u)v & \text{in} \quad Q, \\ w_t = d_3\Delta w + \mu_3 w(1-w) - k(u+v)w & \text{in} \quad Q, \end{cases}
$$

where $\mu_i \geq 0$ for $i = 1, 2, 3$. Hilhorst, Iida, Mimura and Ninomiya [7] proved subsequences of the solution of (2.2) converge to certain functions as k tends to infinity and

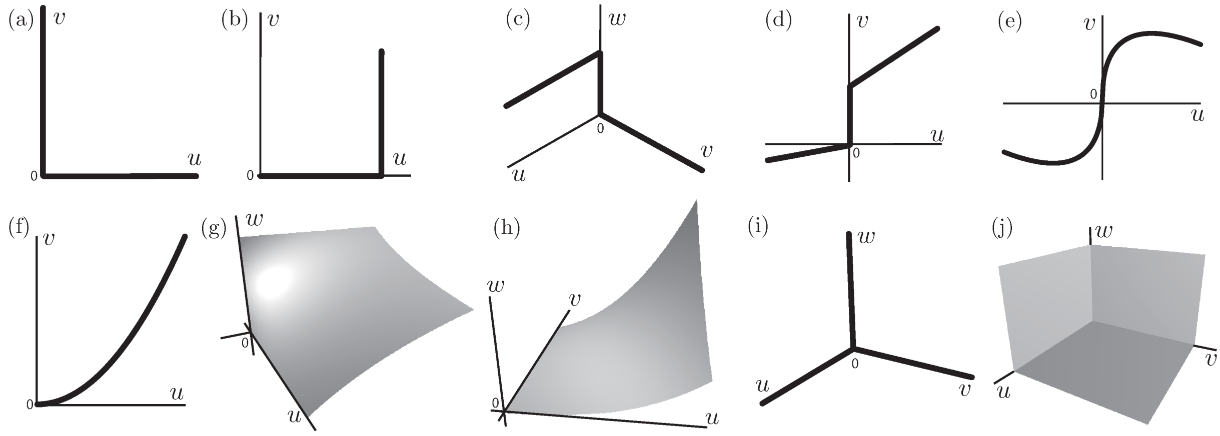


Figure 1. Various reaction limit sets. The limit problems are (a)(b) the two-phase Stefan problem without latent heat or the one-phase Stefan problem, (c)(d) the two-phase Stefan problem, (e) the porous medium equation, (f) a nonlinear diffusion equation, (g)(h) cross-diffusion systems, (i) open problem, (h) our problem.

showed that the species segregate in the limit. However, they did not derive any explicit limit problem. It is still an open problem.

To understand the difficulty of the problem, we begin by examining $(\mathrm{LV})^k$ and its limiting equation as k tends to infinity. Letting $k \to \infty$ in

$$\frac{u_t}{k} = \frac{d_1}{k}\Delta u + \frac{1}{k}\lambda u(1-u) - uv,$$

we can expect that

$$0 = uv$$

if u, u_t and Δu are bounded with respect to k. Hence, the dynamics is restricted to the following one-dimensional set:

$$\mathcal{A}_{\mathrm{LV}} = \{(u,0) \mid u \geq 0\} \cup \{(0,v) \mid v \geq 0\}.$$

This set $\mathcal{A}_{\mathrm{LV}}$ consists of limit points of the fast reaction system:

$$\begin{cases} u_t = -kuv, \\ v_t = -kuv. \end{cases}$$

We call a set of the equilibria of the fast reaction system a *reaction limit set* (or simply RLS). The RLS $\mathcal{A}_{\mathrm{LV}}$ of $(\mathrm{LV})^k$ is shown in Figure 1 (a). The set consists of two axis. The first component diffuses with the diffusion coefficient d_1 on $\{(u,0) \mid u \geq 0\}$, while the second one does with the coefficient d_2 on $\{(0,v) \mid v \geq 0\}$. This may imply the limit is represented by a nonlinear diffusion equation. The flux is discontinuous across the corner in $\mathcal{A}_{\mathrm{LV}}$. This may indicate the presence of a free boundary in the limit problem. Indeed, it was proved as we mentioned. The limiting system as the reaction rate k tends to infinity is represented by the one-phase Stefan problem for the case $d_1 > 0, d_2 = 0$ in [5] and that the limit equation can be described by the two-phase Stefan problem without latent heat for the case $d_1, d_2 > 0$ in [3].

Let us see RLSs of relevant studies of fast reaction limit and reaction-diffusion system approximation. Bouillard et al. [2] considered the following reaction-diffusion system arising in reactive transport.

$$(2.3) \qquad \begin{cases} \dfrac{\partial u}{\partial t} = \Delta u - k((u-1)^+ - \mathrm{sign}^+(v)(u-1)^-) & \text{in} \quad Q, \\ \dfrac{\partial v}{\partial t} = k((u-1)^+ - \mathrm{sign}^+(v)(u-1)^-) & \text{in} \quad Q \end{cases}$$

with non-negative initial data. Here, $\mathrm{sign}^+(x) = 1$ if $x > 0$ and $\mathrm{sign}^+(x) = 0$ if $x = 0$. The RLS of this system is drawn in Figure 1 (b). The diffusion coefficient is 1 on $\{(u,0) \mid 0 \le u \le 1\}$ and that is 0 on $\{(1,v) \mid v > 0\}$. The flux is discontinuous across the corner. They proved that the corresponding limit problems are given by the one-phase Stefan problem. Although problems $(\mathrm{LV})^k$ and (2.3) are different, RLSs are similar and the limit is the same. Hilhorst, King and Röger [8] investigated the fast reaction limit of a reaction-diffusion system arising as a model for host tissue degradation by bacteria. The RLS is similar to those of $(\mathrm{LV})^k$ and (2.3). They showed the convergences to the one-phase Stefan problem and to the two-phase Stefan problem without latent heat.

Hilhorst, Iida, Mimura and Ninomiya [6] proposed the following three-component reaction-diffusion system:

$$(2.4) \qquad \begin{cases} \dfrac{\partial u}{\partial t} = d_1 \Delta u + f_1(u) - ku(1-w) & \text{in} \quad Q, \\ \dfrac{\partial v}{\partial t} = d_2 \Delta v + f_2(v) - kvw & \text{in} \quad Q, \\ \dfrac{\partial w}{\partial t} = ku(1-w) - kvw & \text{in} \quad Q \end{cases}$$

with initial data satisfying $0 \le u_0, v_0, w_0 \le 1$. The RLS of (2.4) is shown in Figure 1 (c). The diffusion coefficients are d_1 on $\{(u,0,1) \mid u > 0\}$, 0 on $\{(0,0,w) \mid 0 \le w \le 1\}$ and d_2 on $\{(0,v,0) \mid v > 0\}$. This suggests us that the limit equation is described by the two-phase Stefan problem with a positive latent heat. In fact, it was proved in [6] that $u^k - v^k + w^k$ converges to the weak solution z of (2.1) with

$$(2.5) \qquad \phi(x) = d_1(x-1)^+ - d_2 x^- \quad x \in \mathbb{R}$$

which is a weak form of the two-phase Stefan problem. Murakawa [12] also proved that the solution of the system

$$
(2.6) \qquad \begin{cases} \dfrac{\partial u}{\partial t} = d\Delta u + f(u) - k(u - \phi(u+v)) & \text{in} \quad Q, \\ \dfrac{\partial v}{\partial t} = k(u - \phi(u+v)) & \text{in} \quad Q \end{cases}
$$

converges to that of the two-phase Stefan problem. Here, ϕ is defined as in (2.5). The corresponding RLS of (2.6) is illustrated in Figure 1 (d). The shapes of the RLSs of (c) and (d) are based on combinations of three lines. Although the number of components of the original system (2.4) is different from that of (2.6), the limits are represented by the same problem. Thus, the RLSs must play an important role in singular limit analysis. It is shown in [12] that the porous medium equation is also approximated by (2.6) when $\phi(x) = |x|^{m-1}x$ ($x \in \mathbb{R}$) for some $m > 1$. The RLS is shown in Figure 1 (e).

Bothe and Hilhorst [1] considered a reversible chemical reaction between two mobile species, and studied the limit to an instantaneous reaction:

$$
(2.7) \qquad \begin{cases} \dfrac{\partial u}{\partial t} = d_1\Delta u - k(r_A(u) - r_B(v)) & \text{in} \quad Q, \\ \dfrac{\partial v}{\partial t} = d_2\Delta v - k(r_B(u) - r_A(v)) & \text{in} \quad Q \end{cases}
$$

(see [1, 4] for the detailed assumptions of r_A and r_B). The RLS of (2.7) is given in Figure 1 (e) for a usual choice of r_A and r_B. They proved that the limit problem becomes a nonlinear diffusion equation (2.1) with $\phi = \left(d_1 \mathrm{id} + d_2 r_B^{-1} \circ r_A\right) \circ \left(\mathrm{id} + r_B^{-1} \circ r_A\right)^{-1}$. The nonlinear diffusivities in the limit problems are determined by the RLSs. We note that the RLSs in both cases (e) and (f) are smooth curves contrary to (a)–(d), so the diffusivities are given by smooth functions.

There are few results dealing with reaction-diffusion systems which possess two- or multi-dimensional RLSs. Iida, Mimura and Ninomiya [10] studied Shigesada-Kawasaki-Teramoto cross-diffusion system [16]:

$$
(2.8) \qquad \begin{cases} \dfrac{\partial z_1}{\partial t} = \Delta[(d_1 + d_2 z_2)z_1] + F_1(z_1, z_2), \\ \dfrac{\partial z_2}{\partial t} = d_3\Delta z_2 + F_2(z_1, z_2). \end{cases}
$$

We note that the diffusion of z_1 depends not only on z_1 but also on z_2. This mixture of diffusion terms is called cross-diffusion, and such systems are called cross-diffusion systems. For a deeper understanding of the cross-diffusion mechanism, they replaced cross-diffusion by a different way of avoiding the congestion of the other species. Then, they proposed the following three-component reaction-diffusion system.

$$\begin{cases} \dfrac{\partial u}{\partial t} = d_1 \Delta u + f_1(u,v,w) - k((1-w)v - wu), \\ \dfrac{\partial v}{\partial t} = (d_1 + d_2)\Delta v + f_2(u,v,w) + k((1-w)v - wu), \\ \dfrac{\partial w}{\partial t} = d_3 \Delta w + f_3(u,v,w). \end{cases}$$

They showed that $(u^k + v^k, w^k)$ approximates the solution (z_1, z_2) of the cross-diffusion system (2.8). For more general cases, see [11, 13, 14]. The RLS is $\{(u,v,w) \mid (1-w)v = uw\}$, that is a two-dimensional smooth set as in Figure 1 (g). Another example of reaction-diffusion system approximation that possesses a two-dimensional RLS is reported in [14]. The RLS of the example is shown in Figure 1 (h). In this case, the limit is described by a nonlinear cross-diffusion system that diffusivity is a fractional type.

All of the above examples illustrate the importance of the shapes of RLSs in presuming the limit problems. Since RLSs in Figure 1 (a)–(f) are one-dimensional lines, the limit problems in all these examples are represented by single nonlinear diffusion equations. The sets in Figure 1 (g), (h) are two-dimensional surfaces. So, the limit is represented by a system of two nonlinear diffusion equations. The existence of corners or points where the diffusion coefficient becomes zero in the RLS indicates the appearance of free boundaries because they create the discontinuity of the flux, which exhibits the interfaces.

Let us look at the RLS of the three-component Lotka-Volterra system (2.2). Figure 1 (i) shows the RLS which consists of three lines. This set is neither associated with a one-dimensional curve nor with a two-dimensional surface by continuous map. This prevents us from deriving the explicit expression of the limit problem. What if we consider a RLS which includes the set (i). For example, the set in Figure 1 (j). A dynamics on the plane, e.g., $\{w = 0\}$, seems to be the same as that of $(\mathrm{LV})^k$. So, first, we restrict the dynamics to the set (j). Then we might be able to consider the fast reaction limit on these surfaces. We consider a system which possesses the set (j) as the RLS. A simple example of such systems is $(\mathrm{RD})^k$ in Section 1. The problem $(\mathrm{RD})^k$ is an artificial problem. But this might be a hint on presuming the limit of the three-component Lotka-Volterra system. Moreover, our results are important from a mathematical point of view.

The RLS of $(\mathrm{RD})^k$ is

$$\mathcal{A}_{\mathrm{RD}} = \{(0,v,w) \mid v \geq 0,\ w \geq 0\} \cup \{(u,0,w) \mid u \geq 0\ w \geq 0\} \cup \{(u,v,0) \mid u \geq 0, v \geq 0\},$$

that is the set in Figure 1 (j). From the above observations, we can imagine the limit problem of the system $(\mathrm{RD})^k$ as k tends to infinity. Since the RLS $\mathcal{A}_{\mathrm{RD}}$ is a two-dimensional surface, the limit problem would be described by a system consists of two nonlinear diffusion equations. Moreover, $\mathcal{A}_{\mathrm{RD}}$ has corners which implies the appearance of free boundaries. Because this has three types of corners, we expect that three types of free boundaries appear and the intersection of those free boundaries. Actually, we obtained such results. We state our results on the fast reaction limit of $(\mathrm{RD})^k$ in the following section.

§ 3. Mathematical results

§ 3.1. Convergence to a nonlinear cross-diffusion system

The following assumptions are imposed on the initial data and on the given functions f_i:

(H1) The initial data $u_0^k, v_0^k, w_0^k \in C(\overline{\Omega})$ satisfy

$$\begin{aligned} &0 \le u_0^k, v_0^k, w_0^k \le M, \\ &u_0^k \rightharpoonup u_0,\ v_0^k \rightharpoonup v_0,\ w_0^k \rightharpoonup w_0 \quad \text{weakly in } L^2(\Omega) \text{ as } k \to \infty \end{aligned}$$

for some positive constant M and for some functions $u_0, v_0, w_0 \in L^\infty(\Omega)$.

(H2) There exist C^1-functions $\tilde{f}_i (i = 1, 2, 3)$ such that for all $\boldsymbol{s} = (s_1, s_2, s_3) \in \mathbb{R}_+^3$,

$$\begin{aligned} &f_i(\boldsymbol{s}) = \tilde{f}_i(\boldsymbol{s}) s_i, \\ &\tilde{f}_i(\boldsymbol{s}) \le 0 \text{ if } s_i \ge M. \end{aligned}$$

Under these assumptions, there exists a unique solution of $(\mathrm{RD})^k$.

We introduce several auxiliary functions to state the limiting equation. For $\boldsymbol{z} = (z_1, z_2) \in \mathbb{R}^2$, we define

$$\varphi(\boldsymbol{z}) := \begin{cases} 0 & \text{if} \quad z_1 > 0,\ z_2 \ge 0, \\ z_1 & \text{if} \quad z_1 \le 0,\ z_1 < z_2, \\ z_2 & \text{if} \quad z_2 < 0,\ z_1 \ge z_2, \end{cases}$$

$$\begin{aligned} &\gamma_1(\boldsymbol{z}) := -\varphi(\boldsymbol{z}), \quad \gamma_2(\boldsymbol{z}) := z_1 - \varphi(\boldsymbol{z}), \quad \gamma_3(\boldsymbol{z}) := z_2 - \varphi(\boldsymbol{z}), \\ &\phi_1(\boldsymbol{z}) := d_2\gamma_2(\boldsymbol{z}) - d_1\gamma_1(\boldsymbol{z}) = d_2 z_1 + (d_1 - d_2)\varphi(\boldsymbol{z}), \\ &\phi_2(\boldsymbol{z}) := d_3\gamma_3(\boldsymbol{z}) - d_1\gamma_1(\boldsymbol{z}) = d_3 z_2 + (d_1 - d_3)\varphi(\boldsymbol{z}), \\ &F_1(\boldsymbol{z}) := f_2(\gamma_1(\boldsymbol{z}), \gamma_2(\boldsymbol{z}), \gamma_3(\boldsymbol{z})) - f_1(\gamma_1(\boldsymbol{z}), \gamma_2(\boldsymbol{z}), \gamma_3(\boldsymbol{z})), \\ &F_2(\boldsymbol{z}) := f_3(\gamma_1(\boldsymbol{z}), \gamma_2(\boldsymbol{z}), \gamma_3(\boldsymbol{z})) - f_1(\gamma_1(\boldsymbol{z}), \gamma_2(\boldsymbol{z}), \gamma_3(\boldsymbol{z})). \end{aligned}$$

The limit functions $\boldsymbol{z} = (z_1, z_2)$ of $(v^k - u^k, w^k - u^k)$ satisfy the following cross-diffusion system:

$$\text{(CD)} \qquad \begin{cases} \dfrac{\partial \boldsymbol{z}}{\partial t} = \Delta \boldsymbol{\phi}(\boldsymbol{z}) + \boldsymbol{F}(\boldsymbol{z}) & \text{in} \quad Q, \\ \dfrac{\partial \boldsymbol{\phi}(\boldsymbol{z})}{\partial \nu} = \boldsymbol{0} & \text{on} \quad \partial\Omega \times (0,T), \\ \boldsymbol{z}(\cdot, 0) = \boldsymbol{z}_0 & \text{in} \quad \Omega, \end{cases}$$

where $\boldsymbol{\phi}(\boldsymbol{z}) = (\phi_1(\boldsymbol{z}), \phi_2(\boldsymbol{z}))$, $\boldsymbol{F}(\boldsymbol{z}) = (F_1(\boldsymbol{z}), F_2(\boldsymbol{z}))$ and $\boldsymbol{z}_0 := (v_0 - u_0, w_0 - u_0)$. This problem is dealt with in a weak sense.

Definition 3.1. A function $\boldsymbol{z} \in L^\infty(Q)^2$ is a weak solution of (CD) with an initial datum $\boldsymbol{z}_0 \in L^\infty(\Omega)^2$ if it satisfies $\phi_i(\boldsymbol{z}) \in L^2(0,T; H^1(\Omega))^2$ and

$$\text{(3.1)} \qquad \int_0^T \left\langle z_i, \frac{\partial \zeta_i}{\partial t} \right\rangle dt + \langle z_{0i}, \zeta_i(\cdot, 0)\rangle = \int_0^T \langle \nabla \phi_i(\boldsymbol{z}), \nabla \zeta_i \rangle \, dt - \int_0^T \langle F_i(\boldsymbol{z}), \zeta_i \rangle \, dt.$$

for all functions $\boldsymbol{\zeta} = (\zeta_1, \zeta_2) \in H^1(Q)^2$ with $\zeta_i(\cdot, T) = 0$ and for $i = 1, 2$. Here and hereafter, $\langle \cdot, \cdot \rangle$ denotes both the inner product in $L^2(\Omega)$ and the duality pairing between $H^1(\Omega)^*$ and $H^1(\Omega)$.

We present our result on the convergence.

Theorem 3.2 ([15])**.** *Assume that* (H1) *and* (H2) *hold. Let* (u^k, v^k, w^k) *be the solution of* $(\mathrm{RD})^k$*. Then, there exist a weak solution* $\boldsymbol{z} = (z_1, z_2) \in (L^\infty(Q) \cap L^2(0,T; H^1(\Omega)) \cap H^1(0,T; H^1(\Omega)^*))^2$ *of* (CD) *and subsequences* $\{u^{k_n}\}$, $\{v^{k_n}\}$ *and* $\{w^{k_n}\}$ *of* $\{u^k\}$, $\{v^k\}$ *and* $\{w^k\}$*, respectively, such that*

$$u^{k_n} \to \gamma_1(\boldsymbol{z}), \ v^{k_n} \to \gamma_2(\boldsymbol{z}), \ w^{k_n} \to \gamma_3(\boldsymbol{z})$$

strongly in $L^2(Q)$*, a.e. in* Q*, and weakly in* $L^2(0,T; H^1(\Omega))$*,*

$$z_1^{k_n} := v^{k_n} - u^{k_n} \to z_1, \ z_2^{k_n} := w^{k_n} - u^{k_n} \to z_2$$

strongly in $L^2(Q)$*, a.e. in* Q*, and weakly in* $L^2(0,T; H^1(\Omega))$ *and* $H^1(0,T; H^1(\Omega)^*)$ *as* k_n *tends to infinity.*

Remark. If the diffusion coefficients satisfy additional conditions (see [15] for more details), we can show the uniqueness of the weak solution of the limit problem (CD). In this case, the convergence in Theorem 3.2 holds for the full sequence (u^k, v^k, w^k) without taking subsequences. Furthermore, we also analyze the rate of the convergence in [15].

Remark. Assume that $f_3(u,v,1)=0$ and that $w_0(x)=1$ for $x\in\Omega$. Then $w(x,t)=1$ for $t\geq 0$, $x\in\Omega$. In this case, the problem $(\mathrm{RD})^k$ coincides with $(\mathrm{LV})^k$ and (CD) corresponds to (2.1). Therefore, Theorem 3.2 is an extension of the result by Dancer et al. [3].

By the conventional argument, we obtain the following a priori estimates:

Lemma 3.3. *Let (u^k,v^k,w^k) be a solution of $(\mathrm{RD})^k$. Set $\boldsymbol{z}^k=(z_1^k,z_2^k)=(v^k-u^k,w^k-u^k)$. Assume that (H1) and (H2) are satisfied. Then, there exists a positive constant C independent of k such that*

$$0\leq u^k,v^k,w^k\leq M \quad in \quad Q, \tag{3.2}$$

$$\iint_Q u^kv^kw^k dxdt\leq \frac{C}{k}, \tag{3.3}$$

$$\|u^k\|_{L^2(0,T;H^1(\Omega))}+\|v^k\|_{L^2(0,T;H^1(\Omega))}+\|w^k\|_{L^2(0,T;H^1(\Omega))}\leq C, \tag{3.4}$$

$$\|\boldsymbol{z}^k\|_{(L^2(0,T;H^1(\Omega))\cap H^1(0,T;H^1(\Omega)^*))^2}\leq C \tag{3.5}$$

$$\begin{aligned}&\|u^k-\gamma_1(\boldsymbol{z}^k)\|_{L^3(Q)}+\|v^k-\gamma_2(\boldsymbol{z}^k)\|_{L^3(Q)}+\|w^k-\gamma_3(\boldsymbol{z}^k)\|_{L^3(Q)}\\ &+\|(d_2v^k-d_1u^k)-\phi_1(\boldsymbol{z}^k)\|_{L^3(Q)}+\|(d_3w^k-d_1u^k)-\phi_2(\boldsymbol{z}^k)\|_{L^3(Q)}\leq Ck^{-1/3}.\end{aligned} \tag{3.6}$$

Sketch of proof. The bounds (3.2) is follows from the maximum principle. Integration of the equation for u^k in Q and (3.2) yield the relation (3.3). Multiply the equation for u^k (resp. v^k, w^k) by u^k (resp. v^k, w^k) and integrate by parts to obtain (3.4). We deduce from $(\mathrm{RD})^k$ that

$$\begin{aligned}\int_0^T\left\langle\frac{\partial z_1^k}{\partial t},\zeta_1\right\rangle dt=&\int_0^T\left\langle\nabla(d_1u^k-d_2v^k),\nabla\zeta_1\right\rangle dt\\ &+\int_0^T\left\langle f_2(u^k,v^k,w^k)-f_1(u^k,v^k,w^k),\zeta_1\right\rangle dt.\end{aligned} \tag{3.7}$$

$$\begin{aligned}\int_0^T\left\langle\frac{\partial z_2^k}{\partial t},\zeta_2\right\rangle dt=&\int_0^T\left\langle\nabla(d_1u^k-d_3w^k),\nabla\zeta_2\right\rangle dt\\ &+\int_0^T\left\langle f_3(u^k,v^k,w^k)-f_1(u^k,v^k,w^k),\zeta_2\right\rangle dt\end{aligned} \tag{3.8}$$

for all $\zeta\in L^2(0,T;H^1(\Omega))$. Applying the Cauchy-Schwarz inequality to (3.7), (3.8) and using (3.4), we obtain the estimate (3.5).

An elementary calculation gives the following property for all non-negative real numbers u,v and w:

$$|u-\gamma_1(v-u,w-u)|^3+|v-\gamma_2(v-u,w-u)|^3+|w-\gamma_3(v-u,w-u)|^3\leq 3uvw.$$

This inequality and (3.3) yield (3.6). $\square$

Sketch of proof of Theorem 3.2. By virtue of (3.2)–(3.5) and the compactness of the embedding $L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^1(\Omega)^*) \subset L^2(Q)$ [17, Theorem 2.1], there exist subsequences $\{u^{k_n}\}$, $\{v^{k_n}\}$, $\{w^{k_n}\}$ and $\{\boldsymbol{z}^{k_n}\}$ and functions u^*, v^*, $w^* \in L^\infty(Q) \cap L^2(0,T;H^1(\Omega))$ and $\boldsymbol{z}^* \in (L^\infty(Q) \cap H^1(0,T;H^1(\Omega)^*) \cap L^2(0,T;H^1(\Omega)))^2$ such that

$$\begin{aligned}
&u^{k_n} \rightharpoonup u^*,\ v^{k_n} \rightharpoonup v^*,\ w^{k_n} \rightharpoonup w^* \quad \text{weakly in } L^2(0,T;H^1(\Omega)),\\
&\boldsymbol{z}^{k_n} \to \boldsymbol{z}^* \quad \text{strongly in } L^2(Q)^2,\ \text{a.e. in } Q,\ \text{and weakly in } L^2(0,T;H^1(\Omega))^2
\end{aligned}$$

as k_n tends to infinity. It follows from the Lipschitz continuities of γ_i $(i = 1, 2, 3)$ and ϕ_i $(i = 1, 2)$ that $\gamma_i(\boldsymbol{z}^{k_n})$ and $\phi_i(\boldsymbol{z}^{k_n})$ also converge to $\gamma_i(\boldsymbol{z}^*)$ and $\phi_i(\boldsymbol{z}^*)$ strongly in $L^2(Q)$ and a.e. in Q, respectively. The estimate (3.6) implies that u^{k_n}, v^{k_n} and w^{k_n} converge to $\gamma_1(\boldsymbol{z}^*)$, $\gamma_2(\boldsymbol{z}^*)$ and $\gamma_3(\boldsymbol{z}^*)$ strongly in $L^2(Q)$ and a.e. in Q, respectively, also $u^* = \gamma_1(\boldsymbol{z}^*)$, $v^* = \gamma_2(\boldsymbol{z}^*)$, $w^* = \gamma_3(\boldsymbol{z}^*)$, $d_2v^* - d_1u^* = \phi_1(\boldsymbol{z}^*)$ and $d_3w^* - d_1u^* = \phi_2(\boldsymbol{z}^*)$ a.e. Since f_i $(i = 1, 2, 3)$ are Lipschitz continuous, we see that $f_i(u^{k_n}, v^{k_n}, w^{k_n})$ converge to $f_i(\gamma_1(\boldsymbol{z}^*), \gamma_2(\boldsymbol{z}^*), \gamma_3(\boldsymbol{z}^*))$ strongly in $L^2(Q)$ and a.e. in Q as k_n tends to infinity. Take $\zeta_i \in H^1(Q)$ with $\zeta_i(\cdot, T) = 0$ in (3.7) and (3.8), integrate by parts, and pass to the limit along the subsequences to obtain (3.1) in which $\boldsymbol{z}$ is replaced with $\boldsymbol{z}^*$. Thus, we observe that $\boldsymbol{z}^*$ is a weak solution of (CD). □

§ 3.2. Free boundaries

In the previous subsection, we have studied the convergence of the solutions of $(\mathrm{RD})^k$ to the weak solution of (CD). The limit problem (CD) can be regarded as a weak form of a free boundary problem. In this subsection, we derive explicit conditions on the free boundaries. Let $\boldsymbol{z}$ be a weak solution of (CD) and put $u = \gamma_1(\boldsymbol{z})$, $v = \gamma_2(\boldsymbol{z})$ and $w = \gamma_3(\boldsymbol{z})$. Set

$$\begin{aligned}
\Omega_1(t) &:= \{x \in \Omega \mid v(x,t) > 0, w(x,t) > 0\},\\
\Omega_2(t) &:= \{x \in \Omega \mid w(x,t) > 0, u(x,t) > 0\},\\
\Omega_3(t) &:= \{x \in \Omega \mid u(x,t) > 0, v(x,t) > 0\},\\
Q_i &:= \cup_{t\in(0,T)}\Omega_i(t) \qquad (i = 1, 2, 3).
\end{aligned}$$

Then it follows from the definition of γ_i that

$$\Omega_i(t) \cap \Omega_j(t) = \emptyset \qquad (i \neq j).$$

We also denote the interfaces by

$$\begin{aligned}
\Gamma_1(t) &:= \partial\Omega_2(t) \cap \partial\Omega_3(t) \cap \Omega,\\
\Gamma_2(t) &:= \partial\Omega_3(t) \cap \partial\Omega_1(t) \cap \Omega,\\
\Gamma_3(t) &:= \partial\Omega_1(t) \cap \partial\Omega_2(t) \cap \Omega,\\
\Gamma_i &:= \cup_{t\in(0,T)}\Gamma_i(t) \qquad (i = 1, 2, 3).
\end{aligned}$$

To avoid some difficulties such as the appearance of multiple junctions among Γ_i, we introduce $\widetilde{\Gamma}_i$ and S as follows:

$$\widetilde{\Gamma}_1 := \left\{ (x,t) \in \Gamma_1 \,\middle|\, \begin{array}{l} \text{there is a neighbourhood } D \text{ of } (x,t) \text{ such that} \\ \quad D = (Q_2 \cup Q_3 \cup \Gamma_1) \cap D \\ \quad \text{and } \Gamma_1 \text{ is an } N-1 \text{ dimensional smooth hypersurface in } D \end{array} \right\}.$$

The interfaces $\widetilde{\Gamma}_2$ and $\widetilde{\Gamma}_3$ are similarly defined. Thus, $\widetilde{\Gamma}_i$ do not include multiple junction points. We denote by n_i the unit normal vector on $\Gamma_i(t)$ oriented from $\Omega_j(t)$ to $\Omega_k(t)$ for $(i,j,k) \in \{(1,2,3),(2,3,1),(3,1,2)\}$. Let S be a set of all points $(x,t) \in \partial\Omega \times (0,T)$ so that there exists a normal segment at (x,t) which is located in $\overline{\Omega_i(t)}$ for some $i \in \{1,2,3\}$.

Now, we are ready to state our result.

Theorem 3.4 ([15]). *Assume that* (H2) *holds. Let* $\boldsymbol{z}$ *be a weak solution of* (CD) *with an initial datum* $\boldsymbol{z}_0 \in L^\infty(\Omega)^2$. *Suppose that the functions* $u = \gamma_1(\boldsymbol{z})$, $v = \gamma_2(\boldsymbol{z})$ *and* $w = \gamma_3(\boldsymbol{z})$ *are smooth on* $\overline{Q_1}$, $\overline{Q_2}$ *and* $\overline{Q_3}$. *Also assume that* Q_i *are* (*piecewise*) *smooth. Then,* u, v *and* w *satisfy*

$$\begin{cases} \dfrac{\partial v}{\partial t} = d_2 \Delta v + f_2(0,v,w), \\ \dfrac{\partial w}{\partial t} = d_3 \Delta w + f_3(0,v,w) \end{cases} \quad in \quad Q_1,$$

$$\begin{cases} \dfrac{\partial w}{\partial t} = d_3 \Delta w + f_3(u,0,w), \\ \dfrac{\partial u}{\partial t} = d_1 \Delta u + f_1(u,0,w) \end{cases} \quad in \quad Q_2, \tag{3.9}$$

$$\begin{cases} \dfrac{\partial u}{\partial t} = d_1 \Delta u + f_1(u,v,0), \\ \dfrac{\partial v}{\partial t} = d_2 \Delta v + f_2(u,v,0) \end{cases} \quad in \quad Q_3, \tag{3.10}$$

$$\begin{cases} v = w = 0 \quad on \quad \Gamma_1, \\ w = u = 0 \quad on \quad \Gamma_2, \\ u = v = 0 \quad on \quad \Gamma_3, \end{cases}$$

$$
\begin{aligned}
(3.11)\quad & d_2\frac{\partial v|_{Q_3}}{\partial n_1}+d_3\frac{\partial w|_{Q_2}}{\partial n_1}=0,\quad d_1\left(\frac{\partial u|_{Q_3}}{\partial n_1}-\frac{\partial u|_{Q_2}}{\partial n_1}\right)=d_2\frac{\partial v|_{Q_3}}{\partial n_1}\quad on\quad \widetilde{\Gamma}_1,\\
& d_3\frac{\partial w|_{Q_1}}{\partial n_2}+d_1\frac{\partial u|_{Q_3}}{\partial n_2}=0,\quad d_2\left(\frac{\partial v|_{Q_1}}{\partial n_2}-\frac{\partial v|_{Q_3}}{\partial n_2}\right)=d_3\frac{\partial w|_{Q_1}}{\partial n_2}\quad on\quad \widetilde{\Gamma}_2,\\
& d_1\frac{\partial u|_{Q_2}}{\partial n_3}+d_2\frac{\partial v|_{Q_1}}{\partial n_3}=0,\quad d_3\left(\frac{\partial w|_{Q_2}}{\partial n_3}-\frac{\partial w|_{Q_1}}{\partial n_3}\right)=d_1\frac{\partial u|_{Q_2}}{\partial n_3}\quad on\quad \widetilde{\Gamma}_3,\\
& \frac{\partial u}{\partial \nu}=\frac{\partial v}{\partial \nu}=\frac{\partial w}{\partial \nu}=0\quad on\quad S,\\
& u(\cdot,0)=\gamma_1(\boldsymbol{z}_0),\ v(\cdot,0)=\gamma_2(\boldsymbol{z}_0),\ w(\cdot,0)=\gamma_3(\boldsymbol{z}_0)\quad in\quad \Omega.
\end{aligned}
$$

Three types of free boundaries appear in the limit problem. Furthermore, the dynamics is governed by a system of equations in each region separated by the free boundaries. On the interface Γ_1, v and w are zero and the fluxes for v and w are balanced as in the left relation in (3.11). There is another condition on the interface. u is usually positive around the interface and it is continuous. But u is not smooth. The right relation in (3.11) implies the flux is discontinuous across the free boundary. The intersection of the three axes $\{(0,0,w)\mid w\ge 0\}$, $\{(u,0,0)\mid u\ge 0\}$ and $\{(0,v,0)\mid v\ge 0\}$ on $\mathcal{A}_{\rm RD}$ indicates the existence of triple (or multiple) junctions. This theorem excludes the multiple junction points by assumption, but these points are included in the limit problem in a weak sense.

Sketch of proof. We check only the free boundary conditions (3.11) because the other properties are obtained straightforwardly or similarly. For $(x_1,t_1)\in\widetilde{\Gamma}_1$, there is a cylinder $D=B(x_1,r)\times(t_1-r,t_1+r)\subset Q$ such that $D=(Q_2\cup Q_3\cup\Gamma_1)\cap D$ and Γ_1 is a smooth hypersurface in D. Noting that $z_1=-u$, $\phi_1(\boldsymbol{z})=-d_1u$ in Q_2 and $z_1=v-u$, $\phi_1(\boldsymbol{z})=d_2v-d_1u$ in Q_3, we deduce from Definition 3.1 for $i=1$ that

$$
\begin{aligned}
&\iint_{D\cap Q_2}\left(\frac{\partial u}{\partial t}-d_1\Delta u-f_1(u,0,w)\right)\zeta\,dxdt-\iint_{D\cap Q_3}\left(\frac{\partial v}{\partial t}-d_2\Delta v-f_2(u,v,0)\right)\zeta\,dxdt\\
&\qquad+\iint_{D\cap Q_3}\left(\frac{\partial u}{\partial t}-d_1\Delta u-f_1(u,v,0)\right)\zeta\,dxdt\\
&\quad=-d_1\iint_{D\cap\Gamma_1}\frac{\partial u|_{Q_2}}{\partial n_1}\zeta\,dxdt-\iint_{D\cap\Gamma_1}\left(d_2\frac{\partial v|_{Q_3}}{\partial n_1}-d_1\frac{\partial u|_{Q_3}}{\partial n_1}\right)\zeta\,dxdt
\end{aligned}
$$

for all $\zeta\in C_0^\infty(D)$. It follows from (3.9) and (3.10) that

$$
d_1\left(\frac{\partial u|_{Q_3}}{\partial n_1}-\frac{\partial u|_{Q_2}}{\partial n_1}\right)=d_2\frac{\partial v|_{Q_3}}{\partial n_1}
$$

on $D\cap\Gamma_1$. Analogously, we deduce from Definition 3.1 for $i=2$ that

$$
d_1\left(\frac{\partial u|_{Q_2}}{\partial n_1}-\frac{\partial u|_{Q_3}}{\partial n_1}\right)=d_3\frac{\partial w|_{Q_2}}{\partial n_1}
$$

on $D \cap \Gamma_1$. Hence, we get (3.11). □

§ 4. Numerical experiments

In this section, numerical experiments are carried out to understand the fast reaction limit of $(\mathrm{RD})^k$ and to capture the free boundaries in the limit. We have already obtained a weak form (CD) of the limit free boundary problem. Therefore, if we have a numerical solution of (CD), the interface is captured immediately from the numerical solution. Thus, all we have to do is to consider numerical scheme for (CD) when we want to capture the interfaces numerically. Murakawa [14] proposed a linear discrete-time scheme to approximate general nonlinear cross-diffusion systems of the type of (CD). The scheme is as follows: We denote by $\tau = T/N_T$ ($N_T \in \mathbb{N}$) the time step size. Put

$$\boldsymbol{Z}^0 = \boldsymbol{z}_0^\tau.$$

Here, $\boldsymbol{z}_0^\tau \in H^1(\Omega)^2$ is an approximation to $\boldsymbol{z}_0 \in L^2(\Omega)^2$. For $n = 1, 2, \ldots, N_T$, find $\boldsymbol{Z}^n$ and $\boldsymbol{\Theta}^n$ such that

$$\text{(4.1)} \qquad \begin{cases} \boldsymbol{\Theta}^n - \dfrac{\tau}{\mu}\Delta\boldsymbol{\Theta}^n = \boldsymbol{\phi}(\boldsymbol{Z}^{n-1}) + \dfrac{\tau}{\mu}\boldsymbol{F}(\boldsymbol{Z}^{n-1}) & \text{in} \quad \Omega, \\ \dfrac{\partial \boldsymbol{\Theta}^n}{\partial \nu} = \boldsymbol{0} & \text{on} \quad \partial\Omega, \\ \boldsymbol{Z}^n = \boldsymbol{Z}^{n-1} + \mu(\boldsymbol{\Theta}^n - \boldsymbol{\phi}(\boldsymbol{Z}^{n-1})) & \text{in} \quad \Omega, \end{cases}$$

where μ is a fixed positive constant (in the simulation, we chose $\mu = 10^4$). Murakawa [14] showed that $\boldsymbol{Z}^n$ and $\boldsymbol{\Theta}^n$ approximate $\boldsymbol{z}(\cdot, \tau n)$ and $\boldsymbol{\phi}(\boldsymbol{z}(\cdot, \tau n))$, respectively. This scheme is quite simple. The scheme amounts to solving two linear elliptic equations, followed by explicit algebraic corrections at each time step. After discretizing the scheme in space, we obtain an easy to implement and stable numerical scheme for (CD). We employ the scheme (4.1) to obtain numerical solutions of (CD) and use a semi-implicit time discretization scheme to get numerical solutions of $(\mathrm{RD})^k$. The finite difference method is adopted to discretize the schemes in space.

We carried out numerical simulations for (CD) and $(\mathrm{RD})^k$ with $\Omega = (0,1)^2$, $d_1 = 4 \times 10^{-5}$, $d_2 = 2 \times 10^{-5}$ and $d_3 = 10^{-5}$. The functions f_i are given by the competition system of Lotka-Volterra type:

$$\begin{cases} f_1(u, v, w) = u(1 - u - 0.2v - 0.6w), \\ f_2(u, v, w) = v(1 - 0.6u - v - 0.2w), \\ f_3(u, v, w) = 3w(1 - 0.2u - 0.6v - w). \end{cases}$$

Figure 2 shows initial data and numerical solutions for (CD) at time $t = 100$, 200, 300, 400. The figures in the first, second and third rows denote the profiles of $u = \gamma_1(\boldsymbol{z})$,

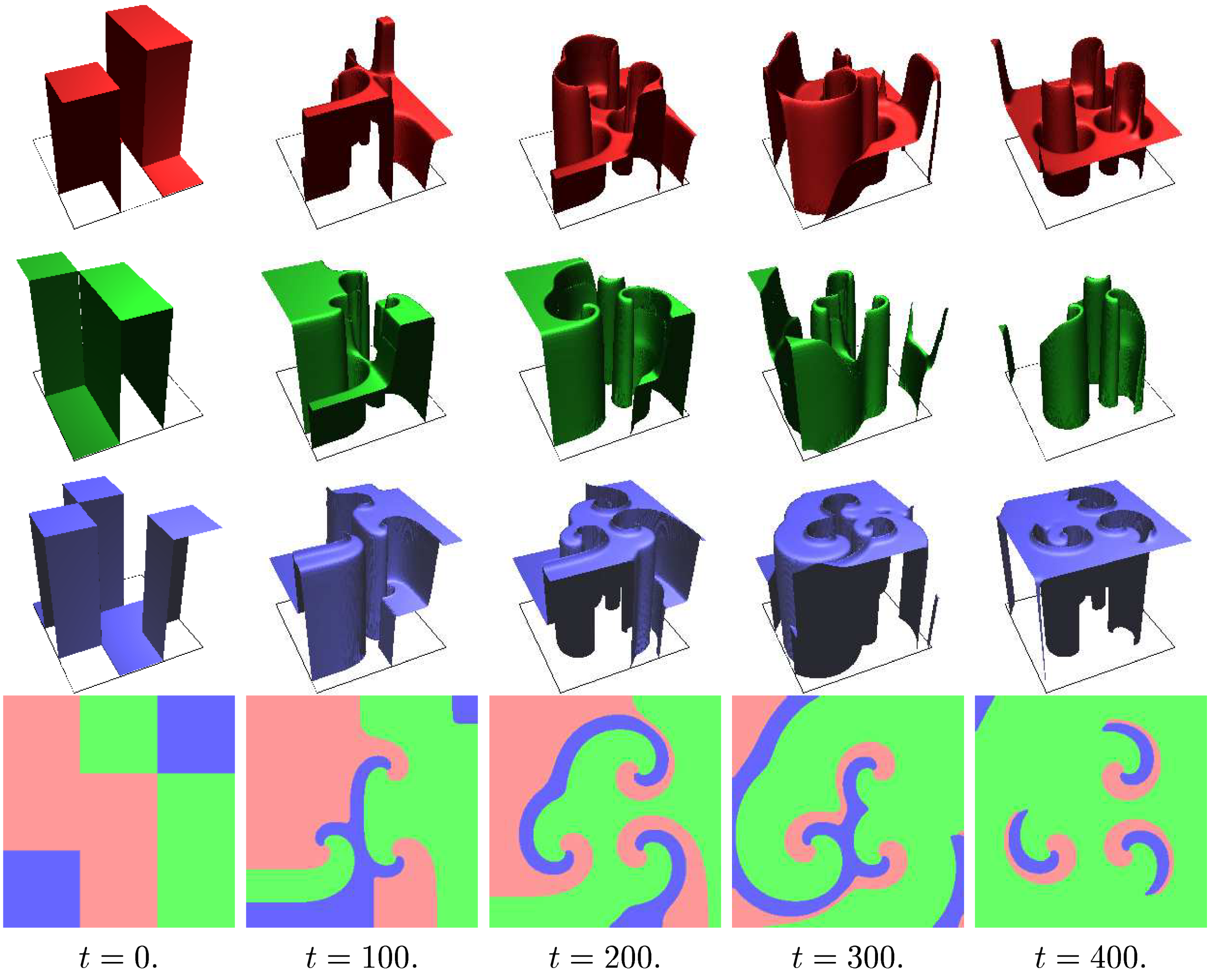
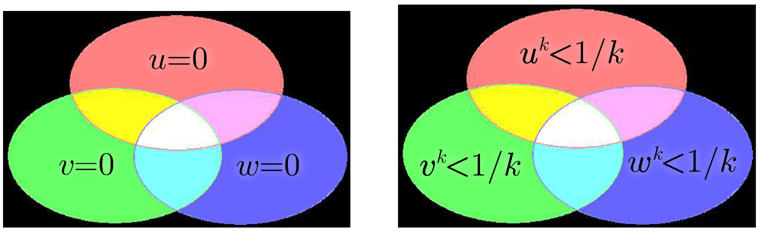


Figure 2. Numerical solutions of (CD).

$v = \gamma_2(\boldsymbol{z})$ and $w = \gamma_3(\boldsymbol{z})$, respectively. Here, $\boldsymbol{z}$ is a numerical solution of (CD). In order to make sure of our theoretical results, we painted the regions with different colors (Figure 3 (a)) in the last row in Figure 2. The domain Ω is completely divided into three regions by the free boundaries, that is, one of the components is zero and others are positive at each point. This fact is reasonable because of the definition of γ_i. We can observe clustering spirals. Looking at the numerical solutions, in particular, v, we can see the discontinuities of the flux across the free boundaries.

Since the numerical solutions for u^k, v^k, w^k are positive almost everywhere, we regard the region $\{x \in Q \mid u^k(x,t) < 1/k\}$ as an approximation of $\Omega_1(t)$ (see Figure 3 (b)). Figure 4 illustrates numerically approximated regions of (CD) and $(\mathrm{RD})^k$ with $k = 10^5$, 10^4, 10^3. We can say similar thing about the numerical solutions of $(\mathrm{RD})^k$ to that of (CD). The domain Ω is divided into three regions, that is, one of the components is close to zero and others are not close to zero at each point except for points near the



(a) for (CD) (b) for $(\mathrm{RD})^k$

Figure 3. Colors for approximated regions which correspond to $\Omega_1(t)$ (salmon), $\Omega_2(t)$ (yellow green) and $\Omega_3(t)$ (royal blue) respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

interfaces. We observe that the numerical solutions of $(\mathrm{RD})^k$ converge to that of (CD) as k becomes large, and the limit free boundaries are captured.

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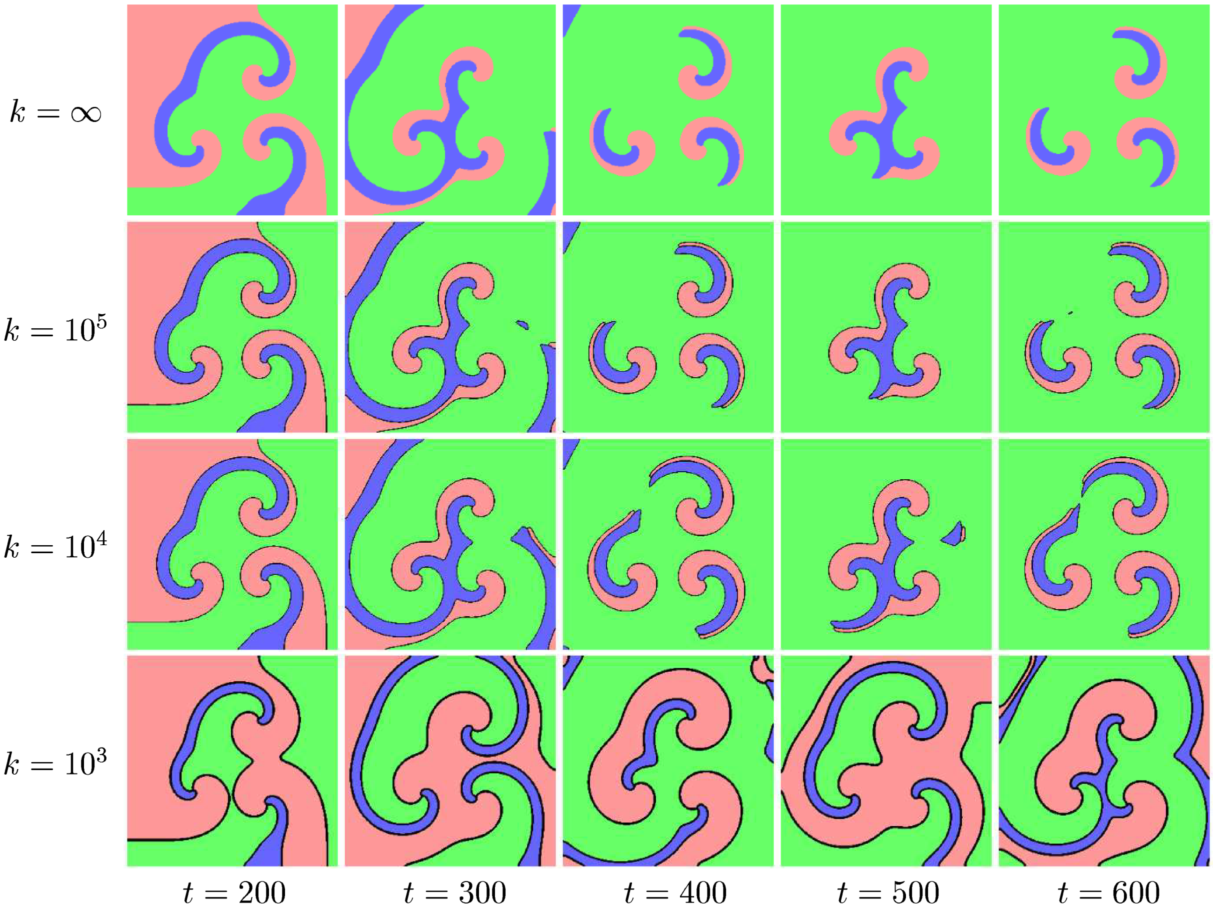

Figure 4. Numerical solutions for various choices of the parameter k. $k = \infty$ implies the limit problem (CD).

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