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Universal bound for stationary patterns of an adsorbate-induced phase transition model

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Abstract. In the catalytic oxidation of carbon monoxide molecules (CO) on platinum surface (Pt), various *pattern formations* of densities of CO molecules have attracted many chemists and mathematicians since the great contributions by Ertl (e.g., [15]). Hildebrand [2] has proposed a reaction-diffusion-advection system to give mathematical understand for such pattern formations from macroscopic point of view. In a previous paper [6], we obtain sufficient conditions of the existence (or nonexistence) of stationary patterns of the system. However, the L^∞-boundedness for all stationary patterns have not yet been obtained. In this paper, we show that all stationary patterns of the system possess a universal L^∞ bound. This result yields a validity of the system from the modelling point of view.

Keywords. reaction-diffusion-advection system, stationary pattern, universal bound

1. Introduction

In the field of surface chemistry, chemical mechanism in a catalytic oxidation of carbon monoxide molecules (CO) on platinum surface (Pt) have been studied. Among other things, owing to great contributions by Ertl (e.g., [15]), several pattern formations of densities of molecules on the Pt surface can be observed by special electron microscopes. In order to reveal the mechanism of such pattern formations from the mathematical view-point, several models of partial differential equations have been studied (e.g., [1]-[7], [9]-[14]). In this paper, we are concerned with the following reaction-diffusion-advection model proposed in [2];

$$
\text{(P)}\quad
\begin{cases}
u_t = d\Delta u + u(1-u)(u+v-1) & \text{in } \Omega\times(0,\infty),\\
v_t = \mathcal{D}\Delta v + \mathcal{D}\alpha\nabla\cdot\{v(1-v)\nabla\chi(u)\} + g(u,v) & \\
 & \text{in } \Omega\times(0,\infty),\\
\dfrac{\partial u}{\partial\nu} = \dfrac{\partial v}{\partial\nu} = 0 & \text{on } \partial\Omega\times(0,\infty),\\
u(\,\cdot\,,0) = u_0 \ge 0,\quad v(\,\cdot\,,0) = v_0 \ge 0 & \text{in } \Omega,
\end{cases}
$$

where $\Omega\subset\mathbb{R}^2$ is a bounded domain with smooth boundary $\partial\Omega$ and ν is the outward unit normal vector on $\partial\Omega$. The domain Ω corresonds to the Pt surface. The unknown functions $u = u(x,t)$ and $v = v(x,t)$ denote a chemical structural state of Pt surface and the adsorbate coverage rate against Pt surface by CO molecules at position $x\in\Omega$ and time $t\in[0,\ \infty)$, respectively. In the first equation, positive coefficient d represents the diffusion of u and the reaction term $u(1-u)(u+v-1)$ is *bistable* which means that the structural state possesses two stable constant equilibria $u = 0$ and $u = 1$. In the advection term $\alpha\nabla\cdot\{v(1-v)\nabla\chi(u)\}$, α is a positive constant and $\chi(u)$ yields a surface potential given by

$$\chi(u) = u^2(2u-3), \tag{1}$$

which is monotone decreasing for $u\in(0,1)$. From a chemical view-point, Δv denotes the diffusion of CO molecules by Fick's law and $\alpha\nabla\cdot\{v(1-v)\nabla\chi(u)\}$ represents viscous flow of CO molecules induced by the gradient of the surface potential $\chi(u)$. Here, $v(1-v)$ means that CO molecules can pass preferentially through vacant adsorbate sites on the surface. Therefore, it can be said that positive coefficient $\mathcal{D}$ represents mobility of CO molecules. The reaction term in the second equation is given by

$$g(u,v) = c(1-v) - ae^{\alpha\chi(u)}v - bv, \tag{2}$$

where a, b and c are positive constants. Here $c(1-v)$ represents adsorption of CO molecules against Pt surface. Both $-ae^{\alpha\chi(u)}$ and $-bv$ denote desorption of CO molecules from the surface into the gas phase. The former is a thermodynamical desorption depending on the surface potential $\chi(u)$ and the latter is a chemical desorption driven by the oxidation.

From the modelling aspect, we are interested in spatio-temporal behaviours of solutions (u,v) which fulfill

$$0 < u < 1 \quad\text{and}\quad 0 < v < 1. \tag{3}$$

Indeed, Tsujikawa and Yagi [14] have proved that, in a suitable functional space, for each initial value (u_0,v_0) satisfying (3) in Ω, (P) has a unique solution (u,v) and it also satisfies (3) for $(x,t)\in\Omega\times(0,\infty)$.

Concerning stationary patterns of (P), we obtain sufficient conditions on the existence (or nonexistence) of nonconstant solutions of the associate stationary problem ([6]);

$$\text{(SP)}\quad \begin{cases} d\Delta u + u(1-u)(u+v-1) = 0 & \text{in } \Omega, \\ \mathcal{D}\Delta v + \mathcal{D}\alpha\nabla\cdot\{v(1-v)\nabla\chi(u)\} + g(u,v) = 0 & \text{in } \Omega, \\ \dfrac{\partial u}{\partial \nu} = \dfrac{\partial v}{\partial \nu} = 0 & \text{on } \partial\Omega, \\ u \geq 0, \quad v \geq 0 & \text{in } \Omega. \end{cases}$$

According to our results in [6, Theorems 1.1 and 1.2], there exist small ranges of d such that (SP) has at least one nonconstant solutions:

Theorem 1. *For any fixed $(\mathcal{D}, \alpha, a, b, c)$, there exists a positive sequence $\{d_j\}_{j=0}^{\infty}$ with*

$$d_0 > d_1 \geq d_2 \geq \cdots \geq d_j \geq \cdots \to 0 \quad (j \to \infty)$$

such that

(i) *if $d \geq d_0$, then (SP) has no nonconstant solution with property (3),*

(ii) *if $d \in (d_{j+1}, d_j)$ and $d_{j+1} \neq d_j$ and j is odd, then (SP) has at least one nonconstant solution (u, v) with property (3).*

In view of Theorem 1, it remains an unsettled question whether all nonconstant solutions of (SP) satisfy (3). Since our paper [6] has found nonconstant solutions in the set of (u, v) satisfying (3), the above question still remains open. In the present paper, we shall prove that all nonconstant solutions of (SP) satisfy (3). This result implies a validity from the modelling point of view.

2. Universal bound for stationary patterns

In this section, we show that any nonconstant solution (u, v) of (SP) satisfies (3) in Ω. Before stating our results, we collect all constant solutions of (SP). It is easily verified that (SP) possesses three constant solutions

$$(u, v) = \left(0, \frac{c}{a+b+c}\right), \quad (u, v) = \left(1, \frac{c}{ae^{-\alpha}+b+c}\right) \tag{4}$$

and (u_*, v_*) with $u_* + v_* - 1 = 0$ and $g(u_*, v_*) = 0$. It is easily verified from (2) that (u_*, v_*) satisfies

$$\frac{ae^{-\alpha}+b}{ae^{-\alpha}+b+c} < u_* < \frac{a+b}{a+b+c}$$

and

$$\frac{c}{a+b+c} < v_* < \frac{c}{ae^{-\alpha}+b+c}.$$

The following theorem is a main result of this paper.

Theorem 2. *Let (u, v) be any solution of (SP) except two constant solutions in (4). Then (u, v) satisfies the following estimates;*

(i) $0 < u(x) < 1$ *for* $x \in \overline{\Omega}$,

(ii) $\dfrac{c}{a+b+c} < \dfrac{1}{|\Omega|}\displaystyle\int_{\Omega} v \,\mathrm{d}x < \dfrac{c}{ae^{-\alpha}+b+c}$,

(iii) $0 < v(x) < 1$ *for* $x \in \overline{\Omega}$.

For the proofs of (i) and (ii), we refer to our previous paper [6, Lemma 2.2]. The L^∞-estimate (iii) for v is a new result and its proof is our main task of this paper. To do so, we prepare the L^2-estimate of ∇u.

Lemma 1. *Let (u, v) be any positive solution of (SP). Then u satisfies*

$$\frac{d}{|\Omega|}\int_{\Omega} |\nabla u|^2 \,\mathrm{d}x \leq \frac{4c}{27(ae^{-\alpha}+b+c)}.$$

Proof. We multiply the first equation by u and integrate the resulting expression to get

$$\begin{aligned} d\int_{\Omega} |\nabla u|^2 \,\mathrm{d}x &= \int_{\Omega} u^2(1-u)(u+v-1)\,\mathrm{d}x \\ &\leq \int_{\Omega} u^2(1-u)v\,\mathrm{d}x. \end{aligned} \tag{5}$$

Since $u^2(1-u) \leq 4/27$ for $0 < u < 1$, then (5) and (ii) of Theorem 2 yield the desired estimate. □

Proof of Theorem 2. Let (u, v) be any solution of (SP) except two constant solutions in (4). We first prove $v \leq 1$ in Ω along a contradiction argument. Suppose that

$$\mathcal{K} = \{x \in \Omega \,:\, v(x) > 1\}$$

possesses a positive measure. In a case when $\partial\mathcal{K}$ is smooth, we can use the divergence theorem in the second equation of (SP) to obtain

$$\begin{aligned} &\int_{\mathcal{K}} \{\, c - (ae^{\alpha\chi(u)} + b + c)v \,\}\,\mathrm{d}x \\ &= -\mathcal{D}\int_{\mathcal{K}} \nabla\cdot\{\, \nabla v + \alpha v(1-v)\,\nabla\chi(u) \,\}\,\mathrm{d}x \\ &= -\mathcal{D}\int_{\partial\mathcal{K}} \underbrace{\nabla v\cdot\nu}_{\leq 0}\,\mathrm{d}\sigma \\ &\quad -\mathcal{D}\alpha\int_{\partial\mathcal{K}} v \underbrace{(1-v)}_{=0 \text{ on } \partial\mathcal{K}\cap\Omega} \chi_u(u) \underbrace{\nabla u\cdot\nu}_{=0 \text{ on } \partial\mathcal{K}\cap\partial\Omega} \mathrm{d}\sigma, \end{aligned} \tag{6}$$

where $\nu = \nu(x)$ denotes the outer unit normal vector at $x \in \partial\mathcal{K}$. By the definition of $\mathcal{K}$ and the Neumann boundary condition on $\partial\Omega$, we observe that

$$\nabla v\cdot\nu \begin{cases} \leq 0 & \text{on } \partial\mathcal{K}\cap\Omega, \\ = 0 & \text{on } \partial\mathcal{K}\cap\partial\Omega \end{cases} \tag{7}$$

and

$$1 - v \begin{cases} = 0 & \text{on } \partial\mathcal{K}\cap\Omega, \\ \leq 0 & \text{on } \partial\mathcal{K}\cap\partial\Omega. \end{cases} \tag{8}$$

Since $\chi_u(u) \leq 0$ by (1) and (i) of Theorem 2, then (6)-(8) imply

$$\int_{\mathcal{K}} \{\, c - (ae^{\alpha\chi(u)} + b + c)v \,\}\,\mathrm{d}x \geq 0.$$

Hence it follows that

$$\frac{1}{|\mathcal{K}|}\int_{\mathcal{K}} v\,\mathrm{d}x \leq \frac{c}{ae^{-\alpha}+b+c} < 1,$$

which yields a contradiction to the definition of $\mathcal{K}$. Then we deduce $v \le 1$ in Ω. Since a similar argument leads to $v \ge 0$ in Ω, we know $0 \le v \le 1$ in Ω provided that $\partial\mathcal{K}$ is smooth.

However if $\partial\mathcal{K}$ possesses singularity, the divergence theorem in (6) is not applicable. Note that any singular point $x_* \in \partial\mathcal{K}$ satisfies $v(x_*) = 1$ and $\nabla v(x_*) = 0$. Indeed, if $v(x_*) > 1$, then $x_* \in \partial\Omega \cap \partial\mathcal{K}$ and there exists a neighbourhood $\mathcal{N}$ of x_* such that $v > 1$ on $\mathcal{N} \cap \partial\mathcal{K}$ by the continuity of v. This fact means $(\mathcal{N} \cap \partial\mathcal{K}) \subset \partial\Omega$, namely, $\partial\mathcal{K}$ is smooth near x_* because of the smoothness of $\partial\Omega$. This yields a contradiction. On the other hand, if $v(x_*) = 1$ and $\nabla v(x_*) \ne 0$, then the implicit function theorem ensures the level set $\{v = 1\}$ is smooth near x_*, which is also a contradiction.

Then, we discuss the case when there exists $x_* \in \partial\mathcal{K}$ such that

$$v(x_*) = 1 \quad \text{and} \quad \nabla v(x_*) = 0. \tag{9}$$

In such a singular case, we recall the Sard theorem which implies that the set of critical values of v has Lebesgue measure zero. Since 1 is a critical value of v by (9), the Sard theorem ensures a sequence $\{\varepsilon_n\}$ with $\lim_{n\to\infty} \varepsilon_n = 0$ such that $1 + \varepsilon_n$ are regular values of v for all $n \in \mathbb{N}$. Hence this fact implies

$$\mathcal{K}_n := \{x \in \Omega \,:\, v(x) > 1 + \varepsilon_n\}$$

possess smooth boundaries $\partial\mathcal{K}_n$. Then we can use the divergence theorem over $\mathcal{K}_n$ to see

$$\begin{aligned}
&\int_{\mathcal{K}_n} \{\, c - (ae^{\alpha\chi(u)} + b + c)v \,\}\, \mathrm{d}x \\
&= -\mathcal{D} \int_{\mathcal{K}_n} \nabla\cdot\{\, \nabla v + \alpha v(1-v)\, \nabla\chi(u) \,\}\, \mathrm{d}x \\
&= -\mathcal{D} \int_{\partial\mathcal{K}_n} \nabla v\cdot\nu \, \mathrm{d}\sigma - \mathcal{D}\alpha \int_{\partial\mathcal{K}_n} v(1-v)\, \nabla\chi(u)\cdot\nu \, \mathrm{d}\sigma.
\end{aligned} \tag{10}$$

The definition of $\mathcal{K}_n$ and the boundary conditions on v imply $\nabla v \cdot \nu \le 0$ on $\partial\mathcal{K}_n$ and $v = 1 + \varepsilon_n$ on $\partial K_n \cap \Omega$. Furthermore, since $\nabla\chi(u)\cdot\nu = 0$ on $\partial\mathcal{K}_n \cap \partial\Omega$ by the boundary condition on u and (1), then we use the divergence theorem again in (10) to see

$$\begin{aligned}
&\int_{\mathcal{K}_n} \{\, c - (ae^{\alpha\chi(u)} + b + c)v \,\}\, \mathrm{d}x \\
&\ge \mathcal{D}\alpha(1+\varepsilon_n)\varepsilon_n \int_{\partial\mathcal{K}_n} \nabla\chi(u)\cdot\nu \, \mathrm{d}\sigma \\
&= \mathcal{D}\alpha(1+\varepsilon_n)\varepsilon_n \int_{\mathcal{K}_n} \Delta\chi(u) \, \mathrm{d}x.
\end{aligned} \tag{11}$$

It follows from (1) and (i) of Theorem 2 that

$$\begin{aligned}
\left| \int_{\mathcal{K}_n} \Delta\chi(u)\, \mathrm{d}x \right| &= \left| \int_{\mathcal{K}_n} \big(\chi_{uu}(u)|\nabla u|^2 + \chi_u(u)\Delta u\big)\, \mathrm{d}x \right| \\
&\le C \left(\int_{\mathcal{K}_n} |\nabla u|^2 \, \mathrm{d}x + \int_{\mathcal{K}_n} |\Delta u| \, \mathrm{d}x \right)
\end{aligned}$$

for some positive constant C independent of n. We recall Lemma 1 to know that $\|\nabla u\|_{L^2(\mathcal{K}_n)}$ is uniformly bounded with respect to n. Furthermore it follows from (i) and (ii) of Theorem 2 that

$$\int_{\mathcal{K}_n} |\Delta u| \, \mathrm{d}x = \frac{1}{d} \int_{\mathcal{K}_n} |u(1-u)(u+v-1)| \, \mathrm{d}x$$

is also uniformly bounded with respect to n. Then letting $n \to \infty$ in (11) leads us to

$$\frac{1}{|\mathcal{K}|} \int_{\mathcal{K}} (ae^{\alpha\chi(u)} + b + c)v \, \mathrm{d}x \le c.$$

Therefore it follows that

$$\frac{1}{|\mathcal{K}|} \int_{\mathcal{K}} v \, \mathrm{d}x \le \frac{c}{ae^{-\alpha} + b + c} < 1,$$

which gives a contradiction to the definition of $\mathcal{K}$. Obviously, a similar procedure leads to $v \ge 0$ in Ω. Then we can deduce $0 \le v \le 1$ in Ω.

Finally we prove the strict inequalities in (iii) of Theorem 2. Suppose for contradiction that $v(x_0) = \min_{\overline{\Omega}} v = 0$ for some $x_0 \in \overline{\Omega}$. The second equation of (SP) can be expressed by

$$\begin{aligned}
&\Delta v + \alpha(1-2v)\chi_u(u)\nabla u\cdot\nabla v \\
&+\alpha v(1-v)\left\{\chi_{uu}(u)|\nabla u|^2 + \chi_u(u)\Delta u\right\} + \frac{g(u,v)}{\mathcal{D}} = 0.
\end{aligned}$$

By using the maximum principle (see e.g., Lou-Ni [8, Lemma 2.1]), we see

$$\frac{g(u(x_0), v(x_0))}{\mathcal{D}} = \frac{c}{\mathcal{D}} \le 0.$$

Hence this is a contradiction. Similarly we can show $v < 1$ in Ω. Therefore we complete the proof of Theorem 2. □

Once we obtain Theorem 2, the elliptic regularity theory and the Sobolev embedding theorem lead us to a priori estimates for $\|u\|_{W^{2,p}}$ and $\|v\|_{W^{2,p}}$ uniformly with respect to $\mathcal{D}$.

Theorem 3. *Let $p > 1$. There exists a positive constant M independent of $\mathcal{D}$ such that any solution (u, v) of* (SP) *satisfies*

$$\|u\|_{W^{2,p}(\Omega)} \le M, \qquad \|v\|_{W^{2,p}(\Omega)} \le M.$$

Proof. The proof is essentially same as that of [6, Theorem 2.4]. □

Thanks to Theorem 3, we can derive a *shadow system* of (SP) as $\mathcal{D} \to \infty$:

Theorem 4. *For any positive sequence $\{\mathcal{D}_n\}$ with $\lim_{n\to\infty} \mathcal{D}_n = \infty$, let (u_n, v_n) be any sequence of solutions of* (SP) *with $\mathcal{D} = \mathcal{D}_n$. Then there exists a positive solution (u_∞, v_∞) of*

$$\begin{cases}
d\Delta u + u(1-u)(u+v-1) = 0 & \text{in } \Omega, \\
\Delta v + \alpha\nabla\cdot\{v(1-v)\nabla\chi(u)\} = 0 & \text{in } \Omega, \\
\dfrac{\partial u}{\partial \nu} = \dfrac{\partial v}{\partial \nu} = 0 & \text{on } \partial\Omega
\end{cases} \tag{12}$$

with $0 < u,\, v < 1$ *in* Ω *and*

$$\int_\Omega g(u,v)\,\mathrm{d}x = 0 \tag{13}$$

such that

$$\lim_{n\to\infty}(u_n, v_n) = (u_\infty, v_\infty) \quad in \quad C(\overline{\Omega}) \times C(\overline{\Omega}),$$

passing to a subsequence.

The proof of Theorem 4 can be carried out by a compactness argument based on the combination of the elliptic regularity, the Sobolev embedding and Theorem 3 (see [7] for detail).

To study the shadow system (12)-(13) is important in the sense that solutions of (12)-(13) can approximate original solutions of (SP) when the movements $\mathcal{D}$ of CO molecules is large. In [7], we also obtain the global bifurcation structure of solutions of (12)-(13) in a simplified one-dimensional case.

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