108. *Note on Chemical Interfacial Reaction Models*

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§ 1. **Introduction.** We consider the following parabolic system with nonlinear boundary conditions. Find $u_i=u_i(x,t)$ $(i=1,2,3)$ satisfying

$$
(\mathrm{P}) \quad \begin{cases}
(1) \quad a_i(x)\dfrac{\partial u_i}{\partial t}=\dfrac{\partial^2 u_i}{\partial x^2}, \quad x\in I\equiv(0,1), & t\in(0,\infty),\\[2mm]
(2) \quad \dfrac{\partial u_i}{\partial x}(0,t)=R_i(u_1(0,t),\ u_2(0,t),\ u_3(0,t)), & t\in(0,\infty),\\[2mm]
(3) \quad \dfrac{\partial u_i}{\partial x}(1,t)=0, & t\in(0,\infty),\\[2mm]
(4) \quad u_i(x,0)=\varphi_i(x), \quad x\in I,
\end{cases}
$$

where a_i and R_i $(i=1,2,3)$ are given functions and φ_i $(i=1,2,3)$ are given initial data. Concerning a_i and R_i $(i=1,2,3)$, we introduce the following assumptions.

(A.1) $a_i\geqq 0$ on $\bar{I}\equiv[0,1]$, $a_i\in C^\infty(\bar{I})$, $a_i>0$ on $[0,1)$.

(R.1) $R_i(u_1,u_2,u_3)\in C^\infty(U)$, where U is an open set in $\boldsymbol{R}^3$ satisfying $U\supset[-\delta,\delta]^3\cup[0,\infty)^3$ with some positive constant δ.

(R.2) For any compact subset K of U, there exists a positive constant c_K such that

$$\sum_{i=1}^3 R_i(u_1,u_2,u_3)u_i^-\leqq c_K\sum_{i=1}^3|u_i^-|^2 \qquad \text{for any } (u_1,u_2,u_3)\in K,$$

where $u_i^-=-\min\{u_i,0\}$.

(R.3) There exist positive constants α_i $(i=1,2,3)$ such that

$$\sum_{i=1}^3\alpha_i R_i(u_1,u_2,u_3)=0 \qquad \text{for all } (u_1,u_2,u_3)\in U.$$

(R.4) There exists a positive constant c such that

$$-\sum_{i=1}^3 R_i(u_1,u_2,u_3)u_i^{2p-1}\leqq c\sum_{i=1}^3|u_i|^{2p}$$

$$\text{for all } (u_1,u_2,u_3)\in[0,\infty)^3 \text{ and } p\in[1,\infty).$$

Our motivation for (P) comes from the chemical interfacial model proposed by Kawano, Kusano, Kondo and Nakashio [3]. They analyzed the kinetics of interfacial reaction by comparing the chemical experiments with numerical simulation of the models. After suitable transformation, their typical model is reduced to (P) with the case,

$$
(5) \quad \begin{aligned}
&a_i(x)=k_i(1-x^2) \qquad (i=1,2,3),\\
&R_1=R_2=-R_3=\frac{u_1u_2-k_7u_3}{k_4+k_5u_2+k_6u_1u_2},
\end{aligned}
$$

where k_i $(i=1,\cdots,7)$ are positive constants determined by chemical substances. It is easily seen that the conditions (A.1), (R.1), (R.2), (R.3) and (R.4) are satisfied by taking

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$$U=\{(u_1, u_2, u_3) : k_4+k_5u_2+k_6u_1u_2>0\},$$
$$\alpha_1=1, \quad \alpha_2=1, \quad \alpha_3=2.$$

In (5), u_i $(i=1,2,3)$ correspond to the concentration of chemical substances, a_i $(i=1,2,3)$ correspond to the velocity distribution function of laminar flow, and R_i $(i=1,2,3)$ are related with the kinetics of the chemical reaction at the interface. We should note that the coefficient a_i $(i=1,2,3)$ in (1) vanish at $x=1$ and the boundary conditions (2) at $x=0$ are nonlinear with the non-monotone properties with respect to (u_1, u_2, u_3).

There are some results on the parabolic equations with nonlinear boundary conditions (e.g. [2]). However, because of non-monotone boundary conditions, the existing theory will not be useful for deriving the global existence of non-negative solutions to (P).

§ 2. Main results. Our first theorem is concerned with the existence, uniqueness and regularity of the problem (P) for the initial data with the compatibility condition.

Theorem 1. *Suppose that* (A.1), (R.1), (R.2), (R.3) *and* (R.4) *hold. Assume that the initial data* $(\varphi_1, \varphi_2, \varphi_3)$ *satisfies*

$$\begin{aligned} &\varphi_i \in H^2(I), \qquad a_i^{-1/2}\varphi_{i,xx} \in L^2(I), \\ &\varphi_i \geqq 0 \qquad on\ \bar{I}, \qquad\qquad\qquad\qquad (i=1,2,3) \\ &\varphi_{i,x}(0)=R_i(\varphi_1(0), \varphi_2(0), \varphi_3(0)), \quad \varphi_{i,x}(1)=0. \end{aligned}$$

Then there exists a unique solution (u_1, u_2, u_3) *of* (P) *such that*

$$\left.\begin{aligned} &u_i \in C([0,\infty); H^2(I)) \cap H^1_{\mathrm{loc}}(0,\infty; H^1(I)) \cap C^\infty(\bar{I}\times(0,\infty)), \\ &u_i \geqq 0 \qquad on\ \bar{I}\times[0,\infty). \end{aligned}\right. \qquad (i=1,2,3)$$

For more general initial data, we obtain the following result.

Theorem 2. *Suppose that* (A.1), (R.1), (R.2), (R.3) *and* (R.4) *hold. Assume that the initial data* $(\varphi_1, \varphi_2, \varphi_3)$ *satisfies*

$$\varphi_i \in L^\infty(I), \quad \varphi_i(x) \geqq 0 \quad on\ I. \qquad (i=1,2,3)$$

Then there exists a unique solution (u_1, u_2, u_3) *of* (P) *such that*

$$\left.\begin{aligned} &u_i \in C([0,\infty); L^2(I)) \cap C^\infty(\bar{I}\times(0,\infty)), \\ &u_i \geqq 0 \qquad on\ \bar{I}\times[0,\infty). \end{aligned}\right. \qquad (i=1,2,3)$$

Outline of the proof of Theorem 1. We construct a non-negative local solution in time by applying the contraction mapping principle, whose validity is assured by the assumptions (A.1), (R.1) and (R.2). In particular, (R.2) is used to prove the non-negativity of the solution. The major part is to derive an a priori L^∞-estimate independent of time. We employ Moser's technique [4] (see also Alikakos [1]). The assumption (R.3) assures an a priori L^1-estimate, and the assumption (R.4) enables us to get successively a priori L^p-estimates which are independent of p.

Outline of the proof of Theorem 2. It is sufficient to approximate the given data by some nice data which satisfy the compatibility condition.

We will discuss the details in [5].

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References

[1] N. D. Alikakos: An application of the invariance principle to reaction-diffusion equations. J. Diff. Eqs., **33**, 201–225 (1979).

[2] D. G. Aronson: A comparison method for stability analysis of nonlinear parabolic problems. SIAM Rev., **20**, 245–264 (1978).

[3] Y. Kawano, K. Kusano, K. Kondo and F. Nakashio: Extraction rate of acetic acid by long-chain alkylamine in horizontal rectangular channel. Kagaku Kōgaku Ronbunshu, **9**, 44–51 (1983) (in Japanese).

[4] J. Moser: A Harnack inequality for parabolic differential equations. Comm. Pure Appl. Math., **17**, 101–134 (1964).

[5] Y. Yamada and S. Yotsutani: Chemical interfacial reaction models (in preparation).