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Large-time behavior of solutions to a reaction-diffusion system with distributed microstructure

by

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Abstract

We study the large-time behavior of a class of reaction-diffusion systems with constant distributed microstructure arising when modeling diffusion and reaction in structured porous media. The main result of this Note is the following: As $t \to \infty$ the macroscopic concentration vanishes, while the microscopic concentrations reach constant concentration profiles independent of the shape of the microstructure.

1. Introduction

In this paper we describe the large-time behavior of solutions to a class of reaction-diffusion systems with distributed microstructure hosting a fast chemical reaction. The idea of distributed microstructure (or, more generally, double porosity) is understood here in the spirit of [1]. The prototypical physical scenario that we have in mind is the same as that discussed in [2]. Namely we consider a gas-liquid reaction

$$A + B \to \text{products}$$

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taking place within the pores $Y$ of a porous media $\Omega$. We assume that the species $A$ arrives by diffusion through air and water parts of $\Omega$ at the reaction place where it meets the other reactant – the mobile species $B$. We are particularly interested in situations when (1) is fast compared to the transport mechanisms involved. Such scenarios play an important role, for instance, in pattern formation in geochemistry [4], describing microbial growth in aggregated soils [5], or in forecasting chemical corrosion of concrete structures [6]. We aim at understanding the large-time dynamics when also the Thiele modulus associated to (1) is large, i.e. when reactants segregate in space leading to the occurrence within the microstructure of an internal free boundary where (1) concentrates. See [7,8] for comments on the general problematic and [3] for a rigorous fast-reaction asymptotics for finite times.

The results of this Note are preliminary in the sense that reaction (1) is not considered yet to be fast, and hence the interplay between $t \to \infty$ and high Thiele moduli is not included. Herein we prove that as $t \to \infty$ the macroscopic concentration $U$ vanishes, while the microscopic concentrations $u$ and $v$ reach constant concentration profiles independent of the shape of the microstructure. $U$ denotes in this context an averaged (macroscopic) concentration of species $A$ living in the gas-filled parts of the pores, while $u$ and $v$ are pore level (microscopic) concentrations of dissolved $A$ and respectively $B$ species.

2. A reaction-diffusion model with distributed microstructure

In the following, we formulate a one-dimensional version of the system of partial-differential equations (PDEs) modeling the structured transport and reaction corresponding to the setting indicated in section 1. However, it is worth noting that the reaction-diffusion model, the reported asymptotic behavior, and the working technique do not depend on the space dimension. Although everything can be rewritten with minimal effort in a $n$-dimensional setting, we prefer, for clarity reasons, to stick to the 1D situation.

Let $\theta := (1 - R)/2, S := (0, T), \Omega := (0, L), Y := (0, R)$, where $T, L, R \in (0, \infty)$. We denote by Problem $(P)$ the following two-scale system in one space dimension:

$$\theta \partial_t U - \theta \xi^2 \partial_{xx} U = -b(U - u|_{y=R}), \quad x \in \Omega, \quad t \in S$$  

$$\partial_t u - d_1 \partial_{yy} u = -\eta(u, v), \quad x \in \Omega, \quad y \in Y, \quad t \in S$$  

$$\partial_t v - d_2 \partial_{yy} v = -\alpha \eta(u, v), \quad x \in \Omega, \quad y \in Y, \quad t \in S$$

with boundary conditions on the microscale

$$d \partial_y u(t, x, R) = -b(u(t, x, R) - U(t, x)), \quad x \in \Omega, \quad t \in S$$

$$\partial_y u(t, x, 0) = \partial_y v(t, x, 0) = \partial_y v(t, x, R) = 0, \quad x \in \Omega, \quad t \in S$$

exterior boundary conditions

$$-D \partial_y U(t, 0) = \delta(U(t, 0) - U^{ext}(t)), \quad t \in S$$

$$D \partial_y U(t, R) = 0, \quad t \in S$$

and initial conditions

$$U(0, x) = U_0(x), \quad x \in \Omega$$

$$u(0, x, y) = u_0(x, y), \quad x \in \Omega, \quad y \in Y$$

$$v(0, x, y) = v_0(x, y), \quad x \in \Omega$$

Here the function $\eta(\cdot, \cdot)$ is positive and locally Lipschitz in each of the variables. The example we have in mind for our problem is

$$\eta(u, v) = \begin{cases} 
ku^p v^q, & \text{if both } u, v \text{ are positive} \\
0, & \text{otherwise}
\end{cases}$$
In (12), \( k \) is the reaction constant, \( p, q \geq 1 \) are partial orders of reaction, \( \alpha \) is a molecular weight, \( b \) and \( \delta \) are interfacial transport parameters, while \( D, d_j \) are diffusion coefficients. All involved parameters are strictly positive constants. Note that the coupling between the micro and macro scales is relatively weak and involves only “regularized” boundary terms [1]. We refer to problem (2)–(12) as problem (P).

Let us assume that:

(H1) \( U^{ext} \in H^1(S), U_0 \in H^1(\Omega), u_0, v_0 \in H^1(\Omega \times Y) \), and there exists a constant \( C_M > 0 \) such that \( 0 \leq U^{ext}, u_0, v_0 \leq C_M \) a.e. and standard compatibility conditions are satisfied.

(H2) There exist constants \( c > 0 \) and \( \mu > 0 \) such that \( U^{ext}(t) \leq \frac{c}{\mu + t} \) and \( \partial_t U^{ext} \leq -\frac{c}{\mu + t} \) for all \( t \geq 0 \).

To simplify the writing, we use the notation \( V_1 := H^1(\Omega), V_2 := L^2(\Omega; H^1(Y)) \), and \( V := V_1 \times [V_2]^2 \).

Our concept of weak formulation for the problem (P) is the following: Find \( U \in L^2(S; V_e) \) and \( u, v \in L^2(S; V_2) \) that satisfy (9)–(11) and

\[
\frac{d}{dt} \int_{\Omega} \theta U \phi + \int_{\Omega} \theta D \partial_x U \partial_x \phi + \theta \delta (U(t,0) - U^{ext}(t)) + \int_{\Omega} b(U - u)|_{y=R}(\phi - \Phi)|_{y=R} \\
+ \frac{d}{dt} \int_{\Omega} u \phi + \int_{\Omega} \int_{Y} d_1 \partial_u \partial_y \phi \Phi + \int_{\Omega} \int_{Y} k u v \phi = 0 \quad \forall (\phi, \Phi) \in V_1 \times V_2, \tag{13}
\]

\[
\frac{d}{dt} \int_{\Omega} v \psi + \int_{\Omega} \int_{Y} d_2 \partial_u \partial_y \psi + \int_{\Omega} \int_{Y} a k u v \psi = 0 \quad \forall \psi \in V_2. \tag{14}
\]

Remark 1 Problem (P) can be derived by means of a periodic homogenization strategy (cf. [11], e.g.). This strategy provides also a proof for the (global-in-time) existence of weak solutions to (P) provided assumption (H1) is satisfied. We illustrated this approach in [3], where in problem (P) the Robin boundary condition (7) is replaced by a non-homogeneous Dirichlet one. The same steps can be repeated here without major modifications.

3. Main result

**Theorem 3.1** Assume (H1) and (H2) to be fulfilled. Then the solution vector \((U, u, v)\) converges uniformly to a stationary solution of (P) as \( t \to \infty \).

**Sketch of the proof:**

We adapt to our reaction-diffusion scenario the working strategy developed in [9]. Multiplying by \( \partial_t U \) and \( \partial_t u \) the PDEs for \( U \) and \( u \) and integrating the results respectively over \( \Omega \) and \( \Omega \times Y \), we obtain:

\[
\theta \int_{\Omega} |\partial_t U|^2 + \theta D \frac{d}{dt} \int_{\Omega} |\partial_x U|^2 + \theta \delta (U(t,0) - U^{ext}(t)) |\partial_t U(t,0)| = -b \int_{\Omega} \partial_t U(U - u)|_{y=R}, \tag{15}
\]

\[
\int_{\Omega} \int_{Y} |\partial_t u|^2 + d_1 \frac{d}{dt} \int_{\Omega} \int_{Y} |\partial_y u|^2 + b \int_{\Omega} \int_{Y} \partial_t (u(t,x,R) - U(t,x)) = -k \int_{\Omega} \int_{Y} \partial_t uu v^q. \tag{16}
\]

Adding the latter two equations, we have

\[
\int_{\Omega} \int_{Y} |\partial_t U|^2 + \frac{d}{dt} \left( \int_{\Omega} \int_{Y} |\partial_y u|^2 \right) + \theta \delta (U(t,0) - U^{ext}(t)) |\partial_t U(t,0)| + b \int_{\Omega} (U(t,x) - u(t,x,R)) |\partial_t U - \partial_t u| = -k \int_{\Omega} \int_{Y} \partial_t uu v^q. \tag{17}
\]

Notice that

\[
\theta \delta (U(t,0) - U^{ext}(t)) |\partial_t U(t,0)| = \theta \delta \left( \frac{1}{2} \frac{d}{dt} U^2(t,0) - \frac{d}{dt} (U^{ext}(t) U(t,0)) + U(t,0) \partial_t U^{ext}(t) \right). \tag{18}
\]
The integration of (17) over \((0, T)\) yields

\[
\theta \int_0^T \int_\Omega |\partial_t U|^2 + \int_0^T \int_\Omega \int_Y |\partial_Y U|^2 + b \int_0^T \int_\Omega (U(t, x) - u(t, x, R))(\partial_t U - \partial_t u)
\]

\[
\leq -k \int_0^T \int_\Omega \int_Y u^p v^q \partial_t u + \theta \delta \int_0^T \int_\Omega \partial_t U(t, 0)(U^{ext}(t) - U(t, 0))
\]

\[
= -k \int_0^T \int_\Omega \int_Y u^p v^q \partial_t u - \theta \delta \int_0^T \int_\Omega \left[ \frac{1}{2} \frac{d}{dt} U^2(t, 0) - \frac{d}{dt} U^{ext}(t) \right]
\]

\[
= -k \int_0^T \int_\Omega \int_Y u^p v^q \partial_t u - \theta \delta(U^2(T, 0) - U(0, 0))
\]

\[
+ \theta \delta(U^{ext}(T)U(T, 0) - U^{ext}(0)U(0, 0)) - \theta k \int_0^T \partial_t U^{ext}(t)U(t, 0)
\]

\[
\leq -k \int_0^T \int_\Omega \int_Y u^p v^q \partial_t u + c,
\]  

(19)

where \(c\) depends on \(\delta, b, \theta, \mu, p,\) and \(q\) but it does not depend on \(T.\) Consequently, (19) shows that

\[
\int_0^T \int_\Omega \int_Y |\partial_t U|^2 + \int_0^T \int_\Omega \int_Y |\partial_Y U|^2 \leq -k \int_0^T \int_\Omega \int_Y u^p v^q \partial_t u + c.
\]  

(20)

Moreover, we also have

\[
\int_0^T \int_\Omega \int_Y |\partial_t U|^2 + d_1 \int_0^T \int_\Omega \int_Y |\partial_t v|^2 \leq -\alpha k \int_0^T \int_\Omega \int_Y u^p v^q \partial_t u.
\]  

(21)

Multiplying by \(U^k\) the PDE for \(U\) and integrating the resulting equation over \((0, T) \times \Omega,\) we get

\[
\int_0^T \int_\Omega \frac{\theta}{k+1} \frac{d}{dt} U^{k+1} + \int_0^T \int_\Omega \theta D k U^{k-1} |\partial_x U|^2 + \int_0^T (-\theta D U^{k} \partial_x U)|_0^T = -b \int_0^T \int_\Omega U^k(U(t, x) - u(t, x, R))
\]  

(22)

Multiplying by \(u^k\) the PDE for \(u\) and integrating now over \((0, T) \times \Omega \times Y,\) we have

\[
\int_0^T \int_\Omega \int_Y \frac{1}{k+1} \frac{d}{dt} u^{k+1} + \int_0^T \int_\Omega \int_Y d_1 k u^{k-1} |\partial_Y u|^2 + \int_0^T (-d_1 u^k \partial_Y u)|_0^T = -k \int_0^T \int_\Omega \int_Y u^{p+k} v^q.
\]  

(23)

Hence, we deduce that

\[
\theta \delta \int_0^\infty U^k(t, L)(U(t, L) - U^{ext}(t)) + k \int_0^\infty \int_\Omega \int_Y u^{p+k} v^q < \infty.
\]  

(24)

Choosing \(k := p,\) (24) becomes

\[
\theta \delta \int_0^\infty U^{p+1}(t, L) + k \int_0^\infty \int_\Omega \int_Y u^{2p} v^q < \infty.
\]  

(25)

Recalling (20), we obtain the estimate
\[ \theta \int_0^T \int_\Omega |\partial_t U|^2 + \int_0^T \int_\Omega \int_\Omega |\partial_t u|^2 \leq -k \int_0^T \int_\Omega \int_Y u^p v \partial_t u + c \]
\[
\leq c + \frac{1}{2} \int_0^T \int_\Omega \int_Y (\partial_t u)^2 + \frac{k}{2} \int_0^T \int_\Omega \int_Y u^{2p} v^2 q \]
\[
= \frac{1}{2} \int_0^T \int_\Omega \int_Y (\partial_t u)^2 + \frac{k^2}{2} \|v\|_\infty^2 \int_0^T \int_\Omega \int_Y u^{2p} v^2 + c. \quad (26)\]

This argument suggests that
\[ \int_0^\infty \int_\Omega |\partial_t U|^2 + \int_0^\infty \int_\Omega \int_\Omega |\partial_t u|^2 < \infty. \quad (27)\]

Quite similarly, we also can prove
\[ \int_0^\infty \int_\Omega \int_Y |\partial_t u|^2 < \infty. \quad (28)\]

Let us now denote by \( \hat{A}(t,x) \), \( \hat{a}(t,x,y) \), and \( \bar{b}(t,x,y) \) the unique solution to (P) in which the reaction term \( \eta(\cdot) \) is replaced by zero. We see that equation for \( \bar{b} \) decouples from the rest of the system\(^1\). Furthermore, a standard comparison argument indicates that
\[ U(t,x) \leq \hat{A}(t,x), \quad u(t,x,y) \leq \hat{a}(t,x,y), \quad v(t,x,y) \leq \bar{b}(t,x,y) \quad (29)\]
for all \( x \in \Omega \) and \( t \in S \). Following an argument from [9], we observe that \( \hat{A} \) is uniformly continuous in \( (t,x) \), while \( \hat{a} \) and \( \bar{b} \) are uniformly continuous in \( (t,y) \). We claim that both \( \hat{a} \) and \( \bar{b} \) are uniformly continuous also with respect to the macro-variable \( x \). As an example, we show the uniform continuity of \( \hat{a} \) in \( x \). Denoting by \( r(t,y) := \hat{a}(t,x_1,y) - \hat{a}(t,x_2,y) \), we have
\[
\partial_t r - d_1 \partial_{yy} r = 0 \text{ in } (0,\infty) \times Y, \quad (30)\]
\[
-d_1 \partial_y^t r(R) = b(r(t,R) - (\hat{A}(t,x_1) - \hat{A}(t,x_2))) \quad (31)\]
\[
d_1 \partial_y^t (t,0) = 0. \quad (32)\]

The function \( r \) inherits from \( \hat{A}(t,x_1) - \hat{A}(t,x_2) = O(|x_1 - x_2|^\alpha) \) for \( 0 < \alpha < 1 \) the desired property [10]. This fact concludes the proof of our claim.

Adapting the proof of (27) and (28) for the PDE system in unknowns \( \hat{A}, \hat{a}, \) and \( \bar{b} \), we obtain that
\[ \int_0^T \int_\Omega |\partial_t \hat{A}|^2 + \int_0^T \int_\Omega \int_\Omega |\partial_t \hat{a}|^2 + \int_0^T \int_\Omega \int_Y |\partial_t \bar{b}|^2 < c, \quad (33)\]
where the constant \( c \) is independent of \( T \). By the Hölder continuity of \( \hat{A} \) w.r.t. \( t \) and that of \( \hat{a} \) and \( \bar{b} \) w.r.t. \( (t,x,y) \), we deduce that for any sequence \( (t_n) \) with \( t_n \to \infty \) as \( n \to \infty \), there is a subsequence that we denote again by \( (t_n) \) such that
\[ \hat{A}(t_n + t) \to \hat{A}, \quad \hat{a}(t_n + t) \to \hat{a}, \quad \bar{b}(t_n + t) \to \bar{b} \quad (34)\]
uniformly in \( t \) \( (0 \leq t \leq 1) \). Here \( \hat{A}, \hat{a}, \) and \( \bar{b} \) are stationary solutions to (P) (in which the reaction term was a priori set to zero). For the case \( U^{ext}(\infty) = 0 \), we have \( \hat{A} = \hat{a} = 0 \), and hence, by the estimate (29), we conclude that \( U \to 0 \) and \( u \to 0 \). For \( v \) we can show that \( \lim_{t \to \infty} \|v - \bar{v}\|_{L^2(Y)} = 0 \), where \( (0,0,\bar{v}) \) denotes a (constant) stationary solution of (P). The constant \( \bar{v} \) is selected by means of the initial condition, i.e. \( \bar{v} = C^* := \frac{1}{|Y|} \int_Y v_0(x,y) \) [13].

\(^1\) The PDE system for \( \hat{A} \) and \( \hat{a} \) has the same structure as that proposed in [12] to describe diffusion of CO\(_2\) in structured coal particles.
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References

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