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STEADY STATE SOLUTIONS FOR BALANCED REACTION DIFFUSION SYSTEMS ON HETEROGENEOUS DOMAINS

W.E. Fitzgibbon*
Department of Mathematics, University of Houston, Houston, TX 77204-3476

S.L. Hollis
Department of Mathematics, Armstrong Atlantic State University, Savannah, GA 31419

J.J. Morgan*
Department of Mathematics, Texas A&M University, College Station, TX 77843-3368

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Abstract. We consider a class of semilinear diffractive-diffusion systems of the form

$$\begin{cases} -d_{A_i}\Delta u_i = f_{A_i}(u) & x \in A \\ -d_{B_i}\Delta \tilde{u}_i = f_{B_i}(\tilde{u}) & x \in B \\ u_i = \tilde{u}_i & \text{on } \partial A \\ d_{A_i}\frac{\partial u_i}{\partial \eta_A} = d_{B_i}\frac{\partial \tilde{u}_i}{\partial \eta_A} & \text{on } \partial A \\ \tilde{u}_i = g_i & \text{on } \partial B \backslash \partial A \end{cases} \tag{P}$$

where A and B are smooth bounded domains in $\Re^n$ such that there exists a smooth bounded domain $\Omega \subseteq \Re^n$ so that A is a strict subdomain of Ω and $\bar{A} \cup B = \Omega$. We assume that $d_{A_i}, d_{B_i} > 0$, each g_i is nonnegative and smooth, and $f_A = (f_{A_i})$ and $f_B = (f_{B_i})$ are locally Lipschitz vector fields which are quasi-positive, nearly balanced, and polynomial bounded. We prove that these conditions guarantee the existence of a nonnegative solution of (P) for the case of $n = 2$. In addition, for the case of $n = 3$, we show that nonnegative solutions of (P) exist provided that f_A, f_B satisfy a quadratic intermediate sum property. In particular, our results imply that, for space dimensions $n = 2, 3$, if (P) arises from standard balanced quadratic mass action kinetics, then nonnegative solutions of (P) are guaranteed. We apply our results to two multicomponent chemical models.

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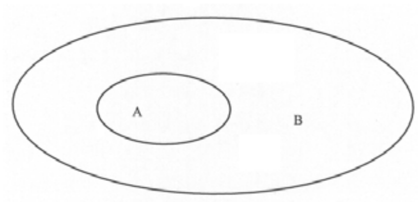

Figure 1.

1. Introduction. Many reactive diffusive processes feature a pronounced dependence of the reaction kinetics and diffusive structure upon the heterogeneity of the domain structure. Systems having reaction kinetics that depend upon domain structure arise in a variety of applications, including geochemistry [15] and experimental chemical reactors [21]. Diffusion through highly heterogeneous media can produce diffractive diffusion. Diffractive diffusion arises in nuclear reactor physics and has been studied in the American and Russian mathematical literature ([11], [12], [17], [18], [19], [20]). However, there is a marked absence of mathematical literature that treats these types of systems and focuses on the presence of complex kinetic structure.

In the work at hand, we are concerned with steady state solutions to systems featuring reaction kinetics and diffusive structure dependent upon the heterogeneity of the domain. We focus on a highly idealized physical scenario whereby m chemical species diffuse and react in a region Ω. We assume that Ω contains an inner core or subvolume, which we shall designate by A, and that A is surrounded by one connected region B that separates ∂A from $\partial\Omega$ as depicted in Figure 1.

We assume that reaction and diffusion transpire throughout Ω, but we assume that the reaction diffusion systems describing the processes differ across the interface ∂A of A and B, and that the distinct systems are coupled by requiring continuity of the state variables (concentration densities) and fluxes across the interface.

The types of systems to be considered are of the form

$$\begin{cases} -d_{A_i}\Delta u_i = f_{A_i}(u) & x \in A \\ -d_{B_i}\Delta \tilde{u}_i = f_{B_i}(\tilde{u}) & x \in B \\ u_i = \tilde{u}_i & \text{on } \partial A \\ d_{A_i}\frac{\partial u_i}{\partial \eta_A} = d_{B_i}\frac{\partial \tilde{u}_i}{\partial \eta_A} & \text{on } \partial A \\ \tilde{u}_i = g_i & \text{on } \partial B \backslash \partial A. \end{cases} \tag{P}$$

Here u_i and $\tilde{u}_i$ represent the concentrations of the i^{th} chemical species in

A and B, respectively, for $i = 1, \ldots, m$. Specific hypotheses concerning the coefficients and functions present in (P) are given in the next section. However, we take some time here to motivate our principle assumptions concerning the vector fields f_A and f_B.

Recall that our primary interest is in models that arise from complex chemistry. To this end, suppose (P) models the steady state behavior for the reaction and diffusion of a chemical process that takes place on the domain Ω. Then the unknowns $u, \tilde{u}$ represent chemical concentrations that are subject to the same basic chemical reactions regardless of whether they take place in A or B, with the only difference being the acceleration or deceleration of reaction rates due to domain properties. In general, if $z_1, \ldots, z_m$ represent m chemical species that interact in k reaction steps on Ω, then the laws of mass action kinetics imply that there exists an $m \times k$ matrix N (termed the *Stoichiometric Matrix*) and reaction rates $R_{q_1}(z), \ldots, R_{q_m}(z)$ (which may also depend upon domain properties) such that

$$f_q(z) = N \begin{pmatrix} R_{q_1}(z) \\ \vdots \\ R_{q_m}(z) \end{pmatrix}, \text{ for } q = A, B,$$

with N independent of z, reaction rates, etc. Now, for the moment, consider the associated kinetic equations (with diffusion ignored). These equations have the form

$$v'(t) = f_A(v(t)) \quad \text{on } A$$

or

$$v'(t) = f_B(v(t)) \quad \text{on } B.$$

We will concentrate on the first of these. If we expect some sort of conservation of total mass, or a weighted conservation of total mass, then we expect something like

$$\sum_{i=1}^{m} b_i v(t) = \sum_{i=1}^{m} b_i v(0) \quad \text{for all } t \geq 0,$$

where $b_1, \ldots, b_m > 0$. However, if we integrate the kinetic equations, then we obtain

$$\sum_{i=1}^{m} b_i v(t) = \sum_{i=1}^{m} \left(b_i v(0) + \int_0^t b_i f_{A_i}(v(s)) ds \right) \quad \text{for all } t \geq 0.$$

Consequently, we can probably expect the conservation above to hold only if

$$\sum_{i=1}^{m} b_i f_{A_i}(z) = 0 \quad \text{for all admissable } z. \tag{A}$$

From the form of f_A above, we would expect this to be a consequence of $(b_1, \cdots, b_m)^T \in \ker(N^T)$; that is, we would expect conservation of mass to be determined by stoichiometry and not by reaction rates. As a result, we would also have

$$\sum_{i=1}^{m} b_i f_{B_i}(z) = 0 \quad \text{for all admissable } z. \tag{B}$$

The assumptions (A) and (B) are typically referred to as balancing assumptions (cf. [5], [7], [8], [9], [10], [13], [14] and the references therein). Interestingly, many chemical systems give rise to a balancing structure. In fact, all single step reversible chemical reactions give rise to a balancing structure ([8]), and many multiple step chemical reactions give rise to similar structure. We will build our analysis around related assumptions.

Our results are quite natural for the case of space dimensions $n = 2$ and $n = 3$, although at first glance, the extra hypothesis that we place on the reaction vector field for space dimension $n = 3$ might seem a little odd. In either case, our results guarantee the existence of nonnegative solutions to systems arising from standard balanced quadratic mass action kinetics.

Our work relies upon estimates developed by localized duality arguments applied to a *nonstandard* scalar steady state diffractive diffusion problem. The scalar diffractive diffusion problem arises from an assumption of near balancing upon the reaction vector field in our model. However, due to the structure of our system, the solutions of the scalar problem are not necessarily continuous across the interface, although their fluxes are continuous. The lack of continuity in the solutions at the interface causes some difficulty in obtaining necessary a priori estimates.

Our subsequent work is organized as follows. We give a precise statement of our problem in Section 2. In Section 3 we develop some estimates for the related, nonstandard scalar equation. We give the proofs of our main results in Section 4. Finally, Section 5 contains two examples to illustrate the applicability of our results.

2. Statements of results. We assume throughout that $n \geq 2$ and Ω, A and B are given as in the introduction. More specifically, we assume Ω is a bounded domain in $\Re^n$ whose boundary $\partial\Omega$ is a $C^{2+\alpha}$ manifold such that Ω lies locally on one side of $\partial\Omega$, and there exist domains $A, B \subseteq \Omega$ such that $\bar{A} \subseteq \Omega$ and $\Omega = \bar{A} \cup B$. In addition, we assume that for each $P \in \partial A$ there exists an $\varepsilon > 0$ such that if we denote $B_\varepsilon(P) = \{x \mid |x - P| < \varepsilon\}$ then there exist local coordinate functions $\phi_1, \dots, \phi_n \in C^3(B_\varepsilon(P), \Re)$ so that

$$\partial A \cap B_\varepsilon(P) = \{x \mid \phi_1(x) = 0\},$$

$$|\nabla\phi_i(x)| \geq \delta > 0 \quad \text{for all } x \in B_\varepsilon(P),$$

and

$$\nabla\phi_i(x) \cdot \nabla\phi_j(x) = 0 \quad \text{for all } x \in B_\varepsilon(P) \text{ if } i \neq j.$$

Finally, we let η_A denote the unit normal vector on ∂A pointing out of A. We consider the system (listed here again for easy reference)

$$\begin{cases} -d_{A_i}\Delta u_i = f_{A_i}(u) & x \in A \\ -d_{B_i}\Delta \tilde{u}_i = f_{B_i}(\tilde{u}) & x \in B \\ u_i = \tilde{u}_i & \text{on } \partial A \\ d_{A_i}\frac{\partial u_i}{\partial \eta_A} = d_{B_i}\frac{\partial \tilde{u}_i}{\partial \eta_A} & \text{on } \partial A \\ \tilde{u}_i = g_i & \text{on } \partial B \backslash \partial A \end{cases} \tag{P}$$

where $f_A, f_B \colon \Re^m_+ \to \Re^m$ are locally Lipschitz, satisfy the quasi-positivity condition:

$$f_{q_i}(z) \geq 0 \text{ for all } z \in \Re^m_+ \text{ with } z_i = 0 \text{ and } q = A, B \tag{QP}$$

and are nearly balanced with the same balancing law:

(BAL) There exist $b_i > 0$ and $K_q \geq 0$ such that

$$\sum_{i=1}^{m} b_i f_{q_i}(z) \leq K_q \text{ for all } z \in \Re^m_+ \text{ and } q = A, B.$$

Furthermore, we assume that each component of f_A and f_B is polynomial bounded, i.e.,

(POLY) There exists a polynomial $P \colon \Re^m \to \Re$ such that

$$|f_{q_i}(z)| \leq |P(z)| \text{ for all } z \in \Re^m_+,\ q = A, B, \text{ and } i = 1, \dots, m.$$

In addition, we assume that $g_i \geq 0$ is smooth and $d_{q_i} > 0$ for each $i = 1, \dots, m$, $q = A, B$. A classical solution of (P) will be defined to be a pair of functions $(u, \tilde{u})$ such that $u \in C^2(A, \Re^m) \cap C^1(\bar{A}, \Re^m)$, $\tilde{u} \in C^2(\bar{B} \backslash \partial A, \Re^m) \cap C^1(\bar{B}, \Re^m)$ and the functions u and $\tilde{u}$ satisfy (P). The above hypotheses are sufficient to obtain the following existence result.

Theorem 2.1. *Suppose that $f_A, f_B : \Re^m_+ \to \Re^m$ are locally Lipschitz and satisfy* (QP), (BAL), *and* (POLY). *In addition, suppose that each g_i is nonnegative and smooth, and $d_{q_i} > 0$ for each $i = 1, \dots, m$, $q = A, B$. Then, if $n = 2$, there exists a componentwise nonnegative classical solution of* (P).

The problem becomes somewhat more complicated for space dimension $n = 3$. In this case, our analysis requires some additional assumptions. Adopting the terminology from [13] and [14], we impose the following quadratic *intermediate sums* condition:

(QUAD) There exist a lower triangular matrix $\mathcal{A} = (a_{i,j})$ with positive diagonal entries and a quadratic polynomial Q: $\Re^m \to \Re$ such that

$$\sum_{j=1}^{i} a_{i,j} f_{q_j}(z) \leq Q(z) \text{ for all } i = 1, \dots, m, q = A, B \text{ and } z \in \Re^m_+.$$

We note that (QUAD) *does not* require each component of f_A and f_B to be bounded by a quadratic polynomial. It simply requires that there is an ordering of the components of f_A and f_B such that the first component is bounded above by a quadratic polynomial and that certain linear combinations of successive components of f_A and f_B can be formed so that higher order terms either cancel each other or are only present with negative coefficients. It should be clear that (QUAD) need only be stated for $i = 1, \dots, (m-1)$ due to (BAL).

We can now state our result for the case $n = 3$.

Theorem 2.2. *Suppose that $n = 3$ and that* (QUAD) *and the hypotheses of Theorem* 2.1 *are satisfied. Then there exists a componentwise nonnegative classical solution of* (P).

It is also possible to give a number of useful adaptations of the results above by giving variations on (BAL) and (QUAD). For example, consider the following assumptions and the subsequent theorem.

(BAL1) There exist $K_q \geq 0$ for $q = A, B$, $k \in \{1, \dots, m\}$, $b_i > 0$, and a polynomial P_1: $\Re^k \to \Re$ such that

$$\sum_{i=1}^{k} b_i f_{q_i}(z) \leq K_q \quad \text{and} \quad \sum_{i=k+1}^{m} b_i f_{q_i}(z) \leq P_1(z_1 \dots, z_k)$$

for all $z \in \Re^m_+$ and $q = A, B$.

(QUAD1) There exists a lower triangular matrix $\mathcal{A} = (a_{i,j})$ with positive diagonal entries and polynomials $Q_1: \Re^k \to \Re$, $Q_2: \Re^m \to \Re$ such that

$$\sum_{j=1}^{i} a_{i,j} f_{q_j}(z) \leq Q_1(z_1, \dots, z_k) \ \forall\ i = 1, \dots, k,\ q = A, B,\ z \in \Re^m_+,$$

and

$$\sum_{j=k+1}^{i} a_{i,j} f_{q_j}(z) \leq Q_2(z) \ \forall\ i = k+1, \dots, m,\ q = A, B,\ z \in \Re^m_+,$$

where Q_1 is quadratic and Q_2 is quadratic in $z_{k+1}, \dots, z_m$.

As we will see below, the first inequality in (BAL1) allows us to obtain a priori estimates for u_i and $\tilde{u}_i$ for $i = 1, \dots, k$. Once that is done, the second inequality in (BAL1) becomes a balancing condition which allows us to obtain a priori estimates for the remaining components. (QUAD1) is used in a similar manner.

Theorem 2.3. *Suppose that* $f_A, f_B: \Re^m_+ \to \Re^m$ *are locally Lipschitz and satisfy* (QP), (BAL1) *and* (POLY). *In addition, suppose that* g_i *is nonnegative and smooth and that* $d_{q_i} > 0$ *for each* $i = 1, \dots, m$, $q = A, B$. *Then, if* $n = 2$ *or if* $n = 3$ *and* (QUAD1) *is satisfied, there exists a componentwise nonnegative classical solution of* (P).

We give an example in the last section to illustrate Theorem 2.3.

3. Preliminary estimates. In this section, we develop some preliminary scalar estimates. We assume g is a fixed nonnegative smooth function, $G_A \in L^q(A)$ and $G_B \in L^q(B)$ with $1 \leq q < \infty$, $d > 0$, and η_A (respectively η_B) denotes the unit normal vector on ∂A (respectively ∂B) pointing out of A (respectively B). Throughout this section we assume

$U \in C^2(A, \Re) \cap C^1(\bar{A}, \Re)$ and $W \in C^2(\bar{B} \backslash \partial A, \Re) \cap C^1(\bar{B}, \Re)$ are nonnegative functions satisfying the system

$$\begin{cases} -\Delta U \le G_A & \text{in } A \\ -\Delta W \le G_B & \text{in } B \\ \frac{\partial U}{\partial \eta_A} = \frac{\partial W}{\partial \eta_A} & \text{on } \partial A \\ \frac{1}{d} W \le U \le dW & \text{on } \partial A \\ W = g & \text{on } \partial B \backslash \partial A. \end{cases} \tag{SC}$$

Remark. At first glance, it might appear as though estimates for solutions of (SC) are a simple matter. However, this is simply not the case.

We begin by obtaining an L^1 estimate for solutions of (SC).

Lemma 3.1. *There exists a constant C dependent upon the L^1 norms of G_A and G_B, but independent of U and W, such that*

$$\int_{\partial A} (U + W) d\sigma + \int_A U \, dx + \int_B W \, dx \ \le C.$$

Proof. Let ϕ and ψ solve, respectively,

$$\begin{cases} -\Delta \phi = 1 & \text{in } A \\ \phi = 0 & \text{on } \partial A \end{cases} \quad \text{and} \quad \begin{cases} -\Delta \psi = \Theta & \text{in } B \\ \psi = 1 & \text{on } \partial A \\ \psi = 0 & \text{on } \partial B \backslash \partial A. \end{cases}$$

Note that $\phi \ge 0$ in A and $\frac{\partial \phi}{\partial \eta_A} < 0$ on ∂A by virtue of the maximum principle. Also, we have the estimates

$$\int_A U \le \int_A U(-\Delta \phi) \le -\int_{\partial A} U \frac{\partial \phi}{\partial \eta_A} + \int_A G_A \phi \le -d \int_{\partial A} W \frac{\partial \phi}{\partial \eta_A} + \int_A G_A \phi \tag{INT3.1}$$

and

$$\int_B W\Theta \le \int_{\partial A} -W \frac{\partial \psi}{\partial \eta_B} + \|G_A\|_{1,A} - \int_{\partial B \backslash \partial A} g \frac{\partial \psi}{\partial \eta_B} + \int_B G_B \psi \tag{INT3.2}$$

(in the first estimate we used the algebraic sign property of the normal derivative). We begin by taking $\Theta = 0$ above. Noting that $\frac{\partial \psi}{\partial \eta_B} > 0$ on the compact set ∂A, we obtain a bound for the L^1 norm of W over ∂A. We now return to (INT3.2) and take $\Theta = 1$. By combining (INT3.1) and (INT3.2) we obtain our result. $\square$

In lieu of the result above, we know that U and W can be bounded a priori on subsets of A and B which lie away from ∂A. We state this result in the following lemma. A proof establishing these interior estimates can be found in either [1] or [6].

Lemma 3.2. *Suppose that $G_A \in L^q(A)$ and $G_B \in L^q(B)$ with $q > \frac{n}{2}$. For every $\varepsilon > 0$ there exists a constant $C_\varepsilon > 0$, independent of U and W, such that if $\Omega_A \subseteq A$ and $\Omega_B \subseteq B$ with dist$(\Omega_A, \partial A)$, dist$(\Omega_B, \partial A) > \varepsilon$, then $U(x)$, $W(y) \le C_\varepsilon$ for all $x \in \Omega_A$ and $y \in \Omega_B$.*

Consequently, we need to concentrate on obtaining estimates near ∂A. Our first set of these estimates is obtained in the proof of the following lemma. The lemma is stated in terms of the resulting estimates for U and W in all of A and B respectively.

Lemma 3.3. *If $1 < p < \infty$ is given such that $\frac{p}{p-1} > \frac{n}{2}$, then there exists a constant $C_p > 0$ dependent upon the L^1 norms of G_A and G_B, but independent of U and W, such that $\|U\|_{p,A}$, $\|W\|_{p,B} < C_p$.*

Proof. We need only develop estimates in a neighborhood of ∂A. To this end, let $P \in \partial A$ and suppose $\{\phi_1, \ldots, \phi_n\}$ is a smooth, orthogonal, local coordinate system for a neighborhood of P such that $\phi_1 = 0$ determines ∂A locally; i.e., there exists an $\varepsilon > 0$ such that $\phi_1, \ldots, \phi_n$ are smooth on $B_\varepsilon(P) = \{x \mid |x - P| < \varepsilon\}$, $\partial A \cap B_\varepsilon(P) = \{x \mid \phi_1(x) = 0\} \cap B_\varepsilon(P)$, $|\nabla \phi_i(x)| \ge \delta > 0$ on $B_\varepsilon(P)$, and $\nabla \phi_i(x) \cdot \nabla \phi_j(x) = 0$ on $B_\varepsilon(P)$ if $i \ne j$. Assume without loss of generality that $\nabla \phi_1(x)$ points out of A at each point $x \in \partial A \cap B_\varepsilon(P)$ (see Figure 2). Then there exist $\alpha_i > 0$ such that

$$\{x \mid |\phi_i(x)| \le \alpha_i,\ \ i = 1, \ldots, n\} \subseteq B_\varepsilon(P) \ \text{ and } \ \{x \mid \phi_1(x) \le 0\} \cap B_\varepsilon(P) \subseteq \bar{A},$$

and near P we can treat U and W as functions of $\phi_1, \ldots, \phi_n$.

If we apply this change of variables to U and W then we obtain

$$\Delta_x U = \sum_{i=1}^{n} \left(U_{\phi_i \phi_i} |\nabla \phi_i|^2 + U_{\phi_i} \Delta_x \phi_i \right)$$
$$\Delta_x W = \sum_{i=1}^{n} \left(W_{\phi_i \phi_i} |\nabla \phi_i|^2 + W_{\phi_i} \Delta_x \phi_i \right).$$

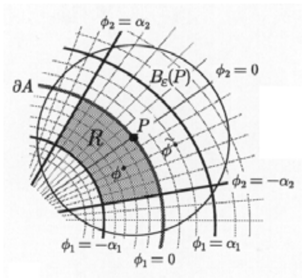

Figure 2.

Consequently, if we define (see Figures 2 and 3)

$$\begin{aligned} &\phi = (\phi_1, \phi_2, \dots, \phi_n), \quad \widetilde{\phi} = (-\phi_1, \phi_2, \dots, \phi_n), \\ &R = \{(\phi_1, \phi_2, \dots, \phi_n) \mid -\alpha_1 < \phi_1 < 0 \text{ and } |\phi_j| < \alpha_j \text{ for } j = 2, \dots, n\}, \\ &\Gamma = \{\phi \mid \phi \in \bar{R} \text{ and } \phi_1 = 0\}, \quad \text{and} \\ &Z(\phi) = U(\phi) + W(\widetilde{\phi}) \text{ for } (\phi_1, \dots, \phi_n) \in R, \end{aligned}$$

then routine calculations yield

$$\begin{cases} -\sum_{i=1}^{n} a_i(\phi) Z_{\phi_i\phi_i}(\phi) \le F(\phi) & \phi \in R \\ Z_{\phi_1}(\phi) = 0 & \phi \in \Gamma \end{cases} \tag{ZEQ}$$

where each $a_i \in C^2(\bar{R})$ with $a_i > 0$ and

$$F(\phi) = \sum_{i=1}^{n} \Big(c_{1,i}(\phi) W_{\phi_i\phi_i}(\widetilde{\phi}) + c_{2,i} U_{\phi_i}(\phi) + c_{3,i}(\phi) W_{\phi_i}(\widetilde{\phi}) \Big) + H,$$

where $c_{1,i} \in C^2(\bar{R})$ with $c_{1,i}(\phi) = 0$ for all $\phi \in \Gamma$, $c_{2,i}$, $c_{3,i} \in C^1(\bar{R})$, and H is an L^1 function dependent upon G_A and G_B. We remark that since $Z(\phi) = U(\phi) + W(\widetilde{\phi})$, Lemma 3.1 yields a bound for Z in each of $L^1(R)$ and $L^1(\Gamma)$. We also note that from Lemma 3.2 and the compactness of the boundary, it is sufficient to obtain bounds for Z in $L^q(R)$ to prove the lemma.

We obtain these estimates for Z as follows. Begin by taking $0 < \beta_i < \alpha_i$ and defining $\mu: \bar{R} \to [0, 1]$ such that μ is smooth, $\frac{\partial \mu}{\partial \eta_R} = 0$ on ∂R, $\mu(\phi) = 1$ for all ϕ such that $-\frac{\beta_i}{2} < \phi_1 < 0$ and $|\phi_j| < \frac{\beta_j}{2}$ for $j = 2, \dots, n$, and

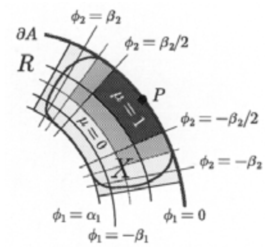

Figure 3.

$\mu(\phi) = 0$ for all ϕ such that either $-\alpha_1 \leq \phi_1 \leq -\frac{3\beta_1}{4}$ or $|\phi_j| \geq \frac{3\beta_j}{4}$ for $j = 2, \dots, n$ (see Figure 3). Now take X to be a smooth bounded domain such that

$$\{\phi \mid -\alpha_1 < \phi_1 < 0 \text{ and } |\phi_j| < 3\alpha_j/4, \quad j = 2, \dots, n\} \subseteq X \subseteq R$$

(see Figure 3). In addition, suppose that $\frac{n}{2} < p < \infty$ and $\Theta \in L^p(R)$ is such that $\Theta \geq 0$ a.e. and $\|\Theta\|_{p,\Omega} = 1$. Note that if η_{Xi} is the i^{th} component of the unit normal vector on ∂X pointing out of X and $M > 0$ is chosen sufficiently large, then there exists a unique, nonnegative solution $y \in W_p^2(X)$ of

$$\begin{cases} -\sum_{i=1}^{n} (a_i y)_{\phi_i \phi_i} + My = \Theta & \phi \in X \\ \sum_{i=1}^{n} \frac{\partial (a_i y)}{\partial \eta_{Xi}} = 0 & \phi \in \partial X. \end{cases} \tag{DUAL}$$

Furthermore, with M chosen in this manner, there exists $C_p > 0$ independent of Θ such that $\|y\|_{2,p,X} \leq C_p$, where $\|\cdot\|_{2,p,X}$ denotes the standard Sobolev norm on $W_p^2(X)$ ([1], [2], [6]). Since $p > \frac{n}{2}$, we can apply Sobolev imbedding results [6] to show $y \in C(\bar{X}) \cap W_p^2(X)$ and obtain a constant $C_p > 0$ independent of Θ so that $\|y\|_{\infty,X} \leq C_p$. In addition, in the case when $p > n$, we have $y \in C^1(\bar{X}) \cap W_p^2(X)$ and C_p can be chosen [6] so that $\|y_{\phi_i}\|_{\infty,X} \leq C_p$ for each $i = 1, \dots, n$.

We proceed via duality. Integration over X with respect to ϕ yields

$$\begin{aligned} \int_X \mu Z \Theta &= \int_X \mu Z \Big(-\sum_{i=1}^{n} (a_i y)_{\phi_i \phi_i} + My \Big) \\ &= \int_X \mu Z M y - \int_X \sum_{i=1}^{n} a_i y (\mu Z)_{\phi_i \phi_i} \end{aligned}$$

$$= M\int_X \mu Z y - \int_X \sum_{i=1}^n a_i y\big(\mu_{\phi_i\phi_i} Z + 2\mu_{\phi_i} Z_{\phi_i} + \mu Z_{\phi_i\phi_i}\big)$$
$$\le M\int_X \mu Z y - \int_X \sum_{i=1}^n \big(a_i y \mu_{\phi_i\phi_i} - 2(a_i y \mu_{\phi_i})_{\phi_i}\big) Z$$
$$- \int_{\Gamma\cap\partial X} 2a_1 y \mu_{\phi_i} Z + \int_X \mu y F.$$

Also,

$$\int_X \mu y F = \int_X \mu y \Big(\sum_{i=1}^n \big(c_{1,i} W_{\phi_i\phi_i}(\widetilde{\phi}) + c_{2,i} U_{\phi_i} + c_{3,i} W_{\phi_i}(\widetilde{\phi})\big) + H\Big)$$
$$= \int_X \Bigg(\sum_{i=1}^n \Big(\big((\mu y c_{1,i})_{\phi_i\phi_i} - (\mu y c_{3,i})_{\phi_i}\big) W(\widetilde{\phi}) - (\mu y c_{2,i})_{\phi_i} U(\phi)\Big) + \mu y H\Bigg)$$
$$+ \int_{\Gamma\cap\partial X} \big(- (\mu y c_{1,1})_{\phi_1} W(\widetilde{\phi}) + \mu y c_{2,1} U(\phi) + \mu y c_{3,1} W(\widetilde{\phi})\big).$$

If we combine these computations with the boundary conditions satisfied by y on Γ and the definition of Z, then we can show there exist functions $g_1, g_2, g_3, g_4 \in C(\bar{X})$ with g_2 independent of the choice of β_i for $i = 1, \dots, n$ so that

$$\int_X \mu Z \Theta \le \int_\Gamma Z y\, g_1 + \int_X \Big(\mu Z g_2 \sum_{i=1}^n |c_{1,i}\, y_{\phi_i\phi_i}| + (Z+H) y\, g_3 + \mu Z g_4 \sum_{i=1}^n |y_{\phi_i}|\Big). \tag{INT3.3}$$

From the conditions that $g_1, \dots, g_4$ satisfy, there exist $K, K_\beta > 0$ so that $\|g_2\|_\infty < K$ and $\|g_i\|_\infty < K_\beta$ for $i = 1, 3, 4$. Now, suppose for the moment that $p > n$. Then we know from our discussion above that $y \in C^1(\bar{X})$ and there exists $C_p > 0$ independent of Θ so that

$$\|y\|_{\infty,X},\ \|y_{\phi_i}\|_{\infty,X},\ \|y\|_{2,p,X} < C_p.$$

Consequently, if we let C be the constant given in Lemma 3.1 then (INT3.3) yields

$$\int_X \mu Z \Theta \le (n + 2 + \|H\|_{1,X}) C C_p K_\beta + C_p K \Big[\int_X \big(\mu Z \sum_{i=1}^n |c_{1,i}|\big)^{\frac{p}{p-1}} \Big]^{\frac{p-1}{p}}. \tag{INT3.4}$$

Now recall that $c_{1,i} \in C(\bar{X})$ with $c_{1,i} = 0$ on Γ, and that the values β_i determine the support of μ. Combining this information with (INT3.4) we obtain (through duality) the existence of $\varepsilon > 0$ such that if $0 < \beta_i < \varepsilon$ for each $i = 1, \dots, n$ and $0 < \delta < \frac{1}{n-1}$, then there exists $C_{\beta,\delta} > 0$ independent of Z such that

$$\|\mu Z\|_{\frac{n}{n-1}-\delta,\Omega} \le C_{\beta,\delta}. \tag{INT3.5}$$

We now return to (INT3.3) and suppose $p > \frac{n}{2}$. Then $y \in C(\bar{X}) \cap W_p^2(\bar{X})$ and there exists $C_p > 0$ independent of Θ such that $\|y\|_{\infty,\bar{X}}$, $\|y\|_{p,X}^{(2)} < C_p$. Then Sobolev imbedding results imply there exists $C_{n,\gamma} > 0$ so that $\|y_{\phi_i}\|_{n+\gamma,\Omega} \le C_{n,\gamma}$ for all $\gamma > 0$ sufficiently small. These estimates and (INT3.3) yield

$$\int_X \mu Z\Theta \le (2 + \|H\|_{1,X}) C C_p K_\beta + C_p K \Big[\int_X \Big(\mu Z \sum_{i=1}^n |c_{1,i}| \Big)^{\frac{p}{p-1}} \Big]^{\frac{p-1}{p}} + \int_X \mu Z g_4 \sum_{i=1}^n |y_{\phi_i}|. \tag{INT3.6}$$

Therefore, if we apply (INT3.5) and the estimate above for y_{ϕ_i} above with appropriate choices for $\delta, \gamma > 0$, then we find

$$\int_X \mu Z\Theta \le (2 + \|H\|_{1,X}) C C_p K_\beta + C_p K \Big[\int_X \Big(\mu Z \sum_{i=1}^n |c_{1,i}| \Big)^{\frac{p}{p-1}} \Big]^{\frac{p-1}{p}} + n K_\beta C_{\beta,\delta} C_{n,\gamma}.$$

Thus, in a manner similar to that used to obtain (INT3.5), we find that there exists $k_p > 0$ independent of Z so that $\|\mu Z\|_{\frac{p}{p-1},X} \le k_p$ for all $p > \frac{n}{2}$. That is, there exists $K_q > 0$ independent of Z so that $\|\mu Z\|_{q,X} \le K_q$ for all $1 \le q < \frac{n}{n-2}$ (where $\frac{n}{n-2}$ is interpreted to be ∞ when $n = 2$). Consequently, if we recall our remark at the beginning of the proof, then we have our result. □

We remark that when $n = 2$, Lemma 3.3 implies that $U \in L^p(A)$ and $W \in L^p(B)$ for all $1 \le p < \infty$, with bounds independent of U and W. This will ultimately give us the necessary estimates to obtain Theorem 2.1 and the first portion of Theorem 2.3. Unfortunately, it falls short of what we need to obtain Theorem 2.2 and the final portion of Theorem 2.3. The following lemma will be used in conjunction with Lemma 3.3 to obtain these latter results.

Lemma 3.4. *Suppose that $n = 3$ and there exists $C > 0$ such that $\|G_A\|_{2,A}$, $\|G_B\|_{2,B}$, $\|U\|_{2,\partial A}$, $\|W\|_{2,\partial A} \leq C$. Then there exists $K_q > 0$ dependent upon C, but otherwise independent of G_A, G_B, U, and W, such that $\|U\|_{q,A}$, $\|W\|_{q,A} \leq C_q$ for all $1 \leq q < \infty$.*

Proof. Proceed as in the proof of Lemma 3.3, but disregard the assumption that $p > \frac{n}{2}$. We have the a priori estimate $\|Z\|_{2,\Gamma} \leq 2C$ (from the hypothesis). Furthermore, for every $1 \leq q < 3$ there exists $C_q > 0$ such that $\|Z\|_{q,G} \leq C_q$ from Lemma 3.3. Using the a priori bound on y in $W^{2,p}(X)$, we can be assured that for every $\delta > 0$ there exists $1 < p < 1 + \delta$ and $K_p > 0$ such that $\|y\|_{3+\delta,X}$, $\|y_{\phi_i}\|_{\frac{3}{2}+\delta,X}$, $\|y\|_{2+\delta,\Gamma} \leq K_p$. If we employ these estimates and the hypothesis in (INT3.3), then we obtain our result by proceeding analogously to the final portion of the proof of Lemma 3.3. $\square$

The proofs of our main results require some fundamental results for scalar diffractive-diffusion problems. To this end, suppose that $d_A, d_B > 0$, $g_A \in L^p(A)$, $g_B \in L^p(B)$, and $h \in H^{1/2}(\partial B \backslash \partial A)$. We consider the problem of determining functions ϕ_A, ϕ_B defined on A, B respectively such that

$$\begin{cases} -d_A \Delta \phi_A = g_A & x \in A \\ -d_B \Delta \phi_B = g_B & x \in B \\ \phi_A = \phi_B & \text{on } \partial A \\ d_A \frac{\partial \phi_A}{\partial \eta_A} = d_B \frac{\partial \phi_B}{\partial \eta_A} & \text{on } \partial A \\ \phi_B = h & \text{on } \partial B \backslash \partial A \end{cases} \tag{SCAL}$$

in some appropriate sense. The notion of a weak solution of (SCAL) is defined in the usual manner. One produces a function $\psi \in H^1(B)$ so that $\psi = h$ on $\partial B \backslash \partial A$ and the support of ψ does not intersect ∂A. Then the substitution $\phi_B = \widetilde{\phi}_B + \psi$ is made in (SCAL) to yield a system similar to (SCAL) with a homogeneous boundary condition on $\partial B \backslash \partial A$. Now define the sets

$$H_{AB} = \{(v_A, v_B) \in H^1(A) \times H^1(B) \mid v_A = v_B \text{ a.e. on } \partial A\}$$

and

$$H_{AB,0} = \big\{(v_A, v_B) \in H^1(A) \times H^1(B) \mid v_B = 0 \text{ a.e. on } \partial B \backslash \partial A \text{ and } v_A = v_B \text{ a.e. on } \partial A\big\}$$

equipped with the inner products $\langle\cdot,\cdot\rangle\colon H_{AB}\times H_{AB}\to\Re$ and $\langle\cdot,\cdot\rangle_0\colon H_{AB,0}\times H_{AB,0}\to\Re$ defined by

$$\big\langle(v_A,v_B),(w_A,w_B)\big\rangle = d_A\int_A \nabla v_A\cdot\nabla w_A + \int_B (d_B\nabla v_B\cdot\nabla w_B + v_B w_B)$$

for all $((v_A,v_B),(w_A,w_B))\in H_{AB}\times H_{AB}$ and

$$\big\langle(v_A,v_B),(w_A,w_B)\big\rangle_0 = d_A\int_A \nabla v_A\cdot\nabla w_A + d_B\int_B \nabla v_B\cdot\nabla w_B$$

for all $((v_A,v_B),(w_A,w_B))\in H_{AB,0}\times H_{AB,0}$. It is a simple matter to show that H_{AB} and $H_{AB,0}$ are Hilbert spaces when they are equipped with these inner products. We say $(\phi_A,\phi_B)\in H_{AB}$ is a weak solution of (SCAL) provided $(\phi_A,\widetilde{\phi}_B)\in H_{AB,0}$ and

$$\int_A d_A\nabla\phi_A\cdot\nabla v_A + \int_B d_B\nabla\widetilde{\phi}_B\cdot\nabla v_B = \int_A g_A v_A + \int_B (g_B v_B - d_B\nabla\psi\cdot\nabla v_B) \tag{WK3.7}$$

for all $(v_A,v_B)\in H_{AB,0}$.

Proposition 3.5. *Let $p>\frac{2n}{n+2}$, $g_A\in L^p(A)$, $g_B\in L^p(B)$, and $h\in H^{1/2}(\partial B\backslash\partial A)$. Then there exists a unique weak solution $(\phi_A,\phi_B)\in H_{AB}$ to* (SCAL). *Furthermore, there exists $K_p>0$ independent of g_A and g_B such that*

$$\|(\phi_A,\phi_B)\|_{H_{AB}} \le K_p\big(\|g_A\|_{p,A}+\|g_B\|_{p,B}+\|h\|_{H^{1/2}(\partial B\backslash\partial A)}\big).$$

Proof. Set $q=\frac{p}{p-1}$. Note that there exist $K_1>0$ independent of h such that the selection of ψ can be made in the manner above with $\|\psi\|_{1,2,B}\le K_1\|h\|_{H^{1/2}(\partial B\backslash\partial A)}$. Furthermore, if $(v_A,v_B)\in H_{AB,0}$, then $(v_A,v_B)\in L^q(A)\times L^q(B)$ and there exists $C_q>0$ independent of (v_A,v_B) such that

$$\|v_A\|_{q,A}+\|v_B\|_{q,B}\le C_p\,\|(v_A,v_B)\|_{H_{AB,0}}.$$

Finally, from the Poincaré inequality there exists $K_2>0$ such that for every $(v_A,v_B)\in H_{AB,0}$

$$\|v_A\|_{1,2,A}+\|v_B\|_{1,2,B}\le K_2\|(v_A,v_B)\|_{H_{AB,0}}.$$

Now define F: $H_{AB,0} \to \Re$ via

$$F(v_A, v_B) = \int_A g_A v_A + \int_B (g_B v_B - d_B \nabla\psi \cdot \nabla v_B)$$

for all $(v_A, v_B) \in H_{AB,0}$. Clearly F is well defined and linear. also,

$$\begin{aligned}|F(v_A, v_B)| &\le \|g_A\|_{p,A}\|v_A\|_{q,A} + \|g_B\|_{p,B}\|v_B\|_{q,B} + d_B\|\psi\|_{1,2,B}\|v_B\|_{1,2,B}\\ &\le \big(\|g_A\|_{p,A} + \|g_B\|_{p,B}\big)C_p\|(v_A, v_B)\|_{H_{AB,0}}\\ &\qquad + d_B K_1\|h\|_{H^{1/2}(\partial B\setminus\partial A)}K_2\|(v_A, v_B)\|_{H_{AB,0}}.\end{aligned}$$

Therefore, F is a bounded linear functional on $H_{AB,0}$. As a result, a simple application of the Riesz Representation Theorem guarantees the existence of a unique $(\phi_A, \widetilde{\phi}_B) \in H_{AB,0}$ that solves (WK3.7). Moreover, $\|(\phi_A, \widetilde{\phi}_B)\|_{H_{AB,0}} = \|F\|$. The result follows. $\square$

The theorem below is well known ([11], [12], [17]). Since our focus does not lie with the properties of the functions g_i in (P), our statement of the result below is given for smooth h in (SCAL). Certainly, if h is smooth, then we have $h \in H^{1/2}(\partial B\setminus\partial A)$. Also, recall from the beginning of Section 2 that we are assuming $n \ge 2$ throughout this work. Consequently, $\frac{n}{2} \ge \frac{2n}{n+2}$, and therefore the results of Proposition 3.5 above can be applied in the setting of the theorem below.

Theorem 3.6. *Let h be a smooth function. If $g_A \in L^p(A)$ and $g_B \in L^p(B)$ with $p > \frac{n}{2}$, then there exists $0 < \alpha < 1$ such that the unique weak solution $(\phi_A, \phi_B) \in H_{AB}$ of* (SCAL) *satisfies $\phi_A \in C^\alpha(\bar{A})$ and $\phi_B \in C^\alpha(\bar{B})$. If there exists $0 < \beta < 1$ such that $g_A \in C^\beta(\bar{A})$ and $g_B \in C^\beta(\bar{B})$, then $\phi_A \in C^2(A)\cap C^1(\bar{A})$, $\phi_B \in C^2(\bar{B}\setminus\partial A)\cap C^1(\bar{B})$, and (ϕ_A, ϕ_B) satisfies* (SCAL) *in the classical sense. In either case, the norm estimates on (ϕ_A, ϕ_B) depend only upon norm estimates for h, g_A and g_B.*

We close this section with the statement of a well known fixed point result [22].

Theorem 3.7. *Let X be a Banach space and suppose that $T\colon X \to X$ is a completely continuous map. If there exists a constant $K > 0$ such that $\|y\|_X \le K$ whenever $0 \le \sigma \le 1$ and $y \in X$ such that $y = \sigma T(y)$, then there exists $x \in X$ such that $T(x) = x$.*

4. Proofs of the main results. Since our results have a common flavor, our analysis begins with a structure which can be applied uniformly.

We begin by truncating our vector field and forcing nonnegativity. To this end, we let $\psi \in C_0^\infty(\Re^m, [0,1])$ and define $F_q(z) = \psi(z) f_q(z^+)$, for $q = A, B$. Note that F_q is Lipschitz. We now create a natural fixed point problem associated with (P). Define

$$T\colon L^2(A,\Re^m) \times L^2(B,\Re^m) \to L^2(A,\Re^m) \times L^2(B,\Re^m)$$

via $T(v,\widetilde{v}) = (u,\tilde{u})$ where $(u,\tilde{u})$ is the unique weak solution of

$$\begin{cases} -d_{A_i}\Delta u_i = F_{A_i}(v) & x \in A \\ -d_{B_i}\Delta \tilde{u}_i = F_{B_i}(\widetilde{v}) & x \in B \\ u_i = \tilde{u}_i & \text{on } \partial A \\ d_{A_i}\frac{\partial u_i}{\partial \eta_A} = d_{B_i}\frac{\partial \tilde{u}_i}{\partial \eta_A} & \text{on } \partial A \\ \tilde{u}_i = g_i & \text{on } \partial B \backslash \partial A \end{cases} \tag{PN}$$

guaranteed by Proposition 3.5. (Note that $(F_{A_i}(v), F_{B_i}(\widetilde{v})) \in L^\infty(A) \times L^\infty(B)$ for all $(v,\widetilde{v}) \in L^2(A) \times L^2(B)$.)

Lemma 4.1. *T is a completely continuous map on $L^2(A) \times L^2(B)$. Furthermore, if $0 \le \lambda \le 1$ and $(u,\tilde{u}) \in L^2(A) \times L^2(B)$ are such that $(u,\tilde{u}) = \lambda T(u,\tilde{u})$, then $u \in C^2(A,\Re^m) \cap C^1(\bar{A})$, $\tilde{u} \in C^2(\bar{B}\backslash\partial A, \Re^m) \cap C^1(\bar{B})$, and $(u,\tilde{u}) = (u^+,\tilde{u}^+)$.*

Proof. From the definitions of F_A and F_B we know there exists $M_\psi > 0$ such that $\|F_{A_i}(v)\|_{\infty,A}$, $\|F_{B_i}(\widetilde{v})\|_{\infty,B} \le M_\psi$ for all $(v,\widetilde{v}) \in L^2(A) \times L^2(B)$. Consequently, from Proposition 3.5, T maps all of $L^2(A) \times L^2(B)$ into a bounded subset of H_{AB}, which is clearly compactly imbedded in $L^2(A) \times L^2(B)$. Similarly, the continuity of T can be easily obtained from Proposition 3.5 since F_A and F_B are Lipschitz. As a result, T is a completely continuous map on $L^2(A) \times L^2(B)$.

Now suppose that $0 \le \lambda \le 1$ and $(u,\tilde{u}) \in L^2(A) \times L^2(B)$ is such that $(u,\tilde{u}) = \lambda T(u,\tilde{u})$. Then $(u,\tilde{u})$ is a weak solution of

$$\begin{cases} -d_{A_i}\Delta u_i = \lambda F_{A_i}(u) & x \in A \\ -d_{B_i}\Delta \tilde{u}_i = \lambda F_{B_i}(\tilde{u}) & x \in B \\ u_i = \tilde{u}_i & \text{on } \partial A \\ d_{A_i}\frac{\partial u_i}{\partial \eta_A} = d_{B_i}\frac{\partial \tilde{u}_i}{\partial \eta_A} & \text{on } \partial A \\ \tilde{u}_i = \lambda g_i & \text{on } \partial B \backslash \partial A. \end{cases} \tag{λPN}$$

Furthermore, from the properties of F_A and F_B, and the first portion of Theorem 3.6, we know there exists $0 < \alpha < 1$ such that $(u, \tilde{u}) \in C^\alpha(\bar{A}, \Re^m) \times C^\alpha(\bar{B}, \Re^m)$. Consequently, if we apply this information to the properties of F_A and F_B, and the second portion of Theorem 3.6, then we have $u \in C^2(A, \Re^m) \cap C^1(\bar{A})$, $\tilde{u} \in C^2(\bar{B} \backslash \partial A, \Re^m) \cap C^1(\bar{B})$ and $(u, \tilde{u})$ satisfies (λPN) in the classical sense. Therefore, if we multiply the partial differential equation for u_i in (λPN) by u_i^- and integrate by parts, then we obtain

$$-d_{A_i} \int_A |\nabla u_i^-|^2 dx + d_{B_i} \int_{\partial A} \tilde{u}_i^- \frac{\partial \tilde{u}_i}{\partial \eta_B} d\sigma \geq 0 \tag{INT4.1}$$

from the quasi-positivity condition (QP). If we perform a similar calculation with $\tilde{u}_i^-$, then after rearranging terms, we are lead to

$$-d_{B_i} \int_{\partial B} \tilde{u}_i^- \frac{\partial \tilde{u}_i}{\partial \eta_B} \partial\sigma - d_{B_i} \int_B |\nabla \tilde{u}_i^-|^2 dx \geq 0. \tag{INT4.2}$$

If we add (INT4.1) and (INT4.2), then we find

$$-d_{B_i} \int_{\partial B \backslash \partial A} \tilde{u}_i^- \frac{\partial \tilde{u}_i}{\partial \eta_B} d\sigma - d_{A_i} \int_A |\nabla u_i^-|^2 dx - d_{B_i} \int_B |\nabla \tilde{u}_i^-|^2 dx \geq 0. \tag{INT4.3}$$

Note that by hypothesis, we have $\tilde{u}_i^- = 0$ on $\partial B \backslash \partial A$. Therefore, we conclude from (INT4.3) that $(u, \tilde{u})$ is nonnegative. □

Proof of Theorem 2.1. Define $U = \sum_{i=1}^m b_i d_{A_i} u_i$, $W = \sum_{i=1}^m b_i d_{B_i} \tilde{u}_i$ and $g = \sum_{i=1}^m b_i d_{B_i} g_i$. Then clearly U and W satisfy (SC) with $H_A = K_A$ and $H_B = K_B$. Consequently, if $n = 2$, then from Lemma 3.3 we have $\|U\|_{q,A}$, $\|W\|_{q,B} < C_q$ for all $1 \leq q < \infty$. This estimate, in turn, implies $\|u_i\|_{q,A}$, $\|\tilde{u}_i\|_{q,B} < C_q/b_i$ for all $1 \leq q < \infty$ and $i = 1, \dots, m$, and we remark that these estimates are independent of λ and the cut-off function ψ. If we now recall (POLY), then we have a bound for $\lambda F_{q_i}(u)$ in every L^p space, for $q = A, B$, $i = 1, \dots, m$ and $1 \leq p < \infty$. As a result, if we apply Theorem 3.6, then we obtain $C_\infty > 0$ independent of λ and ψ such that $\|u_i\|_{\infty,A}$, $\|\tilde{u}_i\|_{\infty,B} < C_\infty$. Therefore, from Theorem 3.7, we have a fixed point for T, and hence a solution of (NP). In addition, a sup-norm bound for this fixed point is obtained independent of the cut-off function. Consequently, by choosing ψ appropriately, we can conclude that (P) has a nonnegative solution when $n = 2$. □

Proof of Theorem 2.2. We proceed as in the proof of Theorem 2.1. First define $U = \sum_{i=1}^{m} b_i d_{A_i} u_i$, $W = \sum_{i=1}^{m} b_i d_{B_i} \tilde{u}_i$, and $g = \sum_{i=1}^{m} b_i d_{B_i} g_i$. As above, U and W satisfy (SC). Consequently, if $n = 3$, then from Lemma 3.3 we have $\|U\|_{q,A}$, $\|W\|_{q,B} < C_q$ for all $1 \le q < 3$. This estimate, in turn, implies $\|u_i\|_{q,A}$, $\|\tilde{u}_i\|_{q,B} < C_q/b_i$ for all $1 \le q < 3$ and $i = 1, \dots, m$, and we remark that these estimates are independent of λ and the cut-off function ψ.

We now employ the intermediate sums condition (QUAD) to improve our estimates. We proceed inductively. First note that

$$\int_A d_1 |\nabla u_1|^2 + \int_B d_{B_1} |\nabla \tilde{u}_1|^2 \le \int_A u_1 Q(u) + \int_B \tilde{u}_1 Q(\tilde{u}). \tag{INT4.4}$$

From Lemma 3.3, there exists $C > 0$ such that

$$\|u_1\|_{1,A}, \|\tilde{u}_1\|_{1,B}, \|Q(u)\|_{4/3,A}, \|Q(\tilde{u})\|_{4/3,B} < C.$$

In addition, from Sobolev Imbedding there exists a constant $K > 0$ such that

$$\|u_1\|_{4,A} + \|\tilde{u}_1\|_{4,B} < K\big(\|u_1\|_{1,2,A} + \|\widetilde{u}_1\|_{1,2,B}\big)$$

and

$$\big(\|u_1\|_{1,2,A} + \|\tilde{u}_1\|_{1,2,B}\big)^2 \le K\Big(C + \int_A d_1 |\nabla u_1|^2 + \int_B d_{B_1} |\nabla \tilde{u}_1|^2\Big).$$

Combining these inequalities with (INT4.4) yields

$$(\|u_1\|_{1,2,A} + \|\tilde{u}_1\|_{1,2,B})^2 < CK^2\big(\|u_1\|_{1,2,A} + \|\widetilde{u}_1\|_{1,2,B} + 1\big).$$

As a result, there exists $L > 0$ such that

$$\|u_1\|_{1,2,A}, \|\widetilde{u}_1\|_{1,2,B} \le L,$$

with L independent of λ and ψ. Now suppose that $1 \le k < m$ and there exists $L > 0$ such that $\|u_i\|_{1,2,A}$, $\|\tilde{u}_i\|_{1,2,B} \le L$ for all $1 \le i \le k$, with L given independent of λ and ψ. If we again employ (QUAD), then we obtain

$$\begin{aligned}\int_A \nabla\left(\sum_{i=1}^{k+1} u_i\right) \cdot \nabla\left(\sum_{i=1}^{k+1} d_{A_i} u_i\right) + \int_B \nabla\left(\sum_{i=1}^{k+1} \tilde{u}_i\right) \cdot \nabla\left(\sum_{i=1}^{k+1} d_{B_i} \tilde{u}_i\right) \\ \le \int_A \sum_{i=1}^{k+1} u_i Q(u) + \int_B \sum_{i=1}^{k+1} \widetilde{u}_i Q(\tilde{u}).\end{aligned} \tag{INT4.5}$$

Consequently, if we argue similarly as above and apply our induction hypothesis, then we obtain $\widetilde{L} > 0$ independent of λ and ψ such that $\|u_{k+1}\|_{1,2,A}$, $\|\tilde{u}_{k+1}\|_{1,2,B} \leq \widetilde{L}$. Therefore, we can conclude that there exists $L > 0$ such that $\|u_i\|_{1,2,A}$, $\|\tilde{u}_i\|_{1,2,B} \leq L$ for all $1 \leq i \leq m$, with L given independent of λ and ψ.

We can now complete our proof. From the estimates above and trace class imbeddings, we have $\|U\|_{3,\partial A}$, $\|W\|_{3,\partial A} \leq C$ where $C > 0$ can be chosen independent of λ and ψ. As a result, Lemma 3.4 implies $\|U\|_{q,A}$, $\|W\|_{q,B} < C_q$ for all $1 \leq q < \infty$, and hence $\|u_i\|_{q,A}$, $\|\tilde{u}_i\|_{q,B} < C_q/b_i$ for all $1 \leq q < \infty$ and $i = 1, \dots, m$, with these estimates being independent of λ and the cut-off function ψ. The proof can now be completed in a manner similar to that of Theorem 2.1. $\square$

Proof of Theorem 2.3. We proceed similarly to the proofs of Theorems 2.1 and 2.2, with adjustments made to accommodate the differences between (BAL)–(QUAD) and (BAL1)–(QUAD1). To this end we first let $U = \sum_{i=1}^{k} b_i d_{A_i} u_i$, $W = \sum_{i=1}^{k} b_i d_{B_i} \tilde{u}_i$ and $g = \sum_{i=1}^{k} b_i d_{B_i} g_i$ and follow the arguments above to obtain $\|u_i\|_{q,A}$, $\|\tilde{u}_i\|_{q,B} < C_q$ for all $1 \leq q < \infty$ and $1 \leq i \leq k$, with C_q independent of λ and the cut-off function ψ. We then take $U = \sum_{i=k+1}^{m} b_i d_{A_i} u_i$, $W = \sum_{i=k+1}^{m} b_i d_{B_i} \tilde{u}_i$ and $g = \sum_{i=k+1}^{m} b_i d_{B_i} g_i$ and note that there exists $d > 0$ such that

$$\begin{cases} -\Delta U \leq P_1(u_1, \dots, u_k) & \text{in } A \\ -\Delta W \leq P_1(\tilde{u}_1, \dots, \tilde{u}_k) & \text{in } B \\ \frac{\partial U}{\partial \eta_A} = \frac{\partial W}{\partial \eta_A} & \text{on } \partial A \\ \frac{1}{d} W \leq U \leq dW & \text{on } \partial A \\ W = g & \text{on } \partial B \backslash \partial A. \end{cases}$$

Since P_1 is a polynomial and we have L^q estimates for $u_i, \tilde{u}_i$ for $1 \leq i \leq k$, we can employ the estimates from Section 3 to obtain estimates for U and W dependent upon our L^q estimates for u_i, $\tilde{u}_i$ for $1 \leq i \leq k$. If we continue as in the proofs of Theorem 2.1 and 2.2, then we obtain L^p estimates for $u_i, \tilde{u}_i$ for $k + 1 \leq i \leq m$ and $1 \leq p < \infty$, dependent upon our earlier estimates for $u_i, \tilde{u}_i$ for $1 \leq i \leq k$, with all estimates independent of λ and the cut-off function ψ. Continuing to follow the proofs above, we obtain our result.

5. Examples. In this section we illustrate the applicability of our results by applying them to two nontrivial chemical models.

Example 5.1. Perhaps the greatest source of interesting problems in this area is the modeling of multi-species chemical reactions. For example, let us consider the following, seemingly simple, reversible reaction in which tin oxide reacts with carbon monoxide to form form metallic tin and carbon dioxide:

$$\mathrm{SnO_2} + 2\mathrm{CO} \rightleftharpoons \mathrm{Sn} + 2\mathrm{CO_2}.$$

We assume that this process takes place on a heterogeneous domain in $\Re^2$ of the type described in the previous sections. Let u_1, u_2, u_3, u_4 denote the concentrations of $\mathrm{SnO_2}$, CO, Sn, $\mathrm{CO_2}$ respectively in A, and $\tilde{u}_1, \tilde{u}_2, \tilde{u}_3, \tilde{u}_4$ the associated counterparts in B. Then we might model the reaction diffusion process for this single step chemical process in the form of the system (P). In this case we have

$$f_A(z) = \begin{pmatrix} 1 \\ 2 \\ -1 \\ -2 \end{pmatrix} \left(k_{Ar} z_3 z_4^2 - k_{Af} z_1 z_2^2\right)$$

and

$$f_B(z) = \begin{pmatrix} 1 \\ 2 \\ -1 \\ -2 \end{pmatrix} \left(k_{Br} z_3 z_4^2 - k_{Bf} z_1 z_2^2\right),$$

where k_{qf}, k_{qr} are forward, reverse effective rates, respectively, for $q = A, B$. Here the terms k_{qf}, k_{qr} are assumed to be smooth, bounded, nonnegative, and possible dependent upon z. Close examination of the vector fields above show that (QP) and (POLY) are clearly satisfied. Furthermore, (BAL) holds with $K_q = 0$ for $q = A, B$, and

$$[b_1, b_2, b_3, b_4] = [1, 1, 1, 1].$$

Consequently, we can conclude from Theorem 2.1 that (P) has a componentwise nonnegative classical solution.

Of course, from the comments in Section 1 this should be no surprise. As stated in that section, all single step reversible chemical processes satisfy (BAL). In addition, it is easy to show that (QP) and (POLY) are satisfied by these systems [8].

Example 5.2. In this example we demonstrate the applicability of our results by considering a somewhat more complex chemical process. More specifically, we consider the interactions of the chemical concentrations of the minimal chlorite-iodite reaction. A somewhat simplified version of this model was considered by Ouyang, Castets, Boissonade, Roux and DeKepper [16]. There the researchers considered the one-dimensional Couette reactor in which chemical concentrations of the minimal chlorite-iodite reaction are fed at both ends of the reactor. The authors employed a simplifying assumption to reduce the complexity of the model equations. A number of spatial patterns were found experimentally, and Ouyang, et al, ran numerical tests on the model to reinforce their findings. The chemical process is described by the following set of reactions steps:

$$\begin{aligned} \mathrm{H}^+ + \mathrm{ClO}_2^- + I^- &\rightharpoonup \mathrm{HOCl} + \mathrm{HOI} \\ \mathrm{H}^+ + \mathrm{HOI} + \mathrm{I}^- &\rightleftharpoons \mathrm{I}_2 + \mathrm{H}_2\mathrm{O} \\ \mathrm{ClO}_2^- + \mathrm{HOI} + \mathrm{H}^+ &\rightharpoonup \mathrm{HIO}_2 + \mathrm{HOCl} \\ \mathrm{HOCl} + \mathrm{I}^- &\rightharpoonup \mathrm{HOI} + \mathrm{Cl}^- \\ \mathrm{HIO}_2 + \mathrm{I}^- + \mathrm{H}^+ &\rightleftharpoons 2\mathrm{HOI} \\ 2\mathrm{HIO}_2 &\rightharpoonup \mathrm{HOI} + \mathrm{IO}_3^- + \mathrm{H}^+ \\ \mathrm{HIO}_2 + \mathrm{HOI} &\rightharpoonup \mathrm{I}^- + \mathrm{IO}_3^- + \mathrm{H}^+ \\ \mathrm{HIO}_2 + \mathrm{HOCl} &\rightharpoonup \mathrm{IO}_3^- + \mathrm{Cl}^- + 2\mathrm{H}^+. \end{aligned}$$

If no simplifying assumptions are made, and the laws of mass action kinetics are employed, then these reaction steps lead to a ten-component reaction-diffusion model. We consider the scenario in which we have a reaction diffusion process taking place on a smooth bounded region Ω of $\Re^3$ which decomposes similarly to the one given in Section 1. Consideration of the associated steady state problem can lead to a system of the form (P) with f_A, f_B described through the following mechanism. First, we denote $u_1 = [\mathrm{ClO}_2^-]$, $u_2 = [\mathrm{Cl}^-]$, $u_3 = [\mathrm{I}^-]$, $u_4 = [\mathrm{HOCl}]$, $u_5 = [\mathrm{HOI}]$, $u_6 = [\mathrm{I}_2]$, $u_7 = [\mathrm{H}_2 O]$, $u_8 = [\mathrm{HIO}_2]$, $u_9 = [\mathrm{IO}_3^-]$ and $u_{10} = [\mathrm{H}^+]$ in A, with corresponding assignments for $\tilde{u}_1, \dots, \tilde{u}_{10}$ in B. We then denote the reaction rates by

$$\begin{gathered} R_1(z) = -k_1 z_1 z_3 z_{10}, R_2(z) = k_{-2} z_6 z_7 - k_2 z_3 z_5 z_{10}, R_3(z) = -k_3 z_1 z_5 z_{10}, \\ R_4(z) = -k_4 z_3 z_4, R_5(z) = k_{-5} z_5^2 - k_5 z_3 z_8 z_{10}, R_6(z) = -k_6 z_8^2, \\ R_7(z) = -k_7 z_5 z_8, \quad \text{and} \quad R_8(z) = -k_8 z_4 z_8, \end{gathered}$$

and make analogous assignments for $\widetilde{R}_i(z)$ with the only changes being the use of $\widetilde{k}_j, \widetilde{k}_{-j}$. Here we assume each $k_j, k_{-j}, \widetilde{k}_j, \widetilde{k}_{-j}$ is nonnegative, bounded, and possibly smoothly dependent upon z. Using standard terminology, we refer to k_j, k_{-j}, $\widetilde{k}_j, \widetilde{k}_{-j}$ as forward and reverse effective rates for the j^{th} reaction step in the regions A and B. We then define the stoichiometric matrix

$$N = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 \\ 1 & 1 & 0 & 1 & 1 & 0 & -1 & 0 \\ -1 & 0 & -1 & 1 & 0 & 0 & 0 & 1 \\ -1 & 1 & 1 & -1 & -2 & -1 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 2 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 \\ 1 & 1 & 1 & 0 & 1 & -1 & -2 & -2 \end{pmatrix}.$$

Then $f_A(z) = NR(z)$ and $f_B(z) = N\widetilde{R}(z)$, where $R(z) = (R_i(z))$ and $\widetilde{R}(z) = (\widetilde{R}_i(z))$ are vector valued functions. It is a simple matter to check that (QP) and (POLY) are satisfied. Also, if we denote N_9 to be the 9×8 matrix obtained by deleting the tenth row from N, then it is easy to see that $(1, 1, \dots, 1)^T \in \ker(N_9^T)$. In addition, $f_{q_{10}}(z) \leq P_1(z_4, z_5, z_6, z_7, z_8)$ for $q = A, B$, where P_1 is a quadratic polynomial. As a result, (BAL1) is satisfied with $b_i = 1$ for all $i = 1, \dots, m$, $K_q = 0$, $k = 9$ and P_1 as above. Finally, if we define

$$\mathcal{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

then it is a simple matter to check (QUAD1). As a result, we can apply Theorem 2.3 to guarantee the existence of a nonnegative solution to (P).

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