

A one-dimensional reaction/diffusion system with a fast reaction¹

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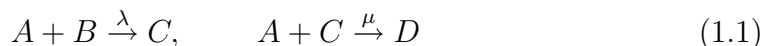
ABSTRACT: We consider a system of second order ordinary differential equations describing steady state for a 3-component chemical system (with diffusion) in the case when one of the reactions is fast. We discuss the existence of solutions and the existence, uniqueness, and characterization of a limit as the rate of the fast reaction approaches infinity.

KEY WORDS: *reaction/diffusion system, boundary value problem, steady state, fast reaction, asymptotics.*

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1. Introduction

From the viewpoint of chemical engineering, our objective is to understand the diffusion controlled rate for a surface reaction $2A + B \rightarrow D$ in terms of a coupled pair of rapid irreversible binary reactions²



involving an intermediate complex C . Mathematically, this will lead us to con-

²The system (1.1) in a ‘film’ (cf., [5]) was also treated as a model problem in [2], there involving much different considerations. For a perspective of one general setting in which problems of this sort arise, see [3] for a discussion of some of the modeling issues arising in the context of bubble reactors. We are here indebted to J. Romanainen, of Kemira Chemicals, for raising the question discussed in this paper.

sider³ the system of ordinary differential equations

$$\begin{aligned} a_1 u'' - \lambda uv - \mu uw &= 0 \\ a_2 v'' - \lambda uv &= 0 & \text{on } (0, 1) \\ a_3 w'' + \lambda uv - \mu uw &= 0 \end{aligned} \tag{1.2}$$

with the boundary conditions

$$\begin{aligned} u = \alpha > 0, \quad v' = 0, \quad w' = 0 & \quad \text{at } x = 0, \\ u' = 0, \quad v = \beta > 0, \quad w' = 0 & \quad \text{at } x = 1 \end{aligned} \tag{1.3}$$

and the paper will be concerned primarily with the limiting behavior as $\lambda \rightarrow \infty$ (with α, β , and μ fixed) for solutions of (1.2)-(1.3). In particular, our objective will be the determination of $q := \int \lambda uv$ for large λ ($\rightarrow \infty$), which corresponds to the rate of production of C and of consumption of B — and also to the rate of production of D , since the assumed boundary conditions for w ensure that the second reaction in (1.1) must go to completion.

This analysis is interesting in its own right — both for the application and as leading to some interesting analysis — but may also serve as a model problem in

³The variables u, v, w of (1.2) represent normalized concentrations of A, B, C , respectively; we have omitted consideration of the reaction product D as well as of any other species whose reactions, if coupled at all with (1.1), are negligible within the membrane. The quadratic terms λuv and μuw are then the usual kinetics for reactions in dilute solution. The variable x represents position transverse to the membrane thickness; we are assuming that this situation is effectively constant in directions parallel to the surface. We have chosen units to scale the membrane thickness to 1 and the diffusion coefficients by a to get $a_j = \mathcal{O}(1)$. Note that this means that the original reaction rates have been multiplied by h^2/a ; as they appear here, we have $\mu = \mathcal{O}(1)$ and $\lambda \gg 1$ (with $\lambda \rightarrow \infty$ later). [It would also have been possible, using the structure of the equation, to normalize the concentrations so as to have $\mu = 1$ as well, but we have chosen not to do this.] The boundary conditions (1.3) correspond to the situation we will be describing.

that the techniques developed here may also be of use for similar situations. To this end, part of our analysis is presented in greater generality than is actually needed for (1.2) and Remark 4 in Section 5 provides some brief further indication of the scope of these ideas.

Following the framework of Chapters 13–15 of [1], which we recommend as a reference for the determination of diffusion controlled reaction rates and applications, we first sketch the heuristic analysis of (1.1) when both λ, μ are effectively infinite. Our point will be that this must be modified — the objective of our analysis from the viewpoint of the application — when the second reaction in (1.1) is less rapid than is appropriate for that argument.

For our purposes, one postulates *steady state* in a thin diffusive layer⁴ (such as a membrane) of thickness h with the concentration of A maintained at A_* on one side ($x = 0$) and, similarly, $B = B_*$ on the other ($x = h$). For both reactions in (1.1) taken to be ‘instantaneous’, we then have a *reaction plane* ($x = x^*h$) within the diffusive layer with pure diffusion of B (i.e., with no reaction in the absence of A) for $x^*h < x < h$ and pure diffusion of A for $0 < x < x^*h$ so one has straight-line concentration profiles. To obtain the overall stoichiometry $2A + B \rightarrow D$, the second reaction in (1.1) must go to completion so we must

⁴Diffusion is, e.g., on the order of $10^{-5}\text{cm}^2/\text{sec}$ — which is slow for a ‘normal’ length scale but fast enough (on the scale of a layer thickness h which may be about 10^{-3}cm) that approach to steady state would be rapid compared to the ‘normal’ time scale; in particular, one would expect quasi-steady state ‘tracking’ of comparatively slower parameter variations.

assume that it takes place at the same reaction plane.⁵ The relevant slopes are $-A_*/x^*h$, $B_*/(1-x^*)h$ and the flux balance for this stoichiometry then gives $a_1A_*/x^* = 2a_2B_*/(1-x^*)$ where a_1, a_2 are the diffusion coefficients for A, B , respectively. As the flux of B necessarily equals the production of D , the surface reaction produces D at the rate

$$\dot{D} =: q = (a_1/2h)A_* + (a_2/h)B_* \quad (1.5)$$

per unit area. Note that the situation is ‘diffusion controlled’ as, even with this approximating assumption of infinitely fast reaction speeds λ, μ in (1.1), the effective composite reaction rate is finite, depending on the diffusion coefficients a_1, a_2 (normalized by the thickness h).

We actually wish to consider (1.1) in a setting with the reaction rate $\mu = \mathcal{O}(1)$ (on the diffusive time scale) but still with the first reaction very much faster: $\lambda \gg 1$. Thus, we take $\lambda \rightarrow \infty$ and anticipate a well-defined reaction plane within the membrane for the first reaction while noting that the second will now be distributed over the region $0 < x < x^*h$ where the component A is available. This means, of course, that in this region one will not have the straight line profile which made possible the simple analysis above.

We do continue to want the second reaction to go to completion, as above, and so assume that the membrane is such as to give ‘no flux conditions’ for the

⁵Otherwise we would get

$$(1+\rho)A + B \rightarrow \rho D + (1-\rho)C \quad (1.4)$$

where ρ here represents the fraction of the C produced which does become involved in the second reaction so $(1-\rho)$ is the remaining fraction which does not become so involved — presumably ‘escaping’ by transport across $x = h$. This problem is not our present concern, but we will comment on it in Section 5, Remark 4.

complex C on each side, so C cannot leave the membrane once produced. This is a somewhat difficult situation to work with, since the Dirichlet conditions for u, v imply ‘potentially infinite’ sources of the reagents A, B which produce it. Thus, a steady state can only be possible if the net production of C would be 0, i.e., if the production of C in the first reaction would always be balanced by its consumption in the second, slower reaction. It is not at all clear *a priori* whether such a balance should occur, but the consumption of C from the second reaction might be expected to ‘grow’ (from a time-dependent viewpoint) as the concentration of C would build up and so one might hope that ‘eventually’ it would become high enough to give this balance — provided enough A remained to maintain the slower reaction at this level.

Section 2 will be devoted to obtaining suitable estimates and showing that one does, in fact, have steady state solutions for finite $\lambda > 0$; the first part of Section 3 obtains an estimate giving enough compactness to ensure, at least for subsequences, some convergence as $\lambda \rightarrow \infty$. These arguments of Sections 2 and 3 already depend somewhat delicately on the interaction of reactions and boundary conditions in our model problem but have a ‘PDE flavor’ and are presented from that point of view, although with final emphasis on the specifically one-dimensional case consistent with our original motivation.

As in the earlier heuristic argument, it is intuitively clear that A, B effectively cannot coexist for very large λ — if they were together they would ‘immediately’ react to form C — so, in the limit $\lambda \rightarrow \infty$ we must have $uv \equiv 0$ (i.e., A, B must occupy distinct geometric regions). Section 3 is concerned with a mathematical demonstration of the corresponding characterization of ‘limit solutions’, for the subsequences noted above, with a return to the specifically one-dimensional

setting for the more detailed convergence analysis.

The chemical engineers' principal concern here would be with the determination, as the parameters α, β (and μ) vary, of the rate of production of D or, equivalently, the rate at which an external supply of B is being consumed by flux into the membrane. [As already noted, this is $q := \int \lambda uv$.] For this determination to be well-defined, it is necessary to show that the characterization of the limit solution implies uniqueness, which is demonstrated in Section 4. This also completes the convergence argument as $\lambda \rightarrow \infty$ by eliminating the need to extract subsequences.

The uniqueness argument seems rather specialized to the ODE context and to the particular system at hand. Indeed, there seems no reason on physical grounds to expect uniqueness generally for problems of this sort. Although we do not, at present, know any actual example of such behavior, one might anticipate 'tracking' (in quasi-steady state), for slowly varying data in the boundary conditions, with the physical selection from among multiple steady states depending hysteresically on the history of that variation.

Finally, we note that the present paper is to be viewed as the initiation of a more complete program of investigation. In particular, we note that: (1) while we are exclusively concerned here with the steady state problem we anticipate related results for the time-dependent evolution and (2) the present results may be viewed as providing the leading term of a singular perturbation expansion in powers of $\varepsilon^{1/3}$ (cf. Remarks 1,2 in Section 5 and [4]) for the small parameter $\varepsilon := 1/\lambda$.

2. Existence of a steady state solution

While our principal interest is with the one-dimensional problem (1.2)-(1.3), the considerations of this section and the next extend to a higher-dimensional setting so the results will be presented in that more general context, especially as this exposition seems likely to provide a deeper understanding of the underlying argument. In this section we present the argument for existence of (at least one) solution of the steady state problem. As already noted in the Introduction, the major difficulty will be to bound the production rate of C (i.e., to bound the generation term $\int \lambda uv$) and then to bound the total amount of C at steady state (i.e., $\int w$).

We will now be considering a bounded region $\Omega \subset \mathbb{R}^m$ (physically, $m = 1, 2, 3$, but mathematically we may have any $m \geq 1$) and the steady state reaction/diffusion system takes the form

$$\begin{cases} a_1 \Delta u - \lambda uv - \mu uw &= 0 \\ a_2 \Delta v - \lambda uv &= 0 \\ a_3 \Delta w + \lambda uv - \mu uw &= 0 \end{cases} \quad \text{on } \Omega \quad (2.1)$$

$$u = \alpha \text{ on } \Gamma_A \text{ with } u_\nu = 0 \text{ on } \partial\Omega \setminus \Gamma_A$$

$$v = \beta \text{ on } \Gamma_B \text{ with } v_\nu = 0 \text{ on } \partial\Omega \setminus \Gamma_B$$

$$w_\nu = 0 \text{ on } \partial\Omega.$$

Here Γ_A, Γ_B are separated portions of the boundary $\partial\Omega$ and α, β are (traces⁶ on Γ_A, Γ_B , respectively, of) functions such that

$$\begin{aligned} \alpha, \beta \in H^1(\Omega) \quad & \text{with } 0 \leq \alpha \leq \bar{\alpha}, \ 0 \leq \beta \leq \bar{\beta} \\ & \text{and } \int_{\Gamma_A} \alpha =: \underline{\alpha} > 0 \end{aligned} \quad (2.2)$$

⁶We need, e.g., $0 \leq \alpha \leq \bar{\alpha}$ only on Γ_A but note that the global assumption involves no further loss of generality: else, just replace α pointwise on Ω by $\min\{\bar{\alpha}, \alpha_+\}$ with $\alpha_+ := \max\{\alpha, 0\}$.

for positive constants $\bar{\alpha}, \bar{\beta}, \underline{\alpha}$. For the region Ω , we assume sufficient regularity for the usual trace theorems; we will later state some further mild conditions (automatic for the one-dimensional case) which will be used in obtaining relevant estimates.

We will prove existence by an argument using the Schauder Fixpoint Theorem. With $M > 0$ to be determined later, we set

$$\begin{aligned} \mathcal{S} = \mathcal{S}_M := \{ (u, v, w) : 0 \leq u \leq \bar{\alpha}, 0 \leq v \leq \bar{\beta}, 0 \leq w, \int_{\Omega} w \leq M \} \\ \subset L^2(\Omega) \times L^2(\Omega) \times L^1(\Omega) \end{aligned} \quad (2.3)$$

and then define on \mathcal{S} a map $\mathcal{M} : (\hat{u}, \hat{v}, \hat{w}) \mapsto (u, v, rw)$ with u, v, w, r given by the steps:

1. Solve for u the linear problem

$$\begin{aligned} a_1 \triangle u - \lambda u \hat{v} - \mu u \hat{w} &= 0 \quad \text{with} \\ u &= \alpha \text{ on } \Gamma_A \text{ and } u_{\nu} = 0 \text{ on } \partial\Omega \setminus \Gamma_A \end{aligned} \quad (2.4)$$

2. Using u from (2.4), solve for v the linear problem

$$\begin{aligned} a_2 \triangle v - \lambda uv &= 0 \quad \text{with} \\ v &= \beta \text{ on } \Gamma_B \text{ and } v_{\nu} = 0 \text{ on } \partial\Omega \setminus \Gamma_B \end{aligned} \quad (2.5)$$

3. Using u, v from (2.4), (2.5), solve for w the linear problem

$$a_3 \triangle w + \lambda uv - \mu uw = 0 \quad \text{with } w_{\nu} = 0 \text{ on } \partial\Omega \quad (2.6)$$

4. Set $r := M/\|w\|_1$ if $\|w\|_1 \geq M$ and $r := 1$ if $\|w\|_1 \leq M$.

There is no question about the solvability of (2.4) when $\hat{v}, \hat{w} \geq 0$. Maximum Principle arguments then give $u \geq 0$ and $u \leq \bar{\alpha}$; we briefly sketch the argument

for the latter. [Take $z := (u - \bar{\alpha})_+ := \max\{0, u - \bar{\alpha}\} \geq 0$ as test function in the weak form of (2.4) — noting that $z = 0$ on Γ_A so the boundary term vanishes after application of the Divergence Theorem, that $\nabla z \cdot \nabla u = |\nabla z|^2$, and that $uz \geq 0$ — to get

$$a_1 \int_{\Omega} |\nabla z|^2 = - \int_{\Omega} [\lambda \hat{v} + \mu \hat{w}] uz \leq 0$$

whence z is a constant, necessarily 0 as $z = 0$ on Γ_A . To show $u \geq 0$ one correspondingly takes $z := u_- := \min\{0, u\} \leq 0$.] Given $u \geq 0$, similar arguments give $0 \leq v \leq \bar{\beta}$ from (2.5). At this point we have an estimate

$$0 \leq \int_{\Omega} \lambda uv =: q \leq \bar{q} \tag{2.7}$$

with $\bar{q} = \lambda \bar{\alpha} \bar{\beta} |\Omega|$ for the moment, although we shall later be at pains to obtain an estimate for \bar{q} independent of λ .

Since $0 \leq u \not\equiv 0$ as $\underline{\alpha} > 0$, the Neumann problem (2.6) is solvable for w : one consequence of the estimates we will shortly obtain is that one has a Fredholm operator of index 0 for which 0 cannot be an eigenvalue, i.e., there cannot be a nontrivial solution of the equation with $\lambda = 0$. Since $Q := \lambda uv \geq 0$, another Maximum Principle argument (now taking $z := w_- := \min\{0, w\} \leq 0$) shows that $w \geq 0$. [We may note here that the positivity $u, v, w \geq 0$ is certainly necessary for a physical interpretation of these as concentrations.] The definition of r now ensures that $\mathcal{M} = \mathcal{M}_M$ maps \mathcal{S}_M to itself for any choice of $M > 0$. We will obtain estimates showing that M may be chosen (large enough) to ensure that $r = 1$ at a fixpoint of \mathcal{M} so one has a solution of (2.1). First, however, to ensure the existence of a fixpoint by the Schauder Theorem we must comment on the continuity and compactness of \mathcal{M} . Taking $z = (u - \alpha)$ as test function in

the weak form of (2.4), one gets

$$\begin{aligned} a_1 \|\nabla u\|^2 &= a_1 \int \nabla u \cdot \nabla \alpha + \int [\lambda \hat{v} + \mu \hat{w}] u \alpha - \int [\lambda \hat{v} + \mu \hat{w}] u^2 \\ &\leq a_1 \|\nabla u\| \|\nabla \alpha\| + \bar{\alpha} [\int \lambda u \hat{v} + \mu \bar{\alpha} M] \end{aligned} \quad (2.8)$$

$$\|\nabla u\|^2 \leq \|\nabla \alpha\|^2 + 2\bar{\alpha}[\lambda \bar{\alpha} \bar{\beta} |\Omega| + \mu \bar{\alpha} M]/a_1$$

and, similarly, $\|\nabla v\|^2 \leq \|\nabla \beta\|^2 + 2\bar{\beta} \bar{q}/a_2$ — giving $H^1(\Omega)$ bounds (whence $L^2(\Omega)$ compactness) for those components. Given this compactness and the uniqueness for the equations, one easily gets continuity of the maps: $\hat{v}, \hat{w} \mapsto u$ and then; $u \mapsto v$.

Most of our effort must be devoted, as indicated in the Introduction, to estimating w . To this end, we first note from (2.6) that

$$\int_{\Omega} [\lambda uv - \mu uw] = a_3 \int_{\Omega} \Delta w = 0 \quad \text{so} \quad \int_{\Omega} \mu uw = \int_{\Omega} \lambda uv =: q \quad (2.9)$$

as $w_{\nu} = 0$ on $\partial\Omega$. Next, we write $w = \overset{\circ}{w} + \omega$ where $\int_{\Omega} \overset{\circ}{w} = 0$ and ω is a constant (so $\omega|\Omega| = \int_{\Omega} w = \|w\|_1$). Now (2.6) gives $-a_3 \Delta \overset{\circ}{w} = [\lambda uv - \mu uw]$ with $\overset{\circ}{w}_{\nu} = 0$ whence, using (2.7),

$$\|\overset{\circ}{w}\|_{\mathcal{W}} \leq K \|\lambda uv - \mu uw\|_1 \leq 2K \bar{q} \quad (2.10)$$

for some suitable space \mathcal{W} depending on the dimension m and the geometry of Ω . For our present purposes, we only need compactness of the embedding⁷ $\mathcal{W} \hookrightarrow L^1(\Omega)$ with the consequent L^1 estimate

$$\|\overset{\circ}{w}\|_1 \leq K \bar{q}. \quad (2.11)$$

⁷This is a very mild restriction on Ω — for a smooth boundary one would expect a ‘shift theorem’ giving $\mathcal{W} = W^{2,1}(\Omega)$. Certainly we have this for the one-dimensional setting with $\mathcal{W} = W^{2,1}(0,1) \hookrightarrow C^{0,1}[0,1]$.

Now suppose we were to have a lower bound on the amount of A in the system:

$$\int_{\Omega} u \geq \underline{\alpha}_1 > 0. \quad (2.12)$$

Observing that $\int u w = \int u \overset{\circ}{w} + \omega \int u$, we get from (2.11) that

$$\begin{aligned} \mu \omega \underline{\alpha}_1 &\leq \mu \omega \int_{\Omega} u = \int_{\Omega} \mu u w - \mu \int_{\Omega} u \overset{\circ}{w} \\ &\leq \bar{q} + \mu \bar{\alpha} \| \overset{\circ}{w} \|_1 \leq \left(1 + \overset{\circ}{K}\right) \bar{q}, \end{aligned} \quad (2.13)$$

with compactness since ω is one-dimensional. As before, this will give continuity as well as compactness for the map: $u, v \mapsto w$ — once we can verify (2.12) — so the Schauder Theorem will apply to ensure existence of a fixpoint of \mathcal{M} . Note that we have bounded $\|w\|_1 = |\Omega|\omega$ independently of the choice of M , so one can choose $M > \left(1 + \overset{\circ}{K}\right) \bar{q} / \mu \underline{\alpha}_1$ and be certain of obtaining $r = 1$ in step 4 at the fixpoint so this gives the desired solution of (2.1).

It seems plausible that our next argument, verifying (2.12), could be modified to apply to more general geometries, but we avoid considerable complication by presenting this only for the case of a region which is cylindrical near Γ_A — i.e., such that we may coordinatize position in Ω near Γ_A by (x, y) with $y \in \mathcal{Y} \subset \mathbb{R}^{m-1}$ for $0 < x < \delta$ so the relevant portion $\Omega_{\delta} \subset \Omega$ has the form $\Omega_{\delta} = (0, \delta) \times \mathcal{Y}$ with $\Gamma_A = \{0\} \times \mathcal{Y}$. We set

$$U(x) := a_1 \int_{\mathcal{Y}} u(x, y) dy \quad \text{for } 0 \leq x \leq \delta.$$

Note that

$$\begin{aligned} 0 < -U'(0) &= -a_1 \int_{\mathcal{Y}} u_x dy \Big|_{x=0} = a_1 \int_{\Gamma_A} u_{\nu} = a_1 \int_{\partial\Omega} u_{\nu} \\ &= \int_{\Omega} a_1 \triangle u = \int_{\Omega} \lambda u v + \int_{\Omega} \mu u w, \\ &\leq 2\bar{q}. \end{aligned} \quad (2.14)$$

Further, for $0 < x < \delta$ and $y \in \partial\mathcal{Y}$ we have $(x, y) \in \partial\Omega \setminus \Gamma_A$ with coincidence of the normals to $\partial\Omega$ and to $\partial\mathcal{Y}$ whence $\int_{\mathcal{Y}} \Delta_y u = \int_{\partial\mathcal{Y}} u_\nu = 0$ for $0 < x < \delta$ so

$$U'' = \int_{\mathcal{Y}} a_1 \Delta u = \int_{\mathcal{Y}} [\lambda uv + \mu uw] \geq 0$$

whence $U'(x) \geq U'(0) \geq -2\bar{q}$ on $(0, \delta)$. Since (2.2) gives $U(0) = a_1 \underline{\alpha} > 0$, we then have $U(x) \geq \max\{0, a_1 \underline{\alpha} - 2\bar{q}x\}$ which gives

$$\int_{\Omega} u \geq \frac{1}{a_1} \int_0^\delta U(x) dx \geq \min \left\{ \frac{\delta \underline{\alpha}}{2}, \frac{a_1 \underline{\alpha}^2}{4\bar{q}} \right\} =: \underline{\alpha}_1. \quad (2.15)$$

This completes the proof of our existence result. ■

3. Estimates; Convergence as $\lambda \rightarrow \infty$

In this section we consider the convergence (for subsequences) of solutions of (1.2)-(1.3) as $\lambda \rightarrow \infty$. The section naturally divides into two parts: showing that all solutions we consider will lie in a fixed compact set, independent of λ , assuring the existence of convergent subsequences with $\lambda = \lambda_k \rightarrow \infty$ and then characterizing the limit functions $[\bar{u}, \bar{v}, \bar{w}]$. The first part essentially consists of bounding $q := \int \lambda uv$ (which is just the production rate of C) and, as in the previous section, it is reasonable to do this in the PDE context for (2.1), obtaining a λ -independent estimate for \bar{q} in (2.7). For the second part, we will first comment briefly on the PDE context but will then return to the one-dimensional setting of (1.2)-(1.3) for detailed treatment. In that context we will obtain convergence

on $[0, x^*]$, where $x^* \in (0, 1)$ is a new unknown variable, to a solution of

$$\begin{aligned} a_1 \bar{u}'' &= \mu \bar{u} \bar{w} = a_3 \bar{w}'', \quad \bar{v} \equiv 0 \quad \text{on } (0, x^*), \\ \bar{u} &= \alpha > 0, \quad -a_1 \bar{u}' = 2q, \quad \bar{w}' = 0 \quad \text{at } x = 0, \\ \bar{u} &= 0, \quad -a_1 \bar{u}' = a_3 \bar{w}' = q \quad \text{at } x = x^* \end{aligned} \tag{3.1}$$

with convergence on $[x^*, 1]$ to

$$\bar{u} \equiv 0, \quad \bar{v} = \beta \frac{x - x^*}{1 - x^*}, \quad \bar{w} = \text{const} = \bar{w}(x^*) =: w^*. \tag{3.2}$$

For the first part, in reconsidering (2.7), it is convenient to introduce a function ϑ on Ω such that⁸

$$\begin{aligned} 0 &\leq \vartheta \leq 1, \quad \Delta \vartheta = 0 \quad \text{on } \Omega \\ \vartheta &= \begin{cases} 0 & \text{on } \Gamma_A \\ 1 & \text{on } \Gamma_B \end{cases} \quad \vartheta_\nu \in L^1(\partial\Omega) \end{aligned} \tag{3.3}$$

Note that the boundary conditions in (3.3) and (2.1) give

$$(1 - \vartheta)u_\nu \equiv 0 \equiv \vartheta v_\nu \quad \text{on } \partial\Omega. \tag{3.4}$$

Now, with $\vartheta_* \in (0, 1)$, set $\Omega_< := \{x \in \Omega : \vartheta \leq \vartheta_*\}$, $\Omega_> := \{x \in \Omega : \vartheta \geq \vartheta_*\}$. On $\Omega_<$ one has $(1 - \vartheta_*) \leq (1 - \vartheta)$ and $\lambda uv \leq a_1 \Delta u$ so one obtains

$$\begin{aligned} (1 - \vartheta_*) \int_{\Omega_<} \lambda uv &\leq \int_{\Omega_<} (1 - \vartheta) a_1 \Delta u \leq \int_{\Omega} (1 - \vartheta) a_1 \Delta u = \\ &= -a_1 \int_{\partial\Omega} u \vartheta_\nu \leq a_1 \bar{\alpha} \int_{\partial\Omega} |\vartheta_\nu|. \end{aligned}$$

⁸To have $0 \leq \vartheta \leq 1$ on Ω just requires interpolation between 0 and 1 on the remainder of $\partial\Omega$. It may be a mild restriction on Ω that this can be done so as to have $\vartheta_\nu \in L^1(\partial\Omega)$. We note that one could omit the equation $\Delta \vartheta = 0$, asking instead only that $\Delta \vartheta \in L^1(\Omega)$ with a minor modification of (3.5). In the one-dimensional case we could take $\vartheta(x) = x$, giving $\bar{q} = 4[a_1\alpha + a_2\beta]$ in (3.5) — although we note that (3.11) gives half that and further note (3.16).

Similarly, one has $\vartheta_* \leq \vartheta$ on $\Omega_{>}$ and $\lambda uv = a_2 \triangle v$ so

$$\begin{aligned} \vartheta_* \int_{\Omega_{>}} \lambda uv &\leq \int_{\Omega_{>}} \vartheta a_2 \triangle v \leq \int_{\Omega} \vartheta a_2 \triangle v = \\ &= -a_2 \int_{\partial\Omega} v \vartheta_\nu \leq a_2 \bar{\beta} \int_{\partial\Omega} |\vartheta_\nu|. \end{aligned}$$

Adding these estimates and minimizing over the choice of ϑ_* gives \bar{q} : one obtains the desired form of (2.7),

$$q := \int_{\Omega} \lambda uv \leq \left[\sqrt{a_1 \bar{\alpha}} + \sqrt{a_2 \bar{\beta}} \right]^2 \int_{\partial\Omega} |\vartheta_\nu| =: \bar{q}. \quad (3.5)$$

From (2.8), taken at the fixpoint of \mathcal{M} , and the similar estimate for v , one has

$$\begin{aligned} \|u\|_{(1)} &\leq \left[\|\nabla \alpha\|^2 + \frac{2\bar{\alpha}\bar{q}}{a_1} + |\Omega| \bar{\alpha}^2 \right]^{1/2} \\ \|v\|_{(1)} &\leq \left[\|\nabla \beta\|^2 + \frac{2\bar{\beta}\bar{q}}{a_2} + |\Omega| \bar{\beta}^2 \right]^{1/2} \end{aligned} \quad (3.6)$$

(where $\|\cdot\|_{(1)}$ denotes the usual $H^1(\Omega)$ -norm) so these are now bounded independently of λ, μ . Similarly, we have (2.11) bounding⁹ $\|\mathring{w}\|_{\mathcal{W}}$ independently of λ, μ . Using (2.12) — whether or not obtained as (2.15), in a somewhat special geometry — one has (2.13) bounding ω independently of λ and of $\mu \geq \mu_*$.

Thus, for solutions (u, v, w) of (2.1) one has

$$(u, v, w) \text{ bounded in } H^1(\Omega) \times H^1(\Omega) \times [\mathcal{W} + \mathbb{R}], \text{ uniformly as } \lambda \rightarrow \infty. \quad (3.7)$$

By compactness it follows that: for any sequence $\lambda = \lambda_k \rightarrow \infty$, there is a subsequence for which one has convergence in, e.g., $L^2(\Omega) \times L^2(\Omega) \times L^1(\Omega)$

$$(u, v, w) \rightarrow (\bar{u}, \bar{v}, \bar{w}).$$

⁹We also note that the bound for $v \in H^1(\Omega)$ immediately bounds $Q = \triangle v \in H^{-1}(\Omega)$ — in terms of \bar{q} , of course, but without assuming an embedding $L^1(\Omega) \hookrightarrow H^{-1}(\Omega)$ which is unavailable for the higher dimensional case. This, in turn, would easily bound \mathring{w} in $H^1(\Omega)$ without using (2.10).

One can also ask of the subsequence that u, v each converge weakly in $H^1(\Omega)$ and pointwise ae on Ω with some similar convergence for w , depending on the nature of \mathcal{W} .

Fixing any such subsequence and its limit, we now turn to the second part of the section: characterization of the limit functions $(\bar{u}, \bar{v}, \bar{w})$.

The first observation is that all the uniform estimates we have obtained also apply in the limit — so $0 \leq \bar{u} \leq \bar{\alpha}$, etc. The product uv converges pointwise ae to $\bar{u}\bar{v}$ and is uniformly dominated by the (integrable) constant $\bar{\alpha}\bar{\beta}$ so $uv \rightarrow \bar{u}\bar{v}$ in $L^1(\Omega)$ by Lebesgue's Dominated Convergence Theorem. Since $\|uv\|_1 \leq \bar{q}/\lambda \rightarrow 0$, one then must have $\bar{u}\bar{v} \equiv 0$ (ae on Ω) as expected. Next, we observe that $|u - \bar{u}|\bar{w}$ is dominated by $\bar{\alpha}\bar{w}$ and converges pointwise to 0 so $u\bar{w} \rightarrow \bar{u}\bar{w}$ in $L^1(\Omega)$; we have $\|uw - u\bar{w}\|_1 \leq \bar{\alpha}\|w - \bar{w}\|_1 \rightarrow 0$ so $uw - u\bar{w} \rightarrow 0$ in $L^1(\Omega)$. Thus, $\mu uw \rightarrow \mu \bar{u}\bar{w}$ in $L^1(\Omega)$. Since Δ is continuous from $H^1(\Omega)$ to $H^{-1}(\Omega)$, hence also continuous between weak topologies, $Q = \Delta v \rightharpoonup \Delta \bar{v} =: \bar{Q} \in H^{-1}(\Omega)$. [Somewhat independently, we note that $L^1(\Omega)$ embeds (isometrically) in the dual space $[C(\bar{\Omega})]^*$ ($= \{\text{measures on } \bar{\Omega}\}$) and that $Q := \lambda uv$ is uniformly bounded in $L^1(\Omega)$ so we have weak-* convergence there: $Q \xrightarrow{*} \bar{Q}$ and \bar{Q} is a measure on $\bar{\Omega}$. We know that $\|\bar{Q}\|_m \leq \bar{q}$.] Since each Q is positive ($\lambda, u, v \geq 0$), one has immediately that \bar{Q} is a positive measure. We similarly note that $\Delta u \rightharpoonup \Delta \bar{u}$ in $H^{-1}(\Omega)$ so $\mu \bar{u}\bar{v} \in L^1(\Omega) \cap H^{-1}(\Omega)$.

Since the boundary conditions are independent of λ , we see that the limit functions satisfy these as well (in some suitable sense; classical for the one-dimensional

case) and so satisfy the limit system

$$\begin{cases} a_1 \triangle \bar{u} - \bar{Q} - \mu \bar{u} \bar{w} &= 0 \\ a_2 \triangle \bar{v} - \bar{Q} &= 0 \\ a_3 \triangle \bar{w} + \bar{Q} - \mu \bar{u} \bar{w} &= 0 \end{cases} \quad \text{on } \Omega \quad (3.8)$$

$$\begin{aligned} \bar{u} &= \alpha \text{ on } \Gamma_A \quad \text{with} \quad \bar{u}_\nu = 0 \text{ on } \partial\Omega \setminus \Gamma_A \\ \bar{v} &= \beta \text{ on } \Gamma_B \quad \text{with} \quad \bar{v}_\nu = 0 \text{ on } \partial\Omega \setminus \Gamma_B \\ \bar{w}_\nu &= 0 \text{ on } \partial\Omega. \end{aligned}$$

Either again taking limits or directly from (3.8), we have

$$\int_{\Gamma_A} \bar{u}_\nu = 2q = 2 \int_{\Gamma_B} \bar{v}_\nu \quad \text{with } q := \langle \bar{Q}, 1 \rangle = \lim_{\lambda \rightarrow \infty} \int_{\Omega} \lambda uv = \int_{\Omega} \mu \bar{u} \bar{w}. \quad (3.9)$$

It is reasonable to conjecture that the distribution \bar{Q} is supported on an interface (of codimension 1) partitioning Ω into the subregions on which one has $\bar{u} > 0$, $\bar{v} > 0$, respectively, where it just gives the jump in the gradient across this ‘reaction surface’. We do not pursue this characterization for the general PDE setting (although, note Remark 3 in Section 5), but now restrict our attention to (1.2)-(1.3) for more detailed treatment.

In the one-dimensional case we have $H^1(0, 1) \hookrightarrow C^{0, (1/2)^-}[0, 1]$ and $\mathcal{W} = W^{2,1}(0, 1) \hookrightarrow C^{0,1}[0, 1]$ so the convergence we have been discussing in the argument for (3.8) implies uniform convergence on $[0, 1]$; we have a pointwise uniform upper bound for w and so for \bar{w} . A key observation in the one-dimensional setting is that the positivity of u'' , v'' means that u' , v' are monotone increasing so, with the boundary conditions $u'(1) = 0 = v'(0)$, one has

$$0 \leq a_2 v'(x) \leq a_2 v'(1) = q = q(\lambda), \quad 0 \leq -a_1 u'(x) \leq -a_1 u'(0) = 2q \quad (3.10)$$

— $a_2 v'(x) = \int_0^x a_2 v'' = \int_0^x \lambda uv \leq \int_0^1 \lambda uv =: q$, etc. This also gives

$$\begin{aligned} \frac{1-x}{a_2} \int_0^x \lambda uv &= (1-x)v'(x) \leq \int_x^1 v' = \beta - v(x) \leq \beta, \\ \frac{x}{a_1} \int_x^1 \lambda uv &\leq -xu'(x) \leq -\int_0^x u' = \alpha - u(x) \leq \alpha; \end{aligned}$$

adding gives $q \leq [a_2\beta/(1-x) + a_1\alpha/x]$ and minimizing over x gives the alternative bound

$$q \leq \left(\sqrt{a_1\alpha} + \sqrt{a_2\beta} \right)^2 = \bar{q} \leq 2(a_1\alpha + a_2\beta) \quad (3.11)$$

in this setting.

We have L^2 -weak convergence for these derivatives¹⁰ so also $0 \leq \bar{v}' \leq q$, $0 \leq -\bar{u}' \leq 2q$ in the limit. This also implies that u, \bar{u} are decreasing and v, \bar{v} increasing on $[0, 1]$. Since we have $\bar{u}\bar{v} \equiv 0$, it follows that $v(0) \rightarrow \bar{v}(0) = 0 < \alpha$ as $\bar{u}(0) = u(0) = \alpha > 0$ and, similarly, $u(1) \rightarrow \bar{u}(1) = 0$. Thus, for each λ (large enough to ensure $v(0) < \alpha$ and $u(1) < \beta$) there is some $\xi = \xi(\lambda) \in (0, 1)$ such that

$$u(x) \geq v(x) \text{ on } [0, \xi), \quad u(x) \leq v(x) \text{ on } (\xi, 1].$$

We have $u(x) \geq \alpha - 2qx$ so we also have $\bar{u}(x) \geq \alpha - 2qx > 0$ for $0 \leq x < \alpha/2q$; similarly, $v(x) \geq \beta - q(1-x) > 0$ for $0 \leq (1-x) < \beta/q$. Thus, $\xi \in [\alpha/2\bar{q}, 1 - \beta/\bar{q}]$. Again extracting a subsequence if necessary, we have convergence $\xi \rightarrow x^*$ for some $x^* \in [\alpha/2\bar{q}, 1 - \beta/\bar{q}]$; in the limit one has (not merely ‘ae’, since u, v, \bar{u}, \bar{v} are continuous)

$$\bar{u} \geq 0, \bar{v} \equiv 0 \text{ on } [0, x^*], \quad \bar{v} \geq 0, \bar{u} \equiv 0 \text{ on } [x^*, 1]. \quad (3.12)$$

Since $\bar{v} \equiv 0$ on $[0, x^*]$, one has $\bar{v}'' = 0$ on $(0, x^*)$ in the sense of distributions; since $\bar{v}'' = \bar{Q}$, this shows that \bar{Q} vanishes on $(0, x^*)$ — i.e., that $\int_a^b \lambda uv \rightarrow 0$ as

¹⁰Actually, one has uniform convergence on compact subsets of $[0, 1] \setminus \{x^*\}$ with $\bar{u}, \bar{v}, \bar{w}$ smooth except at x^* .

$\lambda \rightarrow \infty$ for any $0 < a < b < x^*$. Similarly, $\bar{u} \equiv 0$ on $[x^*, 1]$ so $\bar{Q} = \bar{u}'' - \mu\bar{u}\bar{v}$ vanishes on $(x^*, 1)$. Thus, the support of \bar{Q} can only be in $\{0, x^*, 1\}$. Now choose some small $a > 0$ such that, e.g., $5\bar{q}a < \alpha$ so $\alpha \geq u \geq \alpha/2$ (for large λ) on $[0, 2a]$ whence $u(x) \leq 2u(x+a)$ on $[0, a]$. Then, as $v(x) \leq v(x+a)$ on $[0, a]$, we have $\int_0^a \lambda uv \leq \int_a^{2a} \lambda uv \rightarrow 0$ and we see that the endpoint 0 is not in the support of \bar{Q} . Similarly, we eliminate 1 and see that the support of \bar{Q} is the singleton $\{x^*\}$ so $\bar{Q} = q\delta(x - x^*)$:

$$\begin{aligned} \int_a^b \lambda uv &\rightarrow q := \langle \bar{Q}, 1 \rangle = \lim \int_0^1 \lambda uv & \text{if } x^* \in (a, b) \subset [0, 1], \\ \int_a^b \lambda uv &\rightarrow 0 & \text{for } [a, b] \subset [0, x^*) \cup (x^*, 1]. \end{aligned} \quad (3.13)$$

By interpretation of the differential equations of (3.8), restricted to $(0, x^*) \cup (x^*, 1)$ where $\bar{Q} = 0$ or by taking the limit of (1.2), we obtain the differential equations

$$\begin{aligned} a_1 \bar{u}'' &= \mu \bar{u} \bar{v} = a_3 \bar{w}'' & \text{on } (0, x^*), \\ a_2 \bar{v}'' &= 0 = a_3 \bar{w}'' & \text{on } (x^*, 1) \end{aligned}$$

which can here be interpreted classically so \bar{u}, \bar{w} are smooth on $[0, x^*]$ (with $\bar{v} \equiv 0$) and \bar{v}, \bar{w} are linear on $[x^*, 1]$. In this setting, we still have the original boundary conditions $\bar{u}(0) = \alpha$, $\bar{v}(1) = \beta$, $\bar{w}'(0) = 0 = \bar{w}'(1)$ (whence $\bar{w} = \text{const.}$ on $[x^*, 1]$) and (3.9) just gives $-a_1 \bar{u}'(0) = 2q$, $a_2 \bar{v}'(1) = q$. Since $\bar{v}(x^*) = 0$, it follows that $\bar{v}(x) = \beta(x - x^*)/(1 - x^*)$ on $[x^*, 1]$ so we have verified (3.2) and have

$$q = a_2 \bar{v}'(1) = a_2 \beta / (1 - x^*); \quad (3.14)$$

this is just the jump in $a_2 \bar{v}'$ across x^* . For $a < x^* < b$ we have convergence

$$\begin{aligned} \int_a^b \lambda uv + \int_a^b \mu uv &= a_1 [u'(b) - u'(a)] \rightarrow -a_1 \bar{u}'(a) \\ &\rightarrow q + \int_a^b \mu \bar{u} \bar{v} \end{aligned}$$

and letting $a \rightarrow x^* -$, $b \rightarrow x^* +$ (so $\int_a^b \mu \bar{u} \bar{v} \rightarrow 0$) gives $-a_1 \bar{u}'(x^* -) = q$; similarly, we obtain $a_3 \bar{w}'(x^* -) = q$, completing the verification of (3.1).

Note that (3.1) and the monotone decrease of \bar{u}' give $2q \geq -a_1\bar{u}' \geq q$ on $(0, x^*)$ so, integrating, we have $x^*(2q/a_1) \geq \alpha - 0 \geq x^*(q/a_1)$. Combining this with (3.14) from (3.1) gives

$$\frac{a_1\alpha}{a_1\alpha + 2a_2\beta} \leq x^* \leq \frac{a_1\alpha}{a_1\alpha + a_2\beta}. \quad (3.15)$$

An immediate consequence of (3.15), using (3.14) again, is that

$$a_2\beta + \frac{1}{2}a_1\alpha \leq q \leq a_2\beta + a_1\alpha \quad (3.16)$$

— with the minimal value corresponding (with our normalization) to (1.5), where we also had $\mu \rightarrow \infty$, and the maximal value corresponding to a similar computation of the rate of consumption of B from the reaction $A + B \xrightarrow{\lambda} C$ alone, i.e., $\lambda \rightarrow \infty$ with $\mu = 0$. Of course, the maximal value in (3.16) also provides a new bound \bar{q} in the limit.

4. Uniqueness of the limit solution

In this section we show uniqueness of the solution of the limit problem $(3.1) \cup (3.2)$. Recalling that $\bar{v} = 0$ in $[0, x^*]$, we consider the problem (3.1); note that x^* is here unknown, except for (3.15), with q and $\bar{w}(x^*) =: \bar{w}^*$ also unknown except for (3.16).

Subtracting the first differential equation of (3.1) from the other and integrating twice with the additional conditions at x^* , we obtain $a_3\bar{w} = a_1\bar{u} + a_3\bar{w}^* - 2q(x^* - x)$ whence

$$a_1\bar{u}'' = \mu\bar{u}[a_1\bar{u} + a_3\bar{w}^* - 2q(x^* - x)]/a_3 \quad \text{for } 0 < x < x^*.$$

At this point we suppress the unknowns x^* and q by a substitution: if we set

$$s := \left[\frac{\mu q}{a_1 a_3} \right]^{1/3} (x^* - x), \quad y := \left[\frac{a_1^2 a_3}{\mu q^2} \right]^{1/3} u, \quad \omega := \left[\frac{a_3^2}{\mu q^2 a_1} \right]^{1/3} \bar{w}^*, \quad (4.1)$$

then, with a bit of manipulation, the equation and initial conditions for the new variable $y = y(s) = y(s, \omega)$ take the form:

$$\begin{aligned} y_{ss} &= y(y + \omega - 2s) \\ y(0) &= 0, \quad y_s(0) = 1, \end{aligned} \quad (4.2)$$

with ω an unknown parameter. As $-a_1 \bar{u}'(0) = 2q$, we also have

$$y_s(s_0) = 2 \quad (4.3)$$

where $s = s_0$ corresponds to $x = 0$ so (4.1) gives $s_0 = (\mu q / a_1 a_3)^{1/3} x^*$. We may reformulate this, using (3.14) to eliminate q , as an equation for x^* in terms of s_0 :

$$\gamma(x^*)^3 + x^* - 1 = 0 \quad \left(\gamma := \frac{a_2}{a_1 a_3} \frac{\mu \beta}{s_0^3} \right). \quad (4.4)$$

We note also that, since $\bar{u}, \bar{w} > 0$ on $(0, x^*)$, we must have

$$y > 0, \quad y + \omega - 2s > 0 \quad \text{for } 0 < s < s_0. \quad (4.5)$$

Since the definition (4.3) of s_0 gives $y_s < 2$ on $(0, s_0)$ and so $y(s) - 2s < 0$, it is only the strict positivity of ω which makes it at all possible to have $y + \omega - 2s > 0$; on the other hand, that condition certainly ensures that $y > 0$.

The key idea of our argument is to introduce a function: $\omega \mapsto U(\omega)$ as follows:

Given ω , solve the initial value problem (4.2), for $s > 0$ until y_s attains the value 2, defining $s_0 = s_0(\omega)$ by (4.3) and then setting

$$\gamma = \gamma(\omega) := \frac{a_2}{a_1 a_3} \frac{\mu \beta}{s_0^3(\omega)}, \quad \eta = \eta(\omega) := y(s_0(\omega), \omega), \quad (4.6)$$

— with s_0, γ, η undefined if (4.5) fails. (Note that (4.5) gives $y_{ss} > 0$ so one has uniqueness for the determination of $s_0 > 0$ with $\gamma > 0, \eta > 0$ also unique.) Now solve for $x^* = x^*(\omega)$ as the unique positive root of the cubic (4.4), noting that this gives $0 < x^* < 1$ since $\gamma > 0$, and so determines $q = q(\omega) := a_2\mu\beta/(1 - x^*) > 0$. Finally, set

$$U = U(\omega) := \left[\mu q^2(\omega)/a_1^2 a_3 \right]^{1/3} \eta(\omega). \quad (4.7)$$

While this construction of $U(\omega)$ is independent of our derivation from (3.1), etc., it certainly is motivated by that, and we note from (4.1) (and the derivation) that when ω, \dots do correspond to a solution of (3.1), then $U(\omega)$ is just $\bar{u}(0)$.

The desired uniqueness is then an immediate consequence of the fact, whose proof we defer momentarily, that U is a strictly decreasing function of ω — more precisely, that we will show the following.

Lemma: *There is some $\omega_0 > 0$ such that $U(\cdot)$ is undefined for $\omega \leq \omega_0$ and is defined for $\omega > \omega_0$ with a vertical asymptote at ω_0 . Where defined, $U(\cdot)$ is a strictly decreasing positive function of ω with $U \rightarrow 0$ as $\omega \rightarrow \infty$.*

We keep $\mu, \beta > 0$ fixed for our analysis, but do remark that the definitions of ω_0, y, s_0, η are entirely independent of μ, β and that, for fixed $\omega > \omega_0$, γ obviously increases with the product $\mu\beta$ so x^*, q, U decrease as μ, β increase.

Since $U(\omega)$ should correspond to $\bar{u}(0)$ for a solution of (3.1), we must have

$$U(\omega) = \alpha. \quad (4.8)$$

From our present viewpoint, noting the lemma, we may use (4.8) to determine ω uniquely — with existence of a solution ensured by our previous analysis — and

so, as in the construction of U , to determine y, x^*, q, w^* . This then gives $[\bar{u}, \bar{v}, \bar{w}]$ on $[0, x^*]$ satisfying (3.1) and the boundary conditions and then (3.2) also gives $[\bar{u}, \bar{v}, \bar{w}]$ on $[x^*, 1]$. Thus, the uniqueness of ω implies uniqueness of the triple $[\bar{u}, \bar{v}, \bar{w}]$, which completes the uniqueness proof for the solution of the limit system (3.1)–(3.2). Note that this uniqueness of the limit ensures that $[u, v, w] \rightarrow [\bar{u}, \bar{v}, \bar{w}]$ as following (3.7), but now without considering any extraction of sequences or subsequences.

Proof of the Lemma: From (4.8) and our work in the preceding sections which showed existence of solutions to (3.1)–(3.2) for each $\alpha > 0$, we see that $U(\omega)$ is necessarily defined for some values of ω and that the range of $U(\cdot)$ is $(0, \infty)$. We have already noted that (4.5) cannot hold if $\omega \leq 0$ and a continuity argument then shows that $U(\omega)$ must be undefined for $\omega < \omega_0$ for some $\omega_0 > 0$.

Fix any ω_1 for which $U(\omega_1)$ is defined and set $s_1 := s_0(\omega_1) > 0$ so (4.5) holds on $(0, s_1]$. A standard Maximum Principle argument shows that for $\omega > \omega_1$ we will have a strict increase in y, y_s, y_{ss} at each fixed $s \in (0, s_1]$ so (4.5) holds on $(0, s_1]$ for any $\omega > \omega_1$. Thus, if $U(\omega_1)$ is defined, then $U(\omega)$ is defined for any $\omega > \omega_1$ and we may fix $\omega_0 > 0$ so that $U(\omega)$ is undefined for any $\omega < \omega_0$ and is defined for any $\omega > \omega_0$; we will later show that $U(\omega_0)$ is itself undefined.

Now set $z = z(s) := y_s(s)$. Since $y_{ss} > 0$ by (4.5), $z(\cdot)$ is strictly increasing in s so we can invert to get $s = \sigma(z) = \sigma(z, \omega)$. By the Maximum Principle argument above, we have $z(s, \omega)$ strictly increasing in ω for each fixed $s > 0$ so, inversely, $\sigma(z, \omega)$ must be strictly decreasing in ω for each fixed $z > 1$. In particular, noting that $s_0(\omega) = \sigma(2, \omega)$, we see that $s_0(\cdot)$ is a strictly decreasing function of ω where defined. From (4.6), it then follows immediately that γ is a strictly increasing function of ω . Further, implicit differentiation of (4.4) gives

$dx^*/d\gamma = -(x^*)^3/[3\gamma(x^*)^2+1] < 0$ so we have $x^*(\omega)$ a strictly decreasing function of ω and, immediately, $q = q(\omega) := \mu a_2 \beta / (1 - x^*)$ is also a strictly decreasing function of ω .

Next we wish to show that $\eta = y(s_0)$ is a decreasing function of ω so, with the above, (4.7) would give strict decrease for $U(\cdot)$. [We already know that y is increasing in both s and ω but, since s_0 is decreasing in ω , decrease of $y(s_0)$ is not yet clear.] We now define

$$Y(z, \omega) := [y(\sigma(z, \omega), \omega)]^2$$

— i.e., $Y(z) = y^2(s)$, suppressing the dependence on ω — and conversely $y = \sqrt{Y}$.

By the chain rule,

$$2yz = 2yy_s = \frac{dY}{ds} = \frac{dY}{dz} \frac{dz}{ds} = \frac{dY}{dz} y_{ss} = \frac{dY}{dz} y(y + \omega - 2s),$$

whence

$$\frac{dY}{dz} = \frac{2z}{\sqrt{Y} + \omega - 2\sigma(z, \omega)}, \quad Y(1) = 0. \quad (4.9)$$

[Note that (4.5) ensures positivity of the denominator.] Since $\partial[\omega - 2\sigma]/\partial\omega > 0$, the right hand side in (4.9) is decreasing in ω , so — again by a Maximum Principle argument — Y is (strictly) decreasing as a function of ω for each fixed $z \in (1, 2]$. In particular, $\eta(\omega) = \sqrt{Y(2, \omega)}$ decreases as ω increases.

At this point we note that U cannot be defined (finite) at ω_0 — if it were, then we would have $U(\omega) \leq U(\omega_0) < \infty$ wherever defined, which would contradict our observation that the range of $U(\cdot)$ is all of $(0, \infty)$. We have thus shown that $\omega \mapsto U$ must have a vertical asymptote at $\omega = \omega_0+$ and must then decay monotonically to 0 as $\omega \rightarrow \infty$. This completes the proof of the lemma. ■

It is interesting to consider the dependence of $w^* = w(1) = [\mu a_1/a_3^2]^{1/3} q^{2/3} \omega$ on α . From the Lemma and (4.8) we see that $\omega \rightarrow \infty$ as $\alpha \rightarrow 0$ and $\omega \rightarrow \omega_0 > 0$ as $\alpha \rightarrow \infty$. We then note that when $\alpha \rightarrow \infty$ the estimates (3.16) give $q \rightarrow \infty$ and we have $w^* \rightarrow \infty$. On the other hand, for $\alpha \rightarrow 0$ one has $q \rightarrow a_2 \beta$ and again $w^* \rightarrow \infty$; this does not contradict our estimate (2.13) for w since $\alpha \rightarrow 0$ also gives $\underline{\alpha}_1 \rightarrow 0$. Compare Remark 2 in the next section.

5. Further remarks

Remark 1. We have shown the uniform convergence as $\lambda \rightarrow \infty$ of solutions $[u, v, w]$ of (1.2), (1.3) to the unique solution $[\bar{u}, \bar{v}, \bar{w}]$ of the limit system (3.1) \cup (3.2) and it is then natural to inquire as to the *rate of convergence*. More generally, one might seek more detailed knowledge of the nature of this convergence in terms of a suitable asymptotic expansion, using methods of singular perturbation theory since one obtains¹¹

$$\begin{aligned}\varepsilon u'' &= uv + \varepsilon uw, \\ \varepsilon v'' &= uv, \\ \varepsilon w'' &= -uv + \varepsilon uw\end{aligned}\tag{5.1}$$

on dividing by λ and introducing the small parameter $\varepsilon := 1/\lambda \rightarrow 0+$.

Following the approaches of [6], this program can be carried through to get such an expansion in powers of $\varepsilon^{1/3}$ with a ‘stretched variable’ $\xi := (x - x^*)/\varepsilon^{1/3}$ in the internal interface layer within which the fast reaction $A + B \xrightarrow{\lambda} C$ is strongly

¹¹For expository simplicity, we restrict attention here to the case $a_1 = a_2 = a_3 = a$ with the scaling that $a = 1$ and $\mu = 1$.

active. We note here the principal result to be obtained:

$$\begin{aligned} u(x) &= u(x, \varepsilon) = \bar{u}(x) + \varepsilon^{1/3} z(\xi) + \mathcal{O}(\varepsilon^{2/3}), \\ v(x) &= v(x, \varepsilon) = \bar{v}(x) + \varepsilon^{1/3} z(\xi) + \mathcal{O}(\varepsilon^{2/3}), \\ w(x) &= w(x, \varepsilon) = \bar{w}(x) - \varepsilon^{1/3} z(\xi) + \mathcal{O}(\varepsilon^{2/3}), \end{aligned} \tag{5.2}$$

with an estimate

$$|z(\xi)| \leq \frac{q^{2/3}}{2Ai'(0)} Ai(q^{1/3}|\xi|)$$

where $Ai(\cdot)$ is the Airy function and q is the limit value obtained (for the particular α, β) in Section 4.

In developing this, we have the advantage of our work of the previous sections here, giving the leading terms $[\bar{u}, \bar{v}, \bar{w}]$ and so permitting some simplification of the general techniques of [6] for this application. We do note that the general justificatory results of [6] (cf., in particular, the discussion on pp. 41–82 there) do not apply directly to the present context without some technical modification. All of this more detailed treatment will be deferred to another paper [4], focussing on the singular perturbation analysis of (5.1).

Remark 2. It is interesting to note that setting $\alpha = 0+$ in (3.1)–(3.2) — i.e., considering $\lim_{\alpha \rightarrow 0} \lim_{\lambda \rightarrow \infty}$ — gives $u \equiv 0$, $v = \beta x$ (and w undefined: $w \equiv \infty$), whereas if we set $\alpha = 0$ immediately in (1.3) then we again get $u \equiv 0$, but now with $v \equiv \beta$ and $w \equiv [\text{arbitrary constant} \geq 0]$. We may then ask what happens if $\alpha \rightarrow 0$, $\lambda \rightarrow \infty$ in a coordinated way. For the particular relation $\sqrt{\lambda}\alpha \equiv \text{constant} =: \tilde{\alpha}$, numerical computation shows, and analysis confirms, that one then gets an expansion in powers of $\sqrt{\varepsilon}$ (with $\varepsilon := 1/\lambda \rightarrow 0$, as above). This singular perturbation analysis also will be deferred to [4].

Remark 3. To indicate what might be done to continue the charac-

terization of solutions of the system of partial differential equations (3.8), we introduce $z := a_1 u - a_2 v$. This satisfies $\Delta z = \mu u v$, avoiding the term $Q := \lambda u v$ for which the limit is necessarily singular. Letting $\lambda \rightarrow \infty$, we have $z \rightarrow \bar{z}$ with

$$\begin{aligned}\Delta \bar{z} &= (\mu \bar{w}/a_1) \bar{z}_+ \\ \bar{z} &= a_1 \alpha \text{ on } \Gamma_A, \quad \bar{z} = -a_2 \beta \text{ on } \Gamma_B, \\ \bar{z}_\nu &= 0 \text{ on } \partial\Omega \setminus [\Gamma_A \cup \Gamma_B]\end{aligned}\tag{5.3}$$

where we have noted that $\bar{u}\bar{v} \equiv 0$ with $\bar{u} \geq 0$, $\bar{v} \geq 0$ so $a_1 \bar{u} = \bar{z}_+ (:= \max\{0, \bar{z}\})$ and, similarly, $a_2 \bar{v} = -\bar{z}_-$. Since the coefficient $(\mu \bar{w}/a_1)$ is not actually given,¹² this does not determine \bar{z} (and so \bar{u}, \bar{v}), but it can be useful in extracting information.

For example: assume Γ_A connected with α strictly positive there. If there would then be a (maximal) subregion $\Omega_* \subset \Omega$ not connected to Γ_A on which $u > 0$, then we would have $\bar{z}_+ = \bar{z}$ there and $\bar{z} = 0$ on $\partial\Omega_*$ by the assumed maximality. A Maximum Principle argument would immediately give $\bar{z} \equiv 0$ on Ω_* , contradicting its definition. With a similar argument for \bar{v} to show there cannot be enclosed pockets of B , one has a partition¹³ of Ω into simply connected regions Ω_A and Ω_B , corresponding to $(0, x^*)$ and $(x^*, 1)$ for the one-dimensional

¹²We could also introduce the function $y := a_3 w + 2a_2 v - a_1 u$ and note that this is harmonic. One could then replace (5.3) by the system

$$\Delta \bar{y} \equiv 0, \quad \Delta \bar{z} = (\mu/a_1 a_3) [\bar{y} \bar{z}_+ + \bar{z}_+ \bar{z}]$$

— except that we do not have boundary conditions for y, \bar{y} in any easily available form.

¹³Once one might obtain greater regularity for \bar{u}, \bar{v} , a strong Maximum Principle argument would show that there cannot be any intermediate subregion with $\bar{u}, \bar{v}, \bar{z} \equiv 0$ so the interface is a single surface Σ . One would then wish to investigate the regularity of this interface, a problem of a sort which has been considered in a variety of comparable contexts, and of the distribution \bar{Q} , presumably expressible in terms of a function on Σ which (nominally pointwise)

case.

Remark 4. To see a slightly different setting for some of these ideas, we can consider the situation indicated in (1.4) above, in which the boundary conditions for C no longer ensure confinement to Ω so the second reaction $A+C \xrightarrow{\mu} D$ need not go to completion. Slightly more generally, in the m -dimensional setting we replace (2.1) by

$$\begin{cases} a_1 \triangle u - \lambda uv - \mu uw &= 0 \\ a_2 \triangle v - \lambda uv &= 0 \\ a_3 \triangle w + \lambda uv - \mu uw &= 0 \end{cases} \quad \text{on } \Omega \quad (5.4)$$

$$\begin{aligned} u &= \alpha \text{ on } \Gamma_A \text{ with } u_\nu = 0 \text{ on } \partial\Omega \setminus \Gamma_A \\ v &= \beta \text{ on } \Gamma_B \text{ with } v_\nu = 0 \text{ on } \partial\Omega \setminus \Gamma_B \\ w &= \gamma \text{ on } \Gamma_C \text{ with } w_\nu = 0 \text{ on } \partial\Omega \setminus \Gamma_C \end{aligned}$$

where we modify (2.2) to include the requirement¹⁴ that $\gamma \in H^1(\Omega)$ with $0 \leq \gamma \leq \bar{\gamma}$. It is physically plausible to ask that Γ_A, Γ_C be separated (e.g., that $\Gamma_C = \Gamma_B$) but this is not significant for the first part of the analysis.

We define a map \mathcal{M} essentially as by (2.4), (2.5), (2.6), above — of course, with the new boundary conditions used in (2.6), but also with the use of $\|w\|$ rather than $\|w\|_1$ in defining \mathcal{S}_M and in Step 4. The Maximum Principle arguments to see that $0 \leq u \leq \bar{\alpha}$, $0 \leq v \leq \bar{\beta}$ are exactly as earlier and so is the estimation giving (2.8), etc., to obtain (3.6).

What changes here is the treatment of w , which becomes easier with the present boundary conditions. The Maximum Principle argument to see that would give the derivatives of \bar{u}, \bar{v} and a jump in the derivative of \bar{w} normal to the interface — i.e., the fluxes of A, B to this reaction surface and the local creation rate of C .

¹⁴There is, of course, absolutely no relation of this γ and that of (4.6).

$w \geq 0$ is now essentially as for u . We next estimate w in $H^1(\Omega)$ — without the need for (2.12) or for the splitting $[\overset{\circ}{w} + \omega]$. Note that one now has a Poincaré Inequality

$$\|z\|_{(1)} \leq C_P \|z\| \quad \text{if } z = 0 \text{ on } \Gamma_C \quad (5.5)$$

and that (3.6) bounds $Q := \lambda uv = a_2 \triangle v$ in $H^{-1}(\Omega)$. Taking $z := w - \gamma$ as test function in (2.6), we have

$$\begin{aligned} a_3 \|\nabla z\|^2 &= a_3 \langle \nabla z, \nabla \gamma \rangle + \langle Q, z \rangle - \langle \mu u z, z \rangle - \langle \mu u \gamma, z \rangle \\ &\leq a_3 \|\nabla z\| \|\nabla \gamma\| + \|Q\|_{(-1)} \|z\|_{(1)} + \mu \bar{\alpha} \|\gamma\| \|z\| \\ &\leq \left[a_3 \|\nabla \gamma\| + \left(\|Q\|_{(-1)} + \mu \bar{\alpha} \|\gamma\| \right) C_P \right] \|\nabla z\| \end{aligned}$$

which bounds $\|\nabla z\|$ (uniformly in λ) whence $\|z\|_{(1)}$ by (5.5) with $\|w\|_{(1)} \leq \|z\|_{(1)} + \|\gamma\|_{(1)}$. In particular, this gives existence of steady state solutions.

Since these estimates bound u, v, w in $H^1(\Omega)$, uniformly in λ , we do not need (3.5) to permit extraction of convergent sequences giving (3.8) — with the new boundary conditions for w , of course. [This argument gives $\bar{Q} \in H^{-1}(\Omega)$, but the argument leading to (3.5) still applies, without (2.9), so we may use that to bound $Q := \lambda uv$ in $L^1(\Omega)$ and, as before, get \bar{Q} as a positive measure.] We now define¹⁵ $\rho := q_2/q$, but without expecting $\rho = 1$ so we may have $q_2 \neq q$. Without (2.9) one has $\int_{\Gamma_A} u_\nu = q + q_2$ with $q_2 := \int_\Omega \mu u w$ and we must similarly replace $2q$ by $q + q_2$ in (3.10), with (3.11) holding as before in the one-dimensional case.

The argument for partitioning $(0, 1)$ into $(0, x^*)$ and $(x^*, 1)$ is just as before. Again we have straight line profiles on $[x^*, 1]$ where $\bar{u} \equiv 0$:

$$\bar{v} = \beta \frac{x - x^*}{1 - x^*}, \quad \bar{w} = w^* + [\gamma - w^*] \frac{x - x^*}{1 - x^*}, \quad (5.6)$$

¹⁵Note that the particularly interesting case, corresponding to (1.4), is to have $\gamma \equiv 0$. In this case one must have $w_\nu \geq 0$ on Γ_C so (2.6) then gives $\rho \geq 0$; clearly, $q_2 \geq 0$ so $\rho \leq 1$ always.

with $w^* := \bar{w}(x^*)$ and again we have

$$a_1 \bar{u}'' = \mu \bar{u} \bar{w} = a_3 \bar{w}'' \quad \text{for } 0 < x < x^*$$

but with new boundary conditions: the jump across x^* in \bar{u}' , \bar{v}' , $-\bar{w}'$ is again q , giving $-a_1 \bar{u}'(x^*-) = q = a_2 \beta / (1 - x^*)$, but now

$$a_1 \bar{u} \Big|_0^{x^*-} = a_3 \bar{w} \Big|_0^{x^*-} = q_2 = \rho q.$$

Thus we have $-a_1 \bar{u}'(0) = q + q_2 = (1 + \rho)q$ and $\bar{w} = w^* + [a_1 \bar{u} - (1 + \rho)q(x - x^*)] / a_3$ on $[0, x^*]$. Substitutions much like (4.1) now give

$$y_{ss} = y(y + \omega - (1 + \rho)s) \tag{5.7}$$

$$y(0) = 0, \quad y_s(0) = 1, \quad \text{and } y_s(s_0) = 1 + \rho,$$

corresponding to (4.2), (4.3). Note that we now have *two* unknown parameters to determine — ω and now also ρ .

Temporarily fixing ρ , we use essentially the same construction of $U(\omega) = U(\omega, \rho)$ as earlier and the identical argument shows that U is a decreasing function of ω so (4.8) determines ω , etc. — now, of course, as functions of ρ . Returning to (5.6), we now have

$$w^* + (\beta a_2 / a_3) \rho = \gamma - (\beta a_2 / a_3) \tag{5.8}$$

since $-a_3 \bar{w}' = (1 - \rho)q$ and $a_2 \bar{v}' = q$ at $x = 1$. Using $w^* = w^*(\rho)$ as determined from (4.8), etc., we may consider (5.8) as an equation for the determination of the parameter ρ (and so of the solution). Although relevant information as to ρ -dependence can be obtained by arguments parallel to those used in the proof of the Lemma of Section 4, we do not pursue this; it is not yet clear whether $[w^*(\rho) + (\beta a_2 / a_3) \rho]$ would always be a strictly monotone function of ρ , which would ensure a unique determination.

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