

NONLINEAR DIFFUSIVE BEHAVIOR IN A NEARLY EQUIDIFFUSIVE THREE COMPONENT ELEMENTARY REACTION DIFFUSION SYSTEM

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Abstract. We model the dynamics of the concentrations of chemicals which are involved in aqueous chemical reactions. In particular, we focus our interest in understanding the mechanism behind the dynamics of the coupling which occurs between reactive and diffusive mechanisms which occur on significantly separated time scales. A multiple-scales analysis of a reaction diffusion system provides a simplified model of this coupling. We outline the analysis, provide theory to demonstrate that this model is qualitatively sensible and also compare the asymptotic model to numerical solutions of the full physical model.

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AMS subject classifications. Primary: 34E13, 35K45, 35K55, 35K57. Secondary: 80A30, 80A32

1. Introduction. In modeling the fate of chemical contaminants in water, the primary dynamical influences we consider are diffusion and elementary reaction kinetics. This modeling effort has a number of applications to environmental and physical systems such as lakes, rivers, aquifers, and even bloodstreams. The standard model for such situations is obtained for each species, by adding to a diffusion equation the elementary rate laws for every chemical reaction that the species participates in [8, 14].

A general mathematical study of the combined effects of diffusion and elementary reactions would be interesting, but highly complex. We simplify matters by focusing only on three chemical species which participate in a single, reversible chemical reaction which has a fundamental time scale that is much faster than that of diffusion:



Since the elementary rate law (cf. [15]) for this reaction is given by

$$\frac{d[A]}{dt} = \frac{d[B]}{dt} = -\frac{d[AB]}{dt} = -k_f[A][B] + k_b[AB]$$

where the brackets denote molar concentration, the coupled reaction diffusion dynamics of all three species may be modeled by the following system of PDEs (cf. [1, 2, 3, 4, 8, 11, 12, 16]):

$$\left. \begin{aligned} \partial_t u_1 &= D_1 \Delta u_1 - k_f u_1 u_2 + k_b u_3 \\ \partial_t u_2 &= D_2 \Delta u_2 - k_f u_1 u_2 + k_b u_3 \\ \partial_t u_3 &= D_3 \Delta u_3 + k_f u_1 u_2 - k_b u_3 \\ u_i(x, 0) &= g_i(x) \end{aligned} \right\} \begin{array}{l} x \in \mathbb{R}^n, t > 0 \\ x \in \mathbb{R}^n \end{array} \tag{1.2}$$

Here, u_1 , u_2 , and u_3 represent the molar concentrations of A, B, and AB respectively, D_i are the diffusion coefficients for each species, and k_f and k_b are the kinetic coefficients for the reaction. To put these equations in nondimensional form, we rescale

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and relabel the variables $u_i \rightarrow u_i/K$, $x \rightarrow x/L$, and $t \rightarrow k_b t$. Here, $K \equiv k_b/k_f$ and L is any appropriate characteristic length scale (for instance, the length of a region where concentrations will be measured). The resulting PDEs become:

$$\left. \begin{aligned} \partial_t u_1 &= \delta_1 \Delta u_1 - u_1 u_2 + u_3 \\ \partial_t u_2 &= \delta_2 \Delta u_2 - u_1 u_2 + u_3 \\ \partial_t u_3 &= \delta_3 \Delta u_3 + u_1 u_2 - u_3 \\ u_i(x, 0) &= g_i(x) \end{aligned} \right\} \begin{array}{l} x \in \mathbb{R}^n, t > 0 \\ x \in \mathbb{R}^n \end{array} \quad (1.3)$$

where, $\delta_i = \frac{D_i}{L^2 k_b}$ are dimensionless diffusion coefficients. We seek solutions to system 1.3 in the space:

$$\mathbb{X}((0, T], \mathcal{X}) \equiv \{ \mathbf{u}(t) \in C^0((0, T], \mathcal{X}) : \|\mathbf{u}(t) - \mathbf{u}(0)\|_\infty \leq M \}$$

where

$$\mathcal{X} \equiv \left\{ u \in C^\alpha(\mathbb{R}^n) : \lim_{r \rightarrow \infty} \|u - \gamma\|_{C^\alpha(B_r(0)^c)} = 0 \right\}$$

This space was chosen since under purely diffusive dynamics, its members converge to their associated constant, γ as $t \rightarrow \infty$ (cf. [7]). The utility of this property will become apparent later when we establish existence results for the different equations in our models.

In some specific cases, the analysis of system 1.3 is not difficult to understand. If, for instance, the diffusion coefficients are all the same, then the system can be reformulated into two decoupled linear PDEs and one nonlinear diffusion equation. The new variables $\varphi = u_1 + u_3$ and $\theta = u_2 + u_3$ are what permit this simplified picture. There is a sizeable body of theory which enables the study of scalar, nonlinear diffusion equations (reviews may be found in [5] and [13]). However, if this equidiffusive condition is perturbed even slightly, the system no longer decouples. Nevertheless, as long as this perturbation is kept sufficiently small, we can show that it is still possible to model the system's dynamics with a scalar equation. Our primary goal is to gain an understanding of the mechanism behind the coupling between the diffusive and reactive influences that are at work in system 1.3.

2. Asymptotic analysis of diffusive phenomena. The concept of expanding a reaction diffusion equation or system around a small parameter is not new. In his review articles [9, 10], Wei Ming Ni, et. al. described several efforts of modeling pattern formation through the asymptotic expansion of reaction diffusion equations. Other similar examples are provided by Ward [17]. We employ asymptotic methods as well. However, we apply these methods to system 1.3 in order to gain an understanding of the dynamics which occur on an intermediate time scale. Li and Wright [7] have already characterized the dynamics of this system in the short time and long time regimes. They demonstrated both well posedness and global existence / uniform boundedness of solutions to the system. In addition, they fully characterized the ω -limit set. We wish to complete the picture by understanding the intermediate time regime. To do so, we examine system 1.3 in the weakly diffusive limit of $\delta_i \ll 1$. We first obtain an approximation to the system by expanding around a small parameter related to δ_i . Afterwards, we will comment on the dynamics of the solution to the approximate model.

2.1. Derivation of Weakly Diffusive Solution. In this section, we extend an existing analysis of scalar reaction-diffusion equations to our reaction-diffusion system (cf. [6]). In order to approximate system 1.3 by expansion, we require an order parameter. Let $\delta = \frac{1}{3}(\delta_1 + \delta_2 + \delta_3)$. Then define $\hat{\delta}_i$ by $\delta_i = \delta\hat{\delta}_i$. We see $\hat{\delta}_i \sim O(1)$ and $|\delta_i - \delta| \ll \delta$. This can be thought of as the equidiffusive limit since all species' diffusion coefficients are comparable.

With these definitions, we formally expand system 1.3 around δ . However, one finds that a regular expansion would produce secular behavior. Therefore, we adopt a multiple scales approach with $u_i(x, t) = \sum_j \delta^j u_i^j(x, t_1, t_2)$ and $t_1 = t$, $t_2 = \delta t$. To $O(\delta)$, System 1.3 becomes

$$\begin{aligned} \partial_{t_1} u_1^0 + \delta(\partial_{t_2} u_1^0 + \partial_{t_1} u_1^1) &= \delta\hat{\delta}_1 \Delta u_1^0 - (u_1^0 u_2^0 + \delta(u_1^1 u_2^0 + u_1^0 u_2^1)) + (u_3^0 + \delta u_3^1) \\ \partial_{t_1} u_2^0 + \delta(\partial_{t_2} u_2^0 + \partial_{t_1} u_2^1) &= \delta\hat{\delta}_2 \Delta u_2^0 - (u_1^0 u_2^0 + \delta(u_1^1 u_2^0 + u_1^0 u_2^1)) + (u_3^0 + \delta u_3^1) \\ \partial_{t_1} u_3^0 + \delta(\partial_{t_2} u_3^0 + \partial_{t_1} u_3^1) &= \delta\hat{\delta}_3 \Delta u_3^0 + (u_1^0 u_2^0 + \delta(u_1^1 u_2^0 + u_1^0 u_2^1)) - (u_3^0 + \delta u_3^1) \end{aligned} \quad (2.1)$$

From these, consider first the $O(1)$ approximation:

$$\begin{aligned} \partial_{t_1} u_1^0 &= -u_1^0 u_2^0 + u_3^0 \\ \partial_{t_1} u_2^0 &= -u_1^0 u_2^0 + u_3^0 \\ \partial_{t_1} u_3^0 &= u_1^0 u_2^0 - u_3^0 \\ u_j^0(x, 0) &= g_j(x) \end{aligned} \quad (2.2)$$

These equations are exactly the model for the kinetics of the elementary reaction 1.1 in a non-diffusive or well mixed environment. This system decouples if we introduce the notation $\varphi^0 = u_1^0 + u_3^0$ and $\theta^0 = u_2^0 + u_3^0$. From equation 2.2, we see $\partial_{t_1} \varphi^0 = \partial_{t_1} \theta^0 = 0$. Therefore, $\varphi^0 = A(x, t_2)$ and $\theta^0 = B(x, t_2)$, where, up to initial data, A and B are arbitrary at this point. Hence, we obtain for u_3^0 a scalar equation:

$$\begin{aligned} \partial_{t_1} u_3^0 &= (A - u_3^0)(B - u_3^0) - u_3^0 \\ &= (u_3^0 - r(A, B))(u_3^0 - R(A, B)) \\ &\equiv f(u_3^0, A(x, t_2), B(x, t_2)) \end{aligned}$$

with

$$\begin{aligned} r(A, B) &= \frac{1}{2} \left(A + B + 1 - \sqrt{(A + B + 1)^2 - 4AB} \right) \\ R(A, B) &= \frac{1}{2} \left(A + B + 1 + \sqrt{(A + B + 1)^2 - 4AB} \right) \end{aligned}$$

Upon inspection of the the form of f , we see that r and R correspond to the two equilibrium solutions for the reaction system. In [7], it is pointed out that r is the only physically realizable and stable solution. Furthermore, u_3 is always bounded a finite distance away from R .

One solves this equation by separating variables and integrating the resulting equation:

$$\int^{u_3^0} \frac{ds}{f(s, A(x, t_2), B(x, t_2))} = t_1 + C(x, t_2) \quad (2.3)$$

Here, the lower limit of integration is taken to be arbitrary. This formulation provides a template for describing the coupling between the slow (diffusive) and fast reactive time scales. It allows us to formally write:

$$\begin{aligned} u_1^0(x, t_1, t_2) &= A(x, t_2) - U_3(A(x, t_2), B(x, t_2), t_1 + C(x, t_2)) \\ u_2^0(x, t_1, t_2) &= B(x, t_2) - U_3(A(x, t_2), B(x, t_2), t_1 + C(x, t_2)) \\ u_3^0(x, t_1, t_2) &= U_3(A(x, t_2), B(x, t_2), t_1 + C(x, t_2)) \end{aligned} \quad (2.4)$$

Here, the diffusive influences are associated with t_2 and the reactive influences are associated with t_1 .

U_3 is the function obtained by integrating equation 2.3 and solving the result for u_3^0 .

$$\begin{aligned} u_3^0(x, t_1, t_2) &= U_3(A(x, t_2), B(x, t_2), t_1 + C(x, t_2)) \\ &= \frac{R(A, B) + r(A, B)}{2} - \frac{R(A, B) - r(A, B)}{2} F \left[\frac{R(A, B) - r(A, B)}{2} (t_1 + C) \right] \end{aligned} \quad (2.5)$$

where F may be defined depending on the position of u_3^0 relative to chemical equilibrium.

$$F(z) = \begin{cases} \coth(z) & : u_3^0(x, t_1, t_2) < r(A(x, t_2), B(x, t_2)) \\ \tanh(z) & : u_3^0(x, t_1, t_2) > r(A(x, t_2), B(x, t_2)) \end{cases} \quad (2.6)$$

From this formulation we can see that A , B , and C provide the diffusive (slow time) adjustment to the purely reactive solution of 2.2. At this point, these functions are arbitrary up to their initial data. In order to find definite forms for them, we need to proceed to higher order expansions in the perturbation approach. Therefore, we consider the $O(\delta)$ equations that are obtained from system 2.1

$$\begin{aligned} \partial_{t_1} u_1^1 + \partial_{t_2} u_1^0 &= \hat{\delta}_1 \Delta u_1^0 - (u_1^1 u_2^0 + u_1^0 u_2^1) + u_3^1 \\ \partial_{t_1} u_2^1 + \partial_{t_2} u_2^0 &= \hat{\delta}_2 \Delta u_2^0 - (u_1^1 u_2^0 + u_1^0 u_2^1) + u_3^1 \\ \partial_{t_1} u_3^1 + \partial_{t_2} u_3^0 &= \hat{\delta}_3 \Delta u_3^0 + (u_1^1 u_2^0 + u_1^0 u_2^1) - u_3^1 \end{aligned} \quad (2.7)$$

Now, define $\varphi^1 = u_1^1 + u_3^1$ and $\theta^1 = u_2^1 + u_3^1$. From system 2.7, we see:

$$\begin{aligned} \partial_{t_1} \varphi^1 &= -\partial_{t_2} A + \hat{\delta}_1 \Delta A + (\hat{\delta}_3 - \hat{\delta}_1) \Delta u_3^0 \\ \partial_{t_1} \theta^1 &= -\partial_{t_2} B + \hat{\delta}_1 \Delta B + (\hat{\delta}_3 - \hat{\delta}_2) \Delta u_3^0 \end{aligned}$$

However, $\hat{\delta}_3 - \hat{\delta}_1$ and $\hat{\delta}_3 - \hat{\delta}_2$ are of $O(\delta^2)$. Therefore, the last term in each of these equations may be formally neglected. We see that the right hand sides of the equations for φ^1 and θ^1 are independent of φ^1 and θ^1 . Therefore, we may integrate them explicitly and average over the fast time scale t_1 . In order to avoid secular behavior in φ^1 and θ^1 , we must require that the result vanishes. This leads to the following conditions.

$$\begin{aligned} \partial_{t_2} A &= \hat{\delta}_1 \Delta A \\ \partial_{t_2} B &= \hat{\delta}_2 \Delta B \end{aligned} \quad (2.8)$$

Next, we deduce necessary conditions in order to avoid secular behavior in u_3^1 . The $O(\delta)$ equation for u_3^1 is:

$$\partial_{t_1} u_3^1 = (-\partial_{t_2} + \hat{\delta}_3 \Delta) u_3^0 + ((A - u_3^0)(\theta^1 - u_3^1) + (B - u_3^0)(\varphi^1 - u_3^1)) - u_3^1$$

This may be simplified in several ways. First, recall

$$f(u_3^0, A, B) = (A - u_3^0)(B - u_3^0) - u_3^0$$

Hence, we have

$$\partial_{u_3^0} f(u_3^0, A, B) = -(A - u_3^0 + B - u_3^0) - 1$$

Therefore,

$$\begin{aligned} & ((A - u_3^0)(\theta^1 - u_3^1) + (B - u_3^0)(\varphi^1 - u_3^1)) - u_3^1 \\ &= u_3^1 \partial_{u_3^0} f(u_3^0, A, B) + \{(A - u_3^0)\theta^1 + (B - u_3^0)\varphi^1\} \end{aligned}$$

Once again, from equation 2.3, we may calculate

$$\partial_{t_2} u_3^0 = f(u_3^0, A, B) \partial_{t_2} C$$

Finally, if we note $\partial_{t_1} \ln[f(u_3^0, A, B)] = \partial_{u_3^0} f(u_3^0, A, B)$, we may rewrite the PDE for u_3^1 .

$$\begin{aligned} \partial_{t_1} \left(\frac{u_3^1}{f(u_3^0, A, B)} \right) &= \left\{ -\partial_{t_2} C + \hat{\delta}_3 (\Delta C + (\partial_{t_1} \ln[f(u_3^0, A, B)])|\nabla C|^2) \right\} \\ &+ \frac{(A - u_3^0)\theta^1 + (B - u_3^0)\varphi^1}{f(u_3^0, A, B)} \end{aligned}$$

Secular terms arise unless we can guarantee that the right hand side vanishes when we average over the t_1 time scale. The only secular terms that might come from this process are the ones involving C . In order to avoid secularity, we must enforce the condition:

$$-\partial_{t_2} C + \hat{\delta}_3 \left(\Delta C + \lim_{T \rightarrow \infty} \frac{\ln[f(u_3(x, T, t_2), A, B)]}{T} |\nabla C|^2 \right) = 0$$

The limit may be evaluated. One can show:

$$\begin{aligned} \lim_{T \rightarrow \infty} \frac{\ln[f(u_3(x, T, t_2), A, B)]}{T} &= \partial_{u_3^0} f(u_3^0 = r, A, B) \\ &= -\sqrt{(A + B + 1)^2 - 4AB} \equiv -\kappa(A, B) < 0 \end{aligned} \quad (2.9)$$

In summary, to remove secular behavior, we have three conditions:

$$\left. \begin{aligned} \partial_{t_2} A &= \hat{\delta}_1 \Delta A \\ \partial_{t_2} B &= \hat{\delta}_2 \Delta B \\ \partial_{t_2} C &= \hat{\delta}_3 (\Delta C - \kappa(A, B)|\nabla C|^2) \end{aligned} \right\} x \in \mathbb{R}^n, t_2 > 0$$

$$\left. \begin{aligned} A(x, 0) &= u_1(x, 0) + u_3(x, 0) \\ B(x, 0) &= u_2(x, 0) + u_3(x, 0) \\ C(x, 0) &= -\frac{1}{R-r} \ln \left(\frac{|u_3(x, 0) - r|}{|u_3(x, 0) - R|} \right) \end{aligned} \right\} x \in \mathbb{R}^n, t_2 = 0 \quad (2.10)$$

Coupling these with the $O(1)$ solutions we obtain an approximation for the dynamics of system 1.3 that is meaningful for $t < 1/\delta$. In the next section, we will explore the qualitative and theoretical nature of these dynamics.

2.2. Dynamics of Weakly Diffusive Solution. In this section we explore the behavior of $u_i^0(x, t, \delta t)$ as defined by equations 2.4, 2.5 and 2.6. First, we verify these solutions are well behaved by establishing upper and lower bounds based on their initial data. To do this, it is helpful to first establish bounds on A , B , and C .

LEMMA 2.1. *If A , B , and C satisfy system 2.10, then these functions are bounded above and below by their initial data. Specifically,*

$$\begin{aligned} 0 < A(x, \delta t) < \|A(x, 0)\|_\infty &= \|u_1(x, 0) + u_3(x, 0)\|_\infty < \infty \\ 0 < B(x, \delta t) < \|B(x, 0)\|_\infty &= \|u_2(x, 0) + u_3(x, 0)\|_\infty < \infty \\ 0 < C(x, \delta t) < \|C(x, 0)\|_\infty & \end{aligned}$$

Proof. A and B each satisfy system the Cauchy problem for a diffusion equation. Hence, the first two sets of bounds are a direct result of the parabolic maximum principle. The bounds on C may also be obtained by deriving a maximum principle. To do this define, for any $\epsilon > 0$, the following

$$\xi^\pm \equiv C \pm \epsilon t$$

Then, ξ^\pm satisfies:

$$\partial_{t_2} \xi^\pm = \hat{\delta}_3 (\Delta \xi^\pm - \kappa(A, B) |\nabla \xi^\pm|^2) \pm \epsilon$$

One may now show by contradiction that ξ^+ achieves no minimum and ξ^- achieves no maximum in $\mathbb{R} \times \{t > 0\}$. Since these results are true for any $\epsilon > 0$, we let $\epsilon \rightarrow 0$ to obtain the desired bounds for C . \square

Note that the bounds for C are not quite sharp. $C(x, 0) = 0$ only if $|u_3(x, 0) - r| = |u_3(x, 0) - R|$. With a little elementary algebra, it is possible to demonstrate that this is never the case. Also, note that $C(x, 0) = \infty$ if either $u_3(x, 0) = r$ or $u_3(x, 0) = R$. In [7], it was demonstrated that the latter never occurs. However, $u_3(x, 0) = r$ is equivalent to saying the system is in chemical equilibrium at the point $x \in \mathbb{R}^n$ initially. The consequence of this is that C may not have a finite upper bound at later times. However, in Theorem 2.2 we will see that it is only necessary that C is positive and away from zero by a finite amount for all time. This is always the case.

Lemma 2.1 provides sufficient information for establishing the following theorem concerning the boundedness of u_i^0 .

THEOREM 2.2. *The functions $u_i^0(x, t, \delta t)$ as defined by equations 2.4, 2.5 and 2.6 are bounded below by zero and above by a finite constant.*

Proof. We note for fixed A , B and C , any solution to system 2.2 is bounded below by 0 and above by a finite constant provided $u_i^0(x, 0, 0)$ satisfy similar bounds for $i = 1, 2, 3$ and C is bounded a finite distance away from zero (otherwise F , as defined by equation 2.6 may become singular for small t_1). If A , B and C are not fixed, we see that they serve merely as parameters for the solutions to system 2.2. Variations in A and B serve to move the solution from one integral of the ODE to another. Variations in C serve to move the solution forward or backward along a given integral curve. Since all integral curves are bounded below by zero and above by a finite constant, the same must be true for solutions to system 2.2 \square

Next, we compare the long and short term dynamics of u_i^0 to u_i . By construction, $u_i(x, 0, 0) = u_i(x, 0)$. We demonstrate that in addition to beginning at the same point, these functions end at the same point as well:

$$\lim_{t \rightarrow \infty} u_i^0(x, t, \delta t) = \lim_{t \rightarrow \infty} u_i(x, t)$$

To proceed, we need to introduce some ideas concerning the space \mathcal{X} . Since $u_i(x, t) \in \mathcal{X}$, $\exists \gamma_i(t)$ such that

$$\lim_{|x| \rightarrow \infty} \|u_i(x, t) - \gamma_i(t)\|_{C^\alpha(B_{|x|}(0)^c)} = 0$$

for all $t \geq 0$.

In [7], it was demonstrated that $\gamma_i(t)$ satisfies

$$\begin{aligned} \dot{\gamma}_1(t) &= -\gamma_1(t)\gamma_2(t) + \gamma_3(t) \\ \dot{\gamma}_2(t) &= -\gamma_1(t)\gamma_2(t) + \gamma_3(t) \\ \dot{\gamma}_3(t) &= \gamma_1(t)\gamma_2(t) - \gamma_3(t) \\ \gamma_j(0) &= g_j \end{aligned}$$

Here, g_j is the number such that $\|g_j(x) - g_j\|_{C^\alpha(B_{|x|}(0)^c)} = 0$. In the same reference it was also noted that this system has an explicit solution, and in the equidiffusive case, $\lim_{t \rightarrow \infty} u_i(x, t) = \lim_{t \rightarrow \infty} \gamma_i(t)$, where

$$\begin{aligned} \lim_{t \rightarrow \infty} \gamma_1(t) &= \sigma_1 - \frac{\sigma_1 + \sigma_2 + 1}{2} + \frac{\sqrt{(\sigma_1 + \sigma_2 + 1)^2 - 4\sigma_1\sigma_2}}{2} = \sigma_1 - r(\sigma_1, \sigma_2) \\ \lim_{t \rightarrow \infty} \gamma_2(t) &= \sigma_2 - \frac{\sigma_1 + \sigma_2 + 1}{2} + \frac{\sqrt{(\sigma_1 + \sigma_2 + 1)^2 - 4\sigma_1\sigma_2}}{2} = \sigma_2 - r(\sigma_1, \sigma_2) \\ \lim_{t \rightarrow \infty} \gamma_3(t) &= \frac{\sigma_1 + \sigma_2 + 1}{2} - \frac{\sqrt{(\sigma_1 + \sigma_2 + 1)^2 - 4\sigma_1\sigma_2}}{2} = r(\sigma_1, \sigma_2) \end{aligned}$$

where

$$\begin{aligned} \sigma_1 &= \gamma_1(t) + \gamma_3(t) = \gamma_1(0) + \gamma_3(0) \\ \sigma_2 &= \gamma_2(t) + \gamma_3(t) = \gamma_2(0) + \gamma_3(0) \end{aligned}$$

Next, we consider the long term dynamics of $u_i^0(x, t, \delta t)$. First, a lemma will prove useful.

LEMMA 2.3.

$$\begin{aligned} \lim_{t \rightarrow \infty} A(x, \delta t) &= \sigma_1 \\ \lim_{t \rightarrow \infty} B(x, \delta t) &= \sigma_2 \end{aligned}$$

Proof. Since $A(x, 0) = u_1(x, 0) + u_3(x, 0)$ and $B(x, 0) = u_2(x, 0) + u_3(x, 0)$, and $u_i(x, 0) \in \mathcal{X}$, we know $A(x, 0), B(x, 0) \in \mathcal{X}$. Therefore, since

$$\begin{aligned} \lim_{|x| \rightarrow \infty} \|A(x, 0) - \sigma_1\|_{C^\alpha(B_{|x|}(0)^c)} &= 0 \\ \lim_{|x| \rightarrow \infty} \|B(x, 0) - \sigma_2\|_{C^\alpha(B_{|x|}(0)^c)} &= 0 \end{aligned}$$

and since A and B both satisfy diffusion equations, the desired results are true. \square

Finally, we may establish the primary result concerning the limits of u_i^0 .

THEOREM 2.4. *The following limits exist and are given by*

$$\begin{aligned} \lim_{t \rightarrow \infty} u_1^0(x, t, \delta t) &= \sigma_1 - \frac{\sigma_1 + \sigma_2 + 1}{2} + \frac{\sqrt{(\sigma_1 + \sigma_2 + 1)^2 - 4\sigma_1\sigma_2}}{2} = \sigma_1 - r(\sigma_1, \sigma_2) \\ \lim_{t \rightarrow \infty} u_2^0(x, t, \delta t) &= \sigma_2 - \frac{\sigma_1 + \sigma_2 + 1}{2} + \frac{\sqrt{(\sigma_1 + \sigma_2 + 1)^2 - 4\sigma_1\sigma_2}}{2} = \sigma_2 - r(\sigma_1, \sigma_2) \\ \lim_{t \rightarrow \infty} u_3^0(x, t, \delta t) &= \frac{\sigma_1 + \sigma_2 + 1}{2} - \frac{\sqrt{(\sigma_1 + \sigma_2 + 1)^2 - 4\sigma_1\sigma_2}}{2} = r(\sigma_1, \sigma_2) \end{aligned}$$

Proof. From the definition of F given in equation 2.6, we can see

$$\lim_{t \rightarrow \infty} F \left(\frac{R(A(x, \delta t), B(x, \delta t)) - r(A(x, \delta t), B(x, \delta t))}{2} (t + C(x, \delta t)) \right) = 1$$

provided $R - r > 0$ and $C > 0$. This is always the case. Therefore,

$$\begin{aligned} \lim_{t \rightarrow \infty} u_3^0(x, t, \delta t) &= \lim_{t \rightarrow \infty} \frac{R(A, B) + r(A, B)}{2} - \frac{R(A, B) - r(A, B)}{2} \\ &= \lim_{t \rightarrow \infty} r(A, B) \\ &= r(\sigma_1, \sigma_2) = \lim_{t \rightarrow \infty} u_3(x, t) \end{aligned}$$

Since $u_1^0 = A - u_3^0$ and $u_2^0 = B - u_3^0$, the previous lemma also gives us the desired results for u_1^0 and u_2^0 \square

2.3. Numerical Verification of Asymptotic Model. In the previous section, we presented some analytical and interpretive results which suggest that the asymptotic model for weakly diffusive kinetics is reasonable. In this section we continue by comparing the numerical solution to a specific initial value problem based on 1.3 to the solution predicted by the asymptotic model. Consider the problem

$$\left. \begin{aligned} \partial_t u_1 &= \delta_1 \partial_x^2 u_1 - u_1 u_2 + u_3 \\ \partial_t u_2 &= \delta_2 \partial_x^2 u_2 - u_1 u_2 + u_3 \\ \partial_t u_3 &= \delta_3 \partial_x^2 u_3 + u_1 u_2 - u_3 \end{aligned} \right\} x \in [-1, 1], t > 0$$

$$\left. \begin{aligned} u_1(x, 0) &= 1.25 - p(10x) \\ u_2(x, 0) &= 1.75 + p(10x) \\ u_3(x, 0) &= 0.1 + u_1(x, 0)u_2(x, 0) \end{aligned} \right\} x \in [-1, 1], t = 0 \quad (2.11)$$

$$\partial_x u_i(\pm 1, t) = 0 \quad x = \pm 1, t > 0$$

Here, $p(x)$ is the cubic B-spline on $[-1, 1]$ normalized such that $p(0) = 1$ and $p(x) = 0$ if $x \notin (-1, 1)$. In addition, the diffusion coefficients are chosen to reflect a nearly equidiffusive state. Although the original system was posed on \mathbb{R}^n , this initial value problem is posed on the unit interval with Neumann boundary conditions. With the class of initial data we have chosen, the dynamics will be comparable to the Cauchy problem on \mathbb{R} until information from the support of the initial data begins to interact with the boundary (after $t \sim 1/\delta$). None of our simulations run long enough for this to happen.

$$\delta_1 = 0.00101, \delta_2 = 0.00098, \text{ and } \delta_3 = 0.00101$$

In order to solve this system numerically, we employ a Fourier spectral solver which uses an integrating factor to solve the diffusive part of the problem exactly and RK4 for integrating the reactive part in time. More specifically, under the Fourier transform equations of the form

$$\partial_t \hat{u}_i(k, t) = \delta_i \partial_x^2 \hat{u}_i(k, t) + f(\mathbf{u})$$

become

$$\partial_t \hat{u}_i(k, t) = -\delta_i k^2 \hat{u}_i(k, t) + T_F[f(\mathbf{u})]$$

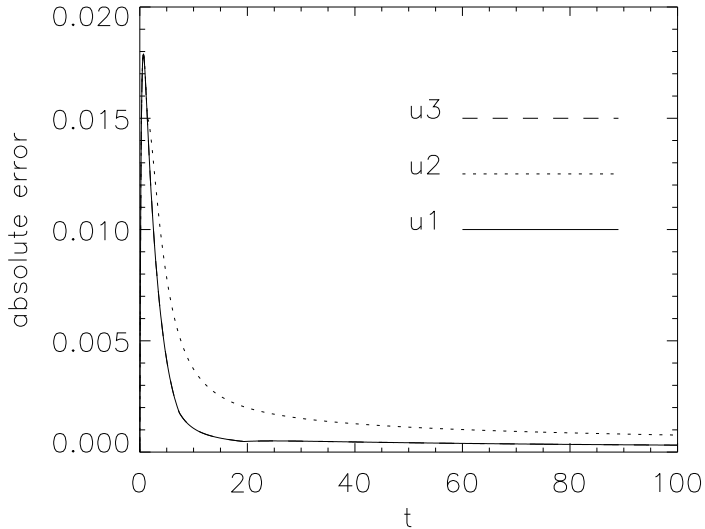


FIG. 2.1. Pictured are the absolute errors ($\|u_i - u_i^0\|_\infty$) between the solutions to the physical system (equation 2.11) and the solutions predicted by the asymptotic model. After an initial reorganization period, the error is $O(\delta)$.

where T_F denotes the Fourier transform. Hence, with the aid of the integrating factor $e^{\delta_i k^2 t}$, this may be written as an ODE in the variable $z_i(k, t) = e^{\delta_i k^2 t} \hat{u}_i(k, t)$ and integrated using RK4.

We apply such a solver to system 2.11 to obtain solutions which has spectral accuracy in space and 4th order accuracy in time. We apply the same solver to system 2.10 in order to obtain the appropriate inputs A , B , and C for the asymptotic model (equations 2.4, 2.5, and 2.6).

The results of this comparison are presented in figures 2.2 and 2.1. Figure 2.2 shows four representative timeslices of the concentrations u_1 , u_2 , and u_3 (solid lines) plotted together with their asymptotic approximations (dotted lines). The differences between solutions are nearly invisible to the eye. Figure 2.1 provides a more quantitative picture of the error between the actual solutions and the asymptotic models. Here, the absolute error in the sup norm $\|\cdot\|_\infty$, is plotted for each species. After the initial short period of reorganization, the error is clearly $O(\delta)$.

3. Conclusion. We have derived a model that captures the mechanism in which weak diffusion perturbs purely reactive dynamics for a three component, elementary chemical reaction. In this case, the model provided a simplified understanding for the dynamics of the full physical system because it essentially reduced a system of three, coupled nonlinear PDEs to a single scalar nonlinear PDE. We have provided both qualitative and quantitative verification for this model in the following forms:

- For a given choice of initial data, the steady state solutions of both the physical system and asymptotic model match.
- Solutions to both the physical system and the asymptotic model are bounded

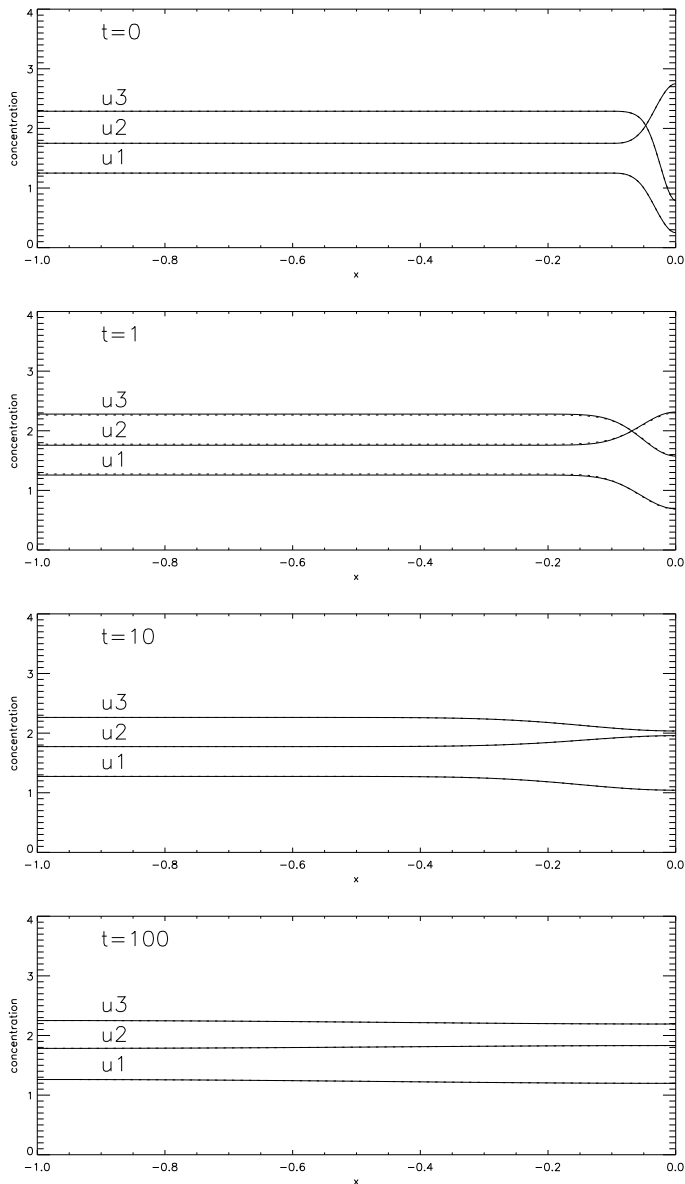


FIG. 2.2. Pictured are representative timeslices of the concentrations of both the solutions to system 2.11 (solid lines) and to the asymptotic model (dotted lines). In most cases, the curves are indistinguishable to the eye.

below by zero and from above by a finite constant which depends on the initial data.

- Numerical solutions of the full physical system agree quite well with solutions to the asymptotic model.

In future work, we are interested in pursuing higher order asymptotic expansions of system 1.3. Such an analysis would permit an understanding of the diffusive cor-

rection to reactive kinetics in extremely non-equidiffusive situations. For instance, a possible choice of diffusion coefficients might obey the scaling $\delta_1 = \delta^2$, $\delta_2 = \delta$, and $\delta_3 = \delta$. This would require an expansion to $O(\delta^2)$ instead of $O(\delta)$. This analysis is physically relevant since there are physical settings such as quiescent or laminar flows where molecular diffusion leads to one of the prominent mixing processes. In such cases, it is not uncommon for chemical species' diffusion coefficients to span a wide range of values.

In addition, we plan to generalize the leading order expansion for a general system of elementary, elementary chemical reactions for an equidiffusive setting. The three component system we investigated in this publication possessed more structure than can typically be expected. Normally, the leading order equations will not decouple completely. Therefore, one would expect to work with a system of coupled integral representations for the secularity constants analogous to equation 2.3. Key difficulties in generalizing this theory will center around finding appropriate conditions on the reaction rate laws that will allow these integral representations to remain well behaved, ensure that limits analogous to the one in equation 2.9 exist, and maintain physical relevance. Such a generalization would provide a useful theory for reducing the number of PDEs needed for modeling such systems.

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