

Singular perturbation analysis of a diffusion/reaction system with a fast reaction*

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June 22, 2010

Abstract

We consider a singularly perturbed system of second-order differential equations describing steady state of a chemical process that involves three species, two reactions (one of which is fast), and diffusion. Formal asymptotic expansion of the solution is constructed. The theorem on estimation of the remainder is proved.

1. Introduction: statement of the problem

We consider a chemical reaction $2A + B \rightarrow \text{product}$ which we decompose as a pair of simultaneous binary reactions involving an intermediate species C :



where λ, μ are the binary reaction rates. We scale our units so $\mu = 1$ and the diffusion coefficient¹ is 1. This reaction in the presence of diffusion can be described in steady state

*J. Math. Anal. Appl., 288, pp. 722–743, (2003).

¹We assume equal diffusion coefficients for convenience of exposition, while emphasizing that for steady state all our arguments for (1.1) would apply with only minimal modification in the more general case with distinct coefficients D_1, D_2, D_3 .

by the system

$$\begin{aligned} u_{xx} - \lambda uv - uw &= 0, \\ v_{xx} - \lambda uv &= 0, \\ w_{xx} + \lambda uv - uw &= 0, \end{aligned} \tag{1.1}$$

where u , v and w represent concentrations of the substances A , B and C , respectively. To this we adjoin the boundary conditions

$$\begin{aligned} u = \alpha > 0, \quad v_x = 0, \quad w_x = 0 & \quad \text{at } x = 0, \\ u_x = 0, \quad v = \beta > 0, \quad w_x = 0 & \quad \text{at } x = 1. \end{aligned} \tag{1.2}$$

Our particular interest will be in the behavior of this system when the first reaction is comparatively extremely fast, i.e., in the asymptotics as $\lambda \rightarrow \infty$.

The study of problem (1.1), (1.2) and its generalization to the spatially multi-dimensional case was initiated in the paper by Seidman and Kalachev [5]. There the chemical engineering context of this problem was extensively discussed and the following results were obtained:

- the existence of a steady state solution of (1.1), (1.2) was proved (in the multi-dimensional case);
- it was proved that the solution converges as $\lambda \rightarrow \infty$ to the solution of a reduced problem associated with (1.1), (1.2);
- the uniqueness of the limit solution was established.

In this paper we inquire about the behavior of the solution in terms of a suitable asymptotic expansion, using the methods of singular perturbation theory for our analysis, and then prove the correct *rate of convergence* for the results of [5].

The paper is organized as follows. The next two sections provide a formal asymptotic analysis of the problem: Section 2 describes the form of the expansion to be obtained, including determination of the appropriate expansion parameter $\lambda^{-1/3}$, and Section 3 shows how the asymptotic algorithm of [6] is used to obtain the first terms of this expansion. With this initial expansion in hand for insight, an independent proof is given in Section 4 for the anticipated $O(\lambda^{-1/3})$ convergence rate for the results of [5], using the infinite dimensional Implicit Function Theorem. Finally, a similar asymptotic analysis is sketched in Section 5 for a related problem in which $\alpha \rightarrow 0$ in (1.2) as $\lambda \rightarrow \infty$, observing that $\alpha \sim 1/\lambda$ gives an expansion in $\lambda^{-1/2}$, rather than in $\lambda^{-1/3}$ as here.

We note that the corresponding time dependent system

$$\begin{aligned} u_t &= u_{xx} - \lambda uv - uw, \\ v_t &= v_{xx} - \lambda uv, \\ w_t &= w_{xx} + \lambda uv - uw, \end{aligned} \tag{1.3}$$

has been considered by Haario and Seidman [3], although with boundary conditions of a quite different type (involving time derivatives of the unknown functions at $x = 1$), to describe reactions in the “film model” for a gas/liquid interface. We are also planning to study the non-stationary system (1.3) subject to non-negative initial conditions and boundary conditions of the form (1.2) with a concern, as here, for the asymptotics as $\lambda \rightarrow \infty$. In that subsequent investigation we will be concerned with the approach to steady

state and especially with descriptions of the development and time-dependent behavior of moving fronts for the limit problem.

2. Asymptotic algorithm

Our goal in this and the next section is to use the boundary function method of [6]) to construct a uniformly valid asymptotic expansion for the solution of the system, viewed in the form (2.1), (1.2). In this section we describe the approach and find the correct expansion parameter and the correct ‘stretched variables’ while in the next section we will show how this method obtains the same characterization of the zeroth order approximation as was developed in [5] and will then determine the next correction terms.

Let us start with a brief explanation of the idea behind the choice of the correct asymptotic sequence with respect to which the expansion will be constructed. Introducing the small parameter $0 < \epsilon := 1/\lambda \ll 1$, the steady state system (1.1) can be written in the form:

$$\begin{aligned}\epsilon u_{xx} &= uv + \epsilon uw, \\ \epsilon v_{xx} &= uv, \\ \epsilon w_{xx} &= -uv + \epsilon uw,\end{aligned}\tag{2.1}$$

which we consider with the boundary conditions (1.2). We use the *boundary function method* (see Vasil’eva, Butuzov and Kalachev [6]) for defining an asymptotic expansion of the solution to (2.1), (1.2) which should be uniformly valid on $[0, 1]$.

The expansion will have the form of a sum of the so-called *regular functions*, approximating the solution of the original problem everywhere in the domain $[0, 1]$ except the vicinity of the point x^* where these functions have discontinuous derivatives² (we denote these functions by \bar{u} , \bar{v} and \bar{w}), and the *boundary functions* (denoted by Πu , Qu , Πv , Qv , Πw , and Qw to the right and left of x^* , respectively) needed to compensate for discontinuities in the derivatives of corresponding regular functions and depending on stretched variables. The correct stretching is determined together with the asymptotic sequence.

Equations defining the regular functions to the leading order (denoted by \bar{u}_0 , \bar{v}_0 and \bar{w}_0 ; these are precisely the ‘limit solutions’ found in [5]) are to be obtained from the original problem by setting ϵ to zero. Thus, we have the equation $\bar{u}_0 \bar{v}_0 = 0$ that must be satisfied by the regular functions of the zero-th order; taking into account the boundary conditions for u and v , we obtain, as in [5],

$$\begin{aligned}\bar{u}_0 &\neq 0, & \bar{v}_0 &= 0 & \text{in } [0, x^*), \\ \bar{u}_0 &= 0, & \bar{v}_0 &\neq 0 & \text{in } (x^*, 1], \\ \bar{u}_0 &= 0, & \bar{v}_0 &= 0 & \text{at } x = x^*,\end{aligned}\tag{2.2}$$

where x^* , as well as \bar{u}_0 and \bar{v}_0 in the subintervals $[0, x^*)$ and $(x^*, 1]$, respectively, are as yet unknown. They, as well as the function \bar{w}_0 , will be found in the next steps of the asymptotic process. We will use the notation $\Pi u(\xi)$, $\Pi v(\xi)$ and $\Pi w(\xi)$ for the boundary functions defined to the right of the point x^* , and the notation $Qu(\xi^*)$, $Qv(\xi^*)$ and $Qw(\xi^*)$ for the boundary functions defined to the left of x^* , where

$$\xi = (x - x^*)/\epsilon^\nu \geq 0, \quad \xi^* = (x^* - x)/\epsilon^\nu \geq 0\tag{2.3}$$

²We are taking advantage of the prior work of [5] to know that there is just one such point x^* , interior to the interval $(0, 1)$.

are the boundary layer (or stretched) variables with ν a constant as yet unknown. The boundary functions describe the corner layer in the vicinity of the point x^* ; they are defined for non-negative values of their arguments and must decay to zero as the corresponding stretched variables approach infinity. No boundary functions are needed in the zero-th order approximation since the limit solution obtained in [5] is already continuous. To define the correct stretching, i.e., the value of ν , as well as to find the correct leading order of the boundary functions we will proceed as follows.

We introduce the notation

$$\Pi u = \epsilon^\mu (\Pi_1 u + \text{higher order terms}), \quad (2.4)$$

and similar representations for Πv , Πw , $Q u$, $Q v$, and $Q w$.

Lemma 2.1: $\mu = \nu = 1/3$.

Proof: Taking into account that $d^2/dx^2 = \epsilon^{-2\nu} d^2/d\xi^2$, we can write for the Π -functions (see Vasil'eva, Butuzov and Kalachev [6] for a detailed description of the corresponding algorithm):

$$\begin{aligned} \epsilon \left(\epsilon^{-2\nu} \frac{d^2 \Pi u}{d\xi^2} \right) &= [\bar{u}(x^* + \epsilon^\nu \xi) + \Pi u(\xi)] [\bar{v}(x^* + \epsilon^\nu \xi) + \Pi v(\xi)] \\ &+ \epsilon [\bar{u}(x^* + \epsilon^\nu \xi) + \Pi u(\xi)] [\bar{w}(x^* + \epsilon^\nu \xi) + \Pi w(\xi)], \end{aligned}$$

with two similar equations involving derivatives of Πv and Πw . Using the representations of type (2.4), etc., for Π -functions, and taking into account that $\bar{u}_0 = 0$ for $x \geq x^*$ and, by virtue of continuity of \bar{v}_0 at x^* , that we have $\bar{v}_0(x^*) = 0$, we can rewrite the above equation in the form:

$$\epsilon^{1-2\nu+\mu} \frac{d^2 \Pi_1 u}{d\xi^2} = \epsilon^\mu \Pi_1 u(\xi) [\bar{v}_{0x}(x^*) \epsilon^\nu \xi + \epsilon^\mu \Pi_1 v(\xi)] + \text{higher order terms}. \quad (2.5)$$

where we assume that the limit from the right $\bar{v}_{0x}(x^*+)$ is non-zero, as we will see below.

Since we expect the boundary functions of the leading order to compensate for the $O(1)$ jumps in the derivatives of regular functions of the zeroth order, we must have

$$\epsilon^{-\nu} \frac{d}{d\xi} (\epsilon^\mu \Pi_1 u) = O(1),$$

with similar relations for $\Pi_1 v$ and $\Pi_1 w$. Thus, we must have $\mu = \nu$ and (2.5) can be rewritten to the leading order as

$$\epsilon^{1-\nu} \frac{d^2 \Pi_1 u}{d\xi^2} = \epsilon^{2\nu} \Pi_1 u(\xi) (\bar{v}_{0x}(x^*) \xi + \Pi_1 v(\xi)) + \dots, \quad (2.6)$$

with similar equations for $\Pi_1 v$ and $\Pi_1 w$. For the Π_1 boundary functions to decay to zero as $\xi \rightarrow \infty$, we need to have at least two terms in (2.6) that are of the same order in ϵ so, necessarily, $1 - \nu = 2\nu$, whence $\nu = \mu = 1/3$. \square

Thus, the asymptotic expansion will take the form:

$$\begin{aligned} u(x, \epsilon) &= \bar{u}_0(x) + \epsilon^{1/3} \bar{u}_1(x) + \epsilon^{2/3} \bar{u}_2(x) + \epsilon \bar{u}_3(x) + \dots \\ &+ \begin{cases} \epsilon^{1/3} \Pi_1 u(\xi) + \epsilon^{2/3} \Pi_2 u(\xi) + \dots & \text{when } \xi > 0, \\ \epsilon^{1/3} Q_1 u(\xi^*) + \epsilon^{2/3} Q_2 u(\xi^*) + \dots & \text{when } \xi^* > 0, \end{cases} \end{aligned} \quad (2.7)$$

with similar expressions for v and w . Recall that x^* is as yet unknown within the interval $[0, 1]$ and, in fact, we must also seek x^* as an expansion

$$x^* = x_0 + \epsilon^{1/3}x_1 + \epsilon^{2/3}x_2 + \dots \quad (2.8)$$

as well. Substituting (2.7) together with this expansion for x^* into (2.1), (1.2), and equating coefficients of like powers of ϵ separately for different types of functions, we obtain the problems for the terms of the asymptotic expansion.

In this context, what was called the ‘limit solution’ in Seidman and Kalachev [5] will now be the leading term in the asymptotics (usually defined by formally setting $\epsilon = 0$ in the original problem). In our case \bar{u}_0 and \bar{v}_0 (as well as \bar{w}_0) are not defined completely by (2.2). We show how (2.7), etc., leads at the zero-th order — in a way somewhat different in its use of the asymptotic algorithm from that of [5] — to the same ‘limit’ problem considered earlier by Seidman and Kalachev [5]. Thus, our previous analysis in [5] provides the existence (and uniqueness — not otherwise obvious) for the zero-th order approximations $[\bar{u}_0, \bar{v}_0, \bar{w}_0]$ of (2.7), etc., together with the unique determination of the leading term x_0 in the expansion of x^* . This, then, provides the basis for the further development of the expansion which describes the behavior of the solution of (1.1), (1.2) for small ϵ (large λ), especially in the neighborhood of x^* (the principal ‘reaction zone’ for $A + B \rightarrow C$).

3. Derivation of terms of the asymptotic expansion

1. Leading order approximation.

Let us recall that we already derived (2.2) for \bar{u}_0 and \bar{v}_0 . It can easily be verified that we obtain relations similar to (2.2) for the functions \bar{u}_i and \bar{v}_i with $i = 1, 2$. In the order $O(\epsilon)$ we obtain the system

$$\begin{aligned} \bar{u}_{0xx} &= \bar{u}_0\bar{v}_3 + \bar{u}_3\bar{v}_0 + \bar{u}_0\bar{w}_0, \\ \bar{v}_{0xx} &= \bar{u}_0\bar{v}_3 + \bar{u}_3\bar{v}_0, \\ \bar{w}_{0xx} &= -\bar{u}_0\bar{v}_3 - \bar{u}_3\bar{v}_0 + \bar{u}_0\bar{w}_0, \end{aligned} \quad (3.1)$$

noting that this has different forms in the subintervals $(0, x_0)$ and $(x_0, 1)$, respectively. In $(0, x_0)$, taking (2.2) into account, we write

$$\bar{u}_{0xx} = \bar{u}_0\bar{w}_0, \quad \bar{v}_0 = 0, \quad \bar{w}_{0xx} = \bar{u}_0\bar{w}_0, \quad (3.2)$$

and in $(x_0, 1)$, we have

$$\bar{u}_0 = 0, \quad \bar{v}_{0xx} = 0, \quad \bar{w}_{0xx} = 0. \quad (3.3)$$

As we have expected, these equations coincide with those in [5].

To (3.2) and (3.3) we must add the additional conditions (1.2) in the zeroth order and the conditions following from the fact that u , v and w are continuous at x_0 . Using the fact that all the boundary functions of the zeroth order are identically zero, we now write down the portion of such conditions relevant to (3.2) and (3.3):

$$\begin{aligned} \bar{u}_0(x_0-) = \bar{u}_0(x_0+) = 0, \quad \bar{v}_0(x_0+) = \bar{v}_0(x_0-) = 0, \\ \bar{w}_0(x_0-) = \bar{w}_0(x_0+) = \text{const}; \end{aligned} \quad (3.4)$$

$$\frac{d\bar{u}_0}{dx}(x_0-) - \frac{dQ_1u}{d\xi^*}(0) = \frac{d\bar{u}_0}{dx}(x_0+) + \frac{d\Pi_1u}{d\xi}(0); \quad (3.5)$$

similar expressions hold for v - and w -functions.

Consider the equations (3.3) for \bar{v}_0 and \bar{w}_0 in the subinterval $(x_0, 1)$ subject to $\bar{v}_0(1) = \beta$ and $\bar{w}_{0x}(1) = 0$. The corresponding solutions are

$$\bar{v}_0(x) = \frac{\beta}{1-x_0}x - \frac{x_0\beta}{1-x_0}, \quad (3.6)$$

$$\bar{w}_0(x) = W = \text{const}, \quad (3.7)$$

where x_0 and W are so far unknown. To obtain additional conditions for the equations (3.2) in the subinterval $[0, x_0]$, we must first consider the problems for the boundary functions Π_1u , Q_1u , etc. For the Π_1 -functions, we have

$$(\Pi_1u)_{\xi\xi} = \Pi_1u[\bar{v}_{0x}(x_0+)(\xi + x_1) + \Pi_1v] = (\Pi_1v)_{\xi\xi} = -(\Pi_1w)_{\xi\xi} \quad (3.8)$$

with x_1 as in (2.8). [Here $(\cdot)_{\xi\xi}$ denotes the second derivative with respect to the variable ξ . In what follows, we will use the notations $(\cdot)_\xi$, $(\cdot)_{\xi^*}$, and $(\cdot)_{\xi^*\xi^*}$ for the first and second derivatives with respect to corresponding stretched variables.] Taking into account the decay conditions at infinity, i.e., that $\Pi_iu(\xi) \rightarrow 0$, $\Pi_iv(\xi) \rightarrow 0$, $\Pi_iw(\xi) \rightarrow 0$ when $\xi \rightarrow \infty$, we obtain

$$\Pi_1u = \Pi_1v = -\Pi_1w. \quad (3.9)$$

In a similar way,

$$\begin{aligned} (Q_1u)_{\xi^*\xi^*} &= [\bar{u}_{0x}(x_0-)(-\xi^* + x_1) + Q_1u]Q_1v \\ &= (Q_1v)_{\xi^*\xi^*} = -(Q_1w)_{\xi^*\xi^*}, \end{aligned} \quad (3.10)$$

and thus

$$Q_1u = Q_1v = -Q_1w. \quad (3.11)$$

From the matching conditions (3.5), etc., together with (3.7), we now obtain

$$\begin{aligned} \bar{u}_{0x}(x_0-) - (Q_1u)_{\xi^*}(0) &= (\Pi_1u)_\xi(0), \\ -(Q_1v)_{\xi^*}(0) &= (\Pi_1v)_\xi(0) + \bar{v}_{0x}(x_0+), \\ \bar{w}_{0x}(x_0-) - (Q_1w)_{\xi^*}(0) &= (\Pi_1w)_\xi(0). \end{aligned} \quad (3.12)$$

Taking into account (3.9) and (3.11), we can derive from (3.12) the relations:

$$\bar{u}_{0x}(x_0-) = -\bar{w}_{0x}(x_0-) = -\bar{v}_{0x}(x_0+) = -\beta/(1-x_0). \quad (3.13)$$

Note that the last equality in (3.13) follows from (3.6). We remark at this point that we have

$$Q_1u(\xi^*) = \Pi_1u(-\xi^*), \text{ etc.} \quad (3.14)$$

as a consequence of (3.13) and the symmetry of the equations (3.8).

Now we have enough conditions to completely define the problem for \bar{u}_0 and \bar{w}_0 in the subinterval $[0, x_0]$. From (3.2), (1.2), (3.4) and (3.13), we have

$$\bar{u}_{0xx} = \bar{u}_0\bar{w}_0, \quad \bar{w}_{0xx} = \bar{u}_0\bar{w}_0, \quad (3.15)$$

$$\bar{u}_0(0) = \alpha, \quad \bar{u}_0(x_0-) = 0, \quad \bar{u}_{0x}(x_0-) = -\beta/(1-x_0), \quad (3.16)$$

$$\bar{w}_{0x}(0) = 0, \quad \bar{w}_{0x}(x_0-) = \beta/(1-x_0). \quad (3.17)$$

Note that the general solution of (3.15) depends on five unknowns (four constants of integration and x_0). To find these unknowns we have exactly five conditions in (3.16), (3.17).

This problem, transformed in an appropriate way, is nothing but the problem analyzed in Seidman and Kalachev [5] and was there proved to have a unique solution. Once x_0 is defined, and $\bar{u}_0(x)$ and $\bar{w}_0(x)$ known the interval $[0, x_0]$, $\bar{v}_0(x)$ for $x \geq x_0$ is also known (see (3.6)). The value $\bar{w}_0(x) \equiv W$ for $x \geq x_0$ can be found from the matching condition $W = \bar{w}_0(x_0-)$. From (2.7) we expect the remainders $u - \bar{u}_0$, etc., to be of order $O(\epsilon^{1/3}) = O(\lambda^{-1/3})$, and in Section 4 we will, indeed, prove this in the sense of uniform approximation.

2. Terms of approximation in the next order.

To get more insight, we now turn to consideration of the next correction terms — those of first order in the expansion parameter $\epsilon^{1/3}$. Note that the equations (3.8), (3.10) for the boundary functions involve the constant x_1 of (2.8). This is as yet unknown, but can be found during solution of the problem for the functions \bar{u}_1 , \bar{v}_1 and \bar{w}_1 . These functions satisfy the following systems obtained analogously to (3.2), (3.3). In $(0, x_0)$, we have

$$\bar{u}_{1xx} = \bar{u}_1\bar{w}_0 + \bar{u}_0\bar{w}_1, \quad \bar{v}_1 = 0, \quad \bar{w}_{1xx} = \bar{u}_1\bar{w}_0 + \bar{u}_0\bar{w}_1, \quad (3.18)$$

and in $(x_0, 1)$, we get

$$\bar{u}_1 = 0, \quad \bar{v}_{1xx} = 0, \quad \bar{w}_{1xx} = 0. \quad (3.19)$$

To (3.18) and (3.19) we must add additional conditions (1.2) in the first order approximation

$$\begin{aligned} \bar{u}_1 = 0, \quad \bar{v}_{1x} = 0, \quad \bar{w}_{1x} = 0 & \quad \text{at } x = 0, \\ \bar{u}_{1x} = 0, \quad \bar{v}_1 = 0, \quad \bar{w}_{1x} = 0 & \quad \text{at } x = 1, \end{aligned} \quad (3.20)$$

and the conditions following from the fact that u , v and w are continuous at x_0 . Taking into account that $\Pi_1 u(0) = Q_1 u(0)$, etc., and that

$$d^2 \bar{u}_0 / dx^2 (x_0-) = d^2 \bar{w}_0 / dx^2 (x_0-) = \bar{u}_0(x_0-)\bar{w}_0(x_0-) = 0; \quad d^2 \bar{v}_0 / dx^2 (x_0+) = 0$$

due to the linearity of \bar{v}_0 on $[x_0, 1]$, the conditions at x_0 can be written as

$$\begin{aligned} \bar{u}_1(x_0-) + \bar{u}_{0x}(x_0-)x_1 &= \bar{u}_1(x_0+) = 0, \\ \bar{v}_1(x_0-) &= \bar{v}_1(x_0+) + \bar{v}_{0x}(x_0+)x_1 = 0, \\ \bar{w}_1(x_0-) + \bar{w}_{0x}(x_0-)x_1 &= \bar{w}_1(x_0+), \end{aligned} \quad (3.21)$$

and

$$\begin{aligned}
\bar{u}_{1x}(x_0-) - (Q_2u)_{\xi^*}(0) &= (\Pi_2u)_{\xi}(0), \\
-(Q_2v)_{\xi^*}(0) &= (\Pi_2v)_{\xi}(0) + \bar{v}_{1x}(x_0+), \\
\bar{w}_{1x}(x_0-) - (Q_2w)_{\xi^*}(0) &= (\Pi_2w)_{\xi}(0).
\end{aligned} \tag{3.22}$$

The equations for the Π_2 - and Q_2 -functions can easily be written out. E.g., for Π_2u we have

$$\begin{aligned}
(\Pi_2u)_{\xi\xi} = & \bar{v}_{0x}(x_0+)(\xi + x_1)\Pi_2u + \Pi_1u\Pi_2v + \Pi_2u\Pi_1v \\
& + [\bar{v}_{0x}(x_0+)x_2 + \bar{v}_{0xx}(x_0+)\{\xi^2/2 + \xi x_1 + x_1^2/2\} + \bar{v}_{1x}(x_0+)(\xi + c)]\Pi_1u.
\end{aligned} \tag{3.23}$$

Note that (3.23) is a linear equation. One term in the square brackets in (3.23) depends on another constant x_2 , again as in (2.8), which will be found together with the regular functions of order $O(\epsilon^{2/3})$, and on the asymptotic terms that must be defined in the earlier stages of the asymptotic algorithm: as soon as these terms are determined the function in the brackets will be known and the equation for Π_2u (as well as the equations for other Π_2 - and Q_2 -functions) will be completely defined.

Just as in the case of the Π_1 - and Q_1 -functions, it can be shown that

$$\Pi_2u = \Pi_2v = -\Pi_2w, \tag{3.24}$$

and

$$Q_2u = Q_2v = -Q_2w. \tag{3.25}$$

By virtue of (3.24), (3.25) we obtain from (3.22):

$$\bar{u}_{1x}(x_0-) = -\bar{w}_{1x}(x_0-) = -\bar{v}_{1x}(x_0+). \tag{3.26}$$

Once again we remark that we have

$$Q_2u(\xi^*) = \Pi_2u(-\xi^*), \text{ etc.} \tag{3.27}$$

as a consequence of (3.26) and the symmetry of the equation (3.23) and the corresponding equation for Q_2u .

Solving the equations (3.19) for \bar{v}_1 , \bar{w}_1 in the interval $(x_0, 1)$ with corresponding conditions in (3.20) and (3.21), we obtain

$$\bar{v}_1 = \frac{\beta x_1}{(1 - x_0)^2}[x - 1], \tag{3.28}$$

$$\bar{w}_1 = \tilde{W} = \text{const}, \tag{3.29}$$

where x_1 and \tilde{W} are as yet unknown. For \bar{u}_1 , \bar{w}_1 in the interval $(0, x_0)$ we have the system (3.18)

$$\bar{u}_{1xx} = \bar{u}_1\bar{w}_0 + \bar{u}_0\bar{w}_1, \quad \bar{w}_{1xx} = \bar{u}_1\bar{w}_0 + \bar{u}_0\bar{w}_1,$$

subject to conditions (3.20) at $x = 0$:

$$\bar{u}_1(0) = 0, \quad \bar{w}_{1x}(0) = 0,$$

and conditions at $x = x_0 -$:

$$\bar{u}_1(x_0-) = \frac{\beta x_1}{1 - x_0}, \quad (3.30)$$

$$\bar{u}_{1x}(x_0-) = -\frac{\beta x_1}{(1 - x_0)^2}, \quad (3.31)$$

$$\bar{w}_{1x}(x_0-) = \frac{\beta x_1}{(1 - x_0)^2}, \quad (3.32)$$

Condition (3.30) follows from (3.21), and (3.31), (3.32) are obtained by substituting (3.28) into (3.26). We have exactly five conditions for defining the five unknowns: four constants of integration and x_1 .

Lemma 3.1: $x_1 = 0$ and $\bar{u}_1 \equiv 0$, $\bar{w}_1 \equiv 0$ on $[0, x_0]$.

Proof: First, notice that $\bar{u}_{1xx} = \bar{w}_{1xx}$, and thus, for constants A, B we have

$$\bar{w}_1 = \bar{u}_1 + Ax + B, \quad (3.33)$$

Differentiating (3.33) once with respect to x and evaluating the resulting expression at $x = x_0$ (substituting (3.31), (3.32) for $\bar{u}_{1x}(x_0-)$ and $\bar{w}_{1x}(x_0-)$ into this expression), we obtain $A = 2x_1\beta/(1 - x_0)^2$ so

$$\bar{w}_1 = \bar{u}_1 + \frac{2x_1\beta}{(1 - x_0)^2}x + B \quad (3.34)$$

and

$$\bar{u}_{1x}(0) = -\frac{2x_1\beta}{(1 - x_0)^2}. \quad (3.35)$$

Let us assume that the problem has a non-trivial solution and come to a contradiction. Suppose $x_1 > 0$. Then $\bar{u}_1(x_0) > 0$, $d\bar{u}_1/dx(0) < 0$ and $d\bar{u}_1/dx(x_0) < 0$. This means that, since $\bar{u}_1(0) = 0$, the function $\bar{u}_1(x)$ must have at least one negative minimum and at least one positive maximum in the interval $(0, x_0)$, and the minimum is attained to the left of where the maximum is attained. Let $\bar{w}_1 \geq 0$ at the maximum of \bar{u}_1 . Then, taking into account that $\bar{u}_0 > 0$, $\bar{w}_0 > 0$ in $(0, x_0)$, we have that $\bar{w}_0\bar{u}_1 + \bar{u}_0\bar{w}_1 > 0$ at this point. On the other hand, at the maximum we have $\bar{u}_{1xx} < 0$, and arrive at a contradiction with the first equation in (3.18). Now let $\bar{w}_1 < 0$ at the maximum of \bar{u}_1 . Then from (3.34) it follows that $\bar{w}_1 < 0$ at the point of minimum of \bar{u}_1 (notice that at this point \bar{u}_1 is negative, and besides, the term $2x_1\beta/(1 - x_0)^2$ in (3.34) is an increasing function of x and the negative minimum lies to the left of the positive maximum). At the minimum of \bar{u}_1 we have $\bar{u}_{1xx} > 0$, but at this point $\bar{w}_0\bar{u}_1 + \bar{u}_0\bar{w}_1 < 0$, which again leads to a contradiction with the first equation in (3.18). A similar argument leads to a contradiction if we assume $x_1 < 0$.

Thus, $x_1 = 0$, and we have for \bar{u}_1 , \bar{w}_1 a system of homogeneous equations with zero boundary conditions. We now show that the solution is trivial: $\bar{u}_1 \equiv 0$, $\bar{w}_1 \equiv 0$.

From (3.34), $\bar{w}_1 = \bar{u}_1 + B$, so if $B = 0$, then $\bar{w}_1 = \bar{u}_1$, and we have

$$\bar{u}_{1xx} = (\bar{w}_0 + \bar{u}_0)\bar{w}_1, \quad \bar{u}_1(0) = \bar{u}_{1x}(x_0) = 0,$$

and thus, by virtue of $(\bar{w}_0 + \bar{u}_0) \geq \text{const} > 0$, we get $\bar{w}_1 \equiv 0$, $\bar{u}_1 \equiv 0$.

Next, suppose $B \neq 0$; without loss of generality we can assume $B < 0$, since otherwise we would consider the solution $(-\bar{u}_1, -\bar{w}_1)$, and also arrive at a contradiction. First, we note that from (3.34), (3.20), $\bar{w}_{1x}(0) = \bar{u}_{1x}(0) = 0$. Substituting (3.34) into the equation for \bar{u}_1 , we obtain:

$$\bar{u}_{1xx} = (\bar{w}_0 + \bar{u}_0)\bar{w}_1 + B\bar{w}_0, \quad \bar{u}_1(0) = \bar{u}_{1x}(0) = 0 \quad (3.36)$$

Since $\bar{w}_0(0) > 0$, $B < 0$ and $\bar{u}_1(0) = 0$, the right-hand side of (3.36) is negative in some neighborhood of $x = 0$. Using this with the conditions $\bar{u}_1(0) = \bar{u}_{1x}(0) = 0$, we see that $\bar{u}_1 < 0$ on some interval in the vicinity of $x = 0$. On the other hand, multiplying (3.36) by $\hat{u} = \min\{0, \bar{u}_1\} \leq 0$, integrating over the interval $[0, x_0]$, rearranging terms and noting that $\hat{u}\bar{u}_1 = \hat{u}^2$, $\hat{u}_x\bar{u}_{1x} = \hat{u}_x^2$, we get

$$\int_0^{x_0} \hat{u}_x^2 dx + \int_0^{x_0} (\bar{w}_0 + \bar{u}_0)\hat{u}^2 dx + B \int_0^{x_0} \bar{w}_0 \hat{u} dx = 0.$$

Each term in the left-hand side of this relation is greater than or equal to zero (since, e.g., $(\bar{w}_0 + \bar{u}_0) \geq \text{const} > 0$, and $B < 0$, $\hat{u} \leq 0$). So, $\hat{u} \equiv 0$, and thus, $\bar{u}_1 \geq 0$ on $(0, x_0)$. We have arrived at a contradiction. \square

All the regular functions of order $O(\epsilon^{1/3})$ in $[0, x_0]$ are now known. From the last condition of (3.21) it follows that $\tilde{W} = 0$, and thus, $\bar{w}_1 \equiv 0$ in $[x_0, 1]$. Substituting $x_1 = 0$ into (3.28), we obtain $\bar{v}_1 \equiv 0$ in $[x_0, 1]$. Thus, all the regular functions of order $O(\epsilon^{1/3})$ are identically zero in the whole interval $[0, 1]$

Now, when x_1 is determined, we may finally define $\Pi_1 u$, $Q_1 u$, $\Pi_1 v$, $Q_1 v$, $\Pi_1 w$, $Q_1 w$. To complete the problems for these boundary functions, we have to substitute $\bar{u}_{0x}(x_0) = -\bar{v}_{0x}(x_0) = -\beta/(1 - x_0)$ and $x_1 = 0$ into the systems (3.8) and (3.10). Note that the equations for Q -functions can be transformed into the equations for Π -functions by symmetrically changing ξ^* to $-\xi$. Therefore, by virtue of (3.9), to find all the Q_1 - and Π_1 -functions, we need to solve only a single equation

$$(\Pi_1 u)_{\xi\xi} = (C\xi + \Pi_1 u) \Pi_1 u \quad \left(C := \frac{\beta}{1 - x_0} \right) \quad (3.37)$$

with the conditions

$$\Pi_1 u(\infty) = 0, \quad (\Pi_1 u)_\xi(0) = \frac{\bar{u}_{0x}(x_0 -)}{2} = -\frac{\beta}{2(1 - x_0)} < 0. \quad (3.38)$$

The last condition follows from the corresponding condition for u -functions in (3.12) together with the relation $(Q_1 u)_{\xi^*}(0) = (\Pi_1 u)_\xi(0)$. We are looking for the non-negative solution to (3.37), (3.38). We can obtain (see Protter and Weinberger [4]) that the unique solution of this problem exists and is bounded from above by the positive solution of the problem

$$P_{\xi\xi} = C\xi P, \quad P(\infty) = 0, \quad P_\xi(0) = -\frac{C}{2} < 0. \quad (3.39)$$

Recognizing that (3.39) is just a scaled version of the defining equation for the well-known Airy function, we see that

$$0 \leq \Pi_1 u(\xi) \leq P(\xi) = -\frac{C^{2/3}}{2\text{Ai}'(0)} \cdot \text{Ai}(C^{1/3}\xi)$$

and recall the decay rate: $\text{Ai}(\eta) \sim \exp(-\frac{2}{3}\eta^{3/2})/\eta^{3/8}$ as $\eta \rightarrow \infty$. This means, in particular, that the discrepancy introduced by $\Pi_1 u(\xi)$ to the boundary condition for u at $x = 1$ is transcendentally small (as are the discrepancies introduced by the other Π_1 , Q_1 -functions; these can easily be written in terms of $\Pi_1 u$, from the boundary conditions for u , v and w at $x = 0$ and $x = 1$).

Let us introduce the new stretched variables $\tilde{\xi} = (x - x_0)/\epsilon^{1/3} \geq 0$, $\tilde{\xi}^* = (x_0 - x)/\epsilon^{1/3} \geq 0$, defined for $x > x_0$ and for $x < x_0$, respectively. These new variables differ from the old variables ξ and ξ^* , respectively, at order $O(\epsilon^{2/3})$ due to the shift of x_0 from x^* . We now define

$$U_1 = \begin{cases} \bar{u}_0(x) + \epsilon^{1/3} Q_1 u(\tilde{\xi}^*) & \text{for } x \in [0, x_0], \tilde{\xi}^* \geq 0, \\ \epsilon^{1/3} \Pi_1 u(\tilde{\xi}) & \text{for } x \in [x_0, 1], \tilde{\xi} \geq 0; \end{cases} \quad (3.40)$$

$$V_1 = \begin{cases} \epsilon^{1/3} Q_1 u(\tilde{\xi}^*) & \text{for } x \in [0, x_0], \tilde{\xi}^* \geq 0, \\ \bar{v}_0(x) + \epsilon^{1/3} \Pi_1 u(\tilde{\xi}) & \text{for } x \in [x_0, 1], \tilde{\xi} \geq 0; \end{cases} \quad (3.41)$$

$$W_1 = \begin{cases} \bar{w}_0(x) - \epsilon^{1/3} Q_1 u(\tilde{\xi}^*) & \text{for } x \in [0, x_0], \tilde{\xi}^* \geq 0, \\ W - \epsilon^{1/3} \Pi_1 u(\tilde{\xi}) & \text{for } x \in [x_0, 1], \tilde{\xi} \geq 0; \end{cases} \quad (3.42)$$

We note that higher order terms of the asymptotic approximation can be constructed as well. The regular functions of higher orders will satisfy linear (non-homogeneous) equations of type (3.18). The boundary functions will satisfy linear equations of type (3.23). Some of the x_k ($k \geq 2$) in the expansion (2.8) for x^* will be non-zero.

From (2.7) we expect that the remainder terms $u - U_1$, $v - V_1$, $w - W_1$ are of order $O(\epsilon^{2/3})$. In the next section we prove the *theorem on estimation of the remainder* for the leading order approximation. The argument that we use in the proof cannot be automatically extended to the case of higher order approximations. We plan to address the analysis of convergence rate of higher order asymptotic solution to the solution of the original problem in the nearest future.

4. Rate of convergence

Our object in this section is to prove the $O(\epsilon^{1/3}) = O(\lambda^{-1/3})$ convergence rate indicated by the expansion (2.7) above. Our proof here, while suggested by the insights suggested by the previous asymptotic analysis, will be independent of that analysis. The key to the present argument is a generalization of the uniqueness argument of [5] together with the use, twice, of the Implicit Function Theorem (IFT). The second use of the IFT is in an infinite dimensional setting \mathcal{Y} , treating $K = \lambda uv$ temporarily as an independent entity in \mathcal{Y} , converging there to a delta function (more precisely, to $\bar{K} = \bar{\kappa} \delta(\cdot - \bar{x}_0)$). The proper choice of norm for this convergence — i.e., the proper choice of the function space \mathcal{Y} — is essential to the computation for Lemma 4.3 below: we find it necessary to take \mathcal{Y} to be $W^{-1,1}(0, 1)$ — the dual space of the Lipschitzian functions.

Let us introduce a shorter notation $\bar{u} := \bar{u}_0$, $\bar{v} := \bar{v}_0$, $\bar{w} := \bar{w}_0$ for the leading order approximation of the solution to (2.1), (1.2).

Theorem 4.1: $\|u - \bar{u}\|_\infty, \|v - \bar{v}\|_\infty, \|w - \bar{w}\|_\infty = O(\epsilon^{1/3})$.

Proof: The proof takes the form of a sequence of lemmas. Before presenting these we

recall our system (1.1), (1.2) in the form

$$\begin{array}{lll}
\text{on } [0, 1] & \text{at } x = 0 & \text{at } x = 1 \\
u'' - K - uw = 0, & u = \alpha > 0, & u' = 0, \\
v'' - K = 0, & v' = 0, & v = \beta > 0, \\
w'' + K - uw = 0, & w' = 0, & w' = 0,
\end{array} \tag{4.1}$$

with $K := \lambda uv$. The following facts are already known from [5]:

1. $u, v, w \geq 0$; and also $u \leq \alpha, v \leq \beta, w \leq M$ uniformly in λ and x .
2. $0 \leq -u', v'$ are monotone increasing; $-u, v$ are monotone increasing.
3. $v'(1) = \kappa, -u'(0) = 2\kappa, \int_0^1 uw \, dx = \kappa$ with $\kappa := \int_0^1 K \, dx$
4. There are limit values $\bar{\kappa}, \bar{u}, \bar{v}, \bar{w}$ such that $\kappa \rightarrow \bar{\kappa}$ and $u, v, w \rightarrow \bar{u}, \bar{v}, \bar{w}$ in H_{weak}^1 (hence, in $C[0, 1]$); in the limit K becomes³ a delta function: $\bar{K} = \bar{\kappa} \delta(\cdot - \bar{x}_0)$.
5. $\bar{u} > 0$ on $[0, \bar{x}_0]$, $\bar{u} \equiv 0$ on $[\bar{x}_0, 1]$; $\bar{v} = \beta(x - \bar{x}_0)/(1 - \bar{x}_0) > 0$ on $(\bar{x}_0, 1]$, $\bar{v} \equiv 0$ on $[0, \bar{x}_0]$, and $\bar{\kappa} = \beta/(1 - \bar{x}_0)$.
6. $dU/d\omega < 0$ (see Lemma 4.2, below).

Lemma 4.1. Define x_0 so that $u(x_0) = v(x_0)$, and set $\zeta := u(x_0) = v(x_0)$. Then $\zeta = O(\epsilon^{1/3})$.

Proof: We temporarily set $\phi := v'(x_0), \psi := -u'(x_0)$. Note that $\phi, \psi \geq 0$ and

$$(u' - v')' = u'' - v'' = -uw$$

so

$$\phi + \psi = -(u' - v')|_{x=1} - \int_{x_0}^1 uw \, dx = \kappa - \int_{x_0}^1 uw \, dx \leq \kappa.$$

On the other hand, setting $[\cdot]_+ = \max\{0, [\cdot]\}$, we use the convexity of u, v to write:

$$\begin{aligned}
\kappa &= \int_0^1 K \, dx = \int_0^1 \lambda uv \, dx \\
&\geq \lambda \int_0^1 [\zeta + \phi(x - x_0)]_+ [\zeta - \psi(x - x_0)]_+ \, dx \\
&= \frac{\lambda}{2} [\zeta^3/\phi + \zeta^3/\psi],
\end{aligned}$$

where the final equality assumes $\zeta \leq \phi x_0, \psi(1 - x_0)$, as is necessarily true for large λ . It follows that

$$\lambda \zeta^3 \leq \frac{2\kappa}{1/\phi + 1/\psi} \leq \kappa^2$$

since either ϕ or $\psi \leq \kappa/2$, so either $1/\phi$ or $1/\psi \geq 2/\kappa$. Thus, $\zeta \leq \kappa^{2/3} \epsilon^{1/3}$. \square

Corollary. Let $\bar{\delta}$ denote a vector consisting of the restrictions of $u(\cdot)$ to $[x_0, 1]$ and of

³In [5] this was interpreted as convergence in the sense of H^{-1} , the dual of $H_0^1(0, 1)$, but we will see here that it is more appropriate to consider this in $\mathcal{Y} = \text{Lip}^*$, the dual of the space $W^{1,\infty}(0, 1)$ of Lipschitz continuous functions.

$v(\cdot)$ to $[0, x_0]$ together with a variety of related terms⁴ boundedly dependent on these. Then $\bar{\delta} = O(\epsilon^{1/3})$.

Proof: It is sufficient to note that $u(\cdot)$ is decreasing so $0 < u(x) \leq \zeta = O(\epsilon^{1/3})$ for $x_0 \leq x \leq 1$ and correspondingly for v on $[0, x_0]$ and then to note that we have uniform bounds for, e.g., $w(\cdot)$ and κ (and $1/\kappa$) in considering the examples noted. \square

We now construct a function $U = U(\omega, \bar{\delta})$ generalizing the function $U = U(\omega)$ introduced in the uniqueness argument in [5] — indeed, $U(\omega)$ of [5] is now $U(\omega, 0)$. This function is defined as follows: First, solve the differential equation⁵

$$\begin{aligned} -\eta'' &= (\eta + \kappa^{-2/3}v)(\eta - \kappa^{-2/3}v + \omega - 2s), \\ \eta(0) &= 0, \quad \eta'(0) = 1 + \frac{1}{\kappa} \int_{x_0}^1 uw \, dx. \end{aligned} \tag{4.2}$$

Note that $\kappa^{-2/3}v$ (more specifically, $\kappa^{-2/3}v(x_0 - \kappa^{-1/3}s)$ for $s > 0$) and the term $\int_{x_0}^1 uw \, dx/\kappa$ occurring in the initial condition were explicitly noted as components of $\bar{\delta}$ so $\eta = \eta(s) = \eta(s; \omega, \bar{\delta})$. Next, solve the equation $\eta'(\tilde{s}) = 2$ for $\tilde{s} = \tilde{s}(\omega, \bar{\delta})$ and then, given \tilde{s} , define $\xi = \xi(\omega, \bar{\delta}) \in (0, 1)$ as the unique real root of the cubic

$$\begin{aligned} &\tilde{\beta}\xi^3 + \sigma\xi - \sigma \\ &\text{with } \sigma = \tilde{s}^3, \quad \tilde{\beta} = \beta + \left[u(1) + \int_{x_0}^1 \int_x^1 uw \, d\hat{x} \, dx \right], \end{aligned}$$

where we note that $\tilde{\beta} - \beta$ is part of $\bar{\delta}$. Finally, set

$$\hat{\kappa} = \hat{\kappa}(\omega, \bar{\delta}) := \frac{\tilde{\beta}}{1 - \xi} = (\tilde{s}/\xi)^3 \tag{4.3}$$

and define

$$U(\omega, \bar{\delta}) := \hat{\kappa}^{2/3} \eta(\tilde{s}) + v(0).$$

We relate U , etc., to our system as follows. Set $y = u - v$, so $y'' = -uw = -(y + v)w$ and set $\tilde{\omega} := (w - u + 2v)|_{x=x_0} = w(x_0) + \zeta$. Since $(w - u + 2v)'' = 0$, we have $(w - u + 2v)' \equiv 2\kappa$ and $w = u - 2v + \tilde{\omega} + 2\kappa(x - x_0)$. Thus

$$\begin{aligned} y'' &= -(y + v)[y - v + \tilde{\omega} + 2\kappa(x - x_0)], \\ y(x_0) &= 0, \quad y'(x_0) = -\kappa + \int_{x_0}^1 uw \, dx \end{aligned} \tag{4.4}$$

If we now set

$$s := -\kappa^{1/3}(x - x_0), \quad \omega := \kappa^{-2/3}\tilde{\omega} = \kappa^{-2/3}[w(x_0) + \zeta],$$

⁴We note $\kappa^{-2/3}v(x_0 - \kappa^{-1/3}s)$ for $s > 0$, $\int_{x_0}^1 uw \, dx/\kappa$, and $\int_{x_0}^1 \int_x^1 uw \, d\hat{x} \, dx$ as examples of the terms taken (e.g., in the proofs of Lemmas 4.2, 4.3, below) to be components of $\bar{\delta}$.

⁵In (4.2), $'$ denotes d/ds for $s > 0$. To see what is going on, note that eventually we will have $s = -\kappa^{1/3}(x - x_0)$, so $s > 0$ will correspond to $x < x_0$.

then $\eta(s) := \kappa^{-2/3}y(x)$ will satisfy (4.2). Note that $\eta' := d\eta/ds = -\kappa^{-1}dy/dx$ and that the initial conditions give $y'(0) = u'(0) = -2\kappa$ so taking $\tilde{s} = \kappa^{1/3}x_0$ corresponding to taking $x = 0$ gives $\eta'(\tilde{s}) = 2$ as specified. This specification of \tilde{s} together with the definitions of η , U and our choices above of s, ω then give $U(\omega, \bar{\delta}) = y(0) + v(0) = u(0) = \alpha$, provided we show that $\hat{\kappa} = \kappa$. To this end we note that

$$\begin{aligned} u(1) - \beta &= y|_{x_0}^1 = \int_{x_0}^1 y' dx = \int_{x_0}^1 [-\kappa - \int_x^1 y'' d\hat{x}] dx \\ &= -\kappa[1 - x_0] + \int_{x_0}^1 \int_x^1 uw d\hat{x} dx \end{aligned}$$

so, with $\tilde{\beta}$ as above and recalling that the choice of \tilde{s} gave $\kappa = [\tilde{s}/x_0]^3$, we see that our definition of ξ gave $\xi = x_0$: we do, indeed, have $\hat{\kappa} = \kappa$.

Lemma 4.2. *Let $\bar{\omega}$ be the limit value for ω when $\bar{\delta} = 0$, i.e., $\bar{\omega} := \bar{\kappa}^{-2/3}\bar{w}(\bar{x}_0)$. Then $dU(\omega, 0)/d\omega < 0$ at $\omega = \bar{\omega}$.*

Proof: This was already shown as one of the principal results of [5], but we take the opportunity to sketch the argument here again.

For $\bar{\delta} = 0$ we have $\eta = \eta(s, \omega)$ satisfying: $\eta'' = \eta(\eta + \omega - 2s)$ with $\eta(0) = 0$, $\eta'(0) = 1$ and note that on the relevant interval we have $\eta, (\eta + \omega - 2s) > 0$ so $\eta'' > 0$ and $z = z(s, \omega)$ is positive and strictly increasing: $z > 0$, $z' = z_s > 0$. Further, η_ω satisfies:

$$\eta_\omega'' = [2\eta + \omega - 2s]\eta_\omega + \eta \quad \text{with } \eta_\omega(0) = 0 = \eta_\omega'(0) [= z_\omega(0)]$$

so $\eta_\omega > 0$ and $\eta_\omega' = z_\omega > 0$. [Note that the strict inequality for η_ω is for $0 < s \leq \tilde{s}$.] Solving: $z(s, \omega) = \zeta$ gives $s = \sigma(\zeta, \omega)$ for $1 \leq \zeta \leq 2$ and $z_s \sigma_\omega + z_\omega = 0$ then gives $\sigma_\omega < 0$ for $\zeta > 1$; note that $\tilde{s} = \sigma(2, \omega)$ so $d\tilde{s}/d\omega < 0$. At the same time we note that implicit differentiation of the defining cubic gives $d\xi/d\tilde{s} = 3\tilde{s}^2(1 - \xi)/[3\beta\xi^2 + \tilde{s}^3] > 0$ so ξ must also be a strictly decreasing function of ω as is $\hat{\kappa} = \beta/(1 - \xi)$.

The trick now is to reformulate the differential equation using $t = \eta'$ as independent variable, since this is strictly increasing on the relevant interval $[0, \tilde{s}]$. We now write $Y(t, \omega) = \eta(\sigma(t, \omega), \omega)$ and note that

$$Y' \left[= \frac{\partial Y}{\partial t} \right] = \frac{\partial \eta / \partial s = t}{\partial \eta' / \partial s = \eta''} = \frac{t}{Y(Y + \omega - 2\sigma)} \quad \text{with } Y(1) = 0.$$

[This is singular at $t = 1$, so a power series computation⁶ is needed there to get started.] Now Y_ω satisfies

$$Y_\omega' = -t[Y(Y + \omega - 2\sigma)]^{-2} [(2Y + \omega - 2\sigma)Y_\omega + (1 - 2\sigma_\omega)] \quad \text{with } Y_\omega(1) = 0$$

so, as we already know $\sigma_\omega < 0$, we have $Y_\omega < 0$. In particular, $d[\eta(\tilde{s}, \omega)]|_{\omega=\bar{\omega}} = Y_\omega(2, \bar{\omega}) < 0$ — i.e., $\eta(\tilde{s}, \omega)$ is a strictly decreasing function of ω . Since we have already noted that $\hat{\kappa}$

⁶Note that the original ode for η (as a function of s) is analytic in s, ω so η is analytic in s, ω . From the ode and the data, we see that at $s = 0$ one has $\eta = 0$, $\eta' = 1$, $\eta'' = 0$, and $\eta''' = \omega$ so η has an expansion $\eta = s + (\omega/6)s^2 + [\text{higher order terms}]$. This gives $t = \eta' = 1 + (\omega/2)s^2 + [\text{higher order terms}]$ and we may invert this to get $\eta^2 \sim s^2 \sim 2(t - 1)/\omega$ whence η^2 (and so η) is strictly decreasing in ω for small enough $t - 1 > 0$.

is a strictly decreasing function of ω , the asserted result now follows from the definition: $U := \hat{\kappa}^{2/3}\eta(\tilde{s})$. \square

Lemma 4.3. $x_0 = \bar{x}_0 + O(\epsilon^{1/3})$, $\kappa = \bar{\kappa} + O(\epsilon^{1/3})$.

Proof: One easily sees that U is well-defined and suitably differentiable for $(\omega, \bar{\delta})$ near $(\bar{\omega}, 0)$. By Lemma 4.2 we have $\partial U / \partial \omega|_{(\bar{\omega}, 0)} \neq 0$, so the Implicit Function Theorem ensures that one can locally solve for ω the equation

$$U(\omega, \bar{\delta}) = \alpha$$

to get $\omega = \omega(\bar{\delta})$ for $\bar{\delta}$ in a neighborhood of 0 with $\omega = \bar{\omega} + O(\bar{\delta})$. Then

$$\begin{aligned} x_0 &= \xi(\omega(\bar{\delta}), \bar{\delta}) = \bar{x}_0 + O(\epsilon^{1/3}) \\ \kappa &= \hat{\kappa}(\omega(\bar{\delta}), \bar{\delta}) = \bar{\kappa} + O(\epsilon^{1/3}) \end{aligned}$$

as desired, using the Corollary to Lemma 4.1 and, as in [5], $\xi(\bar{\omega}, 0) = \bar{x}_0$, $\hat{\kappa}(\bar{\omega}, 0) = \bar{\kappa}$. \square

We next wish to estimate the norm of $\Delta = (K - \bar{K})$. Since \bar{K} has the form $\bar{K} = \kappa\delta(\cdot - \bar{x}_0)$ with both κ and \bar{x}_0 to be determined from the problem, we must be careful in our choice of the norm to use for this estimation: it turns out that the right space to work with is

$$\mathcal{Y} = \text{Lip}^* := [\text{dual space of } \{\text{Lipschitzian functions}\}] = [W^{1,\infty}(0, 1)] =: W^{-1,1}(0, 1).$$

Lemma 4.4. $\|K - \bar{K}\|_{\mathcal{Y}} = O(\epsilon^{1/3})$.

Proof: Let f be any function in $\text{Lip} = W^{1,\infty}(0, 1)$ with $\|f\|_{\text{Lip}} = 1$, i.e., $|f(x)| \leq 1$ and $|f(x_1) - f(x_2)| \leq |x_1 - x_2|$ on $[0, 1]$. Then

$$\begin{aligned} \langle \Delta, f \rangle &= \int_0^1 K f dx - \bar{\kappa} f(\bar{x}_0) \\ &= \int_0^1 K [f - f(\bar{x}_0)] dx + (\kappa - \bar{\kappa}) f(\bar{x}_0). \end{aligned}$$

Note that $|f(\bar{x}_0)| \leq 1$ and we have already shown that $(\kappa - \bar{\kappa}) = O(\epsilon^{1/3})$. Also

$$\begin{aligned} \left| \int_0^1 K [f(x) - f(x_0)] dx \right| &\leq \int_0^1 K |x - x_0| dx \\ &= \int_0^1 v'' |x - x_0| dx = - \int_0^{x_0} v''(x - x_0) dx + \int_{x_0}^1 v''(x - x_0) dx \\ &= \int_0^{x_0} v' dx + v'(x - x_0)|_{x_0}^1 - \int_{x_0}^1 v' dx \\ &= v|_0^{x_0} - v|_{x_0}^1 + (1 - x_0)v'(1) = 2\zeta - v(0) - \beta + \kappa(1 - x_0) \\ &= 2\zeta - v(0) + [-u(1) + \int_{x_0}^1 \int_x^1 uw d\xi dx] = O(\epsilon^{1/3}). \end{aligned}$$

This proves Lemma 4.4. \square

Now consider the ‘solution operators’ $\mathbf{S}_j : \gamma_j \mapsto \omega_j$ ($j = 1, 2$) such that

$$\begin{cases} \omega_1'' - \bar{w}\omega_1 = \gamma_1; & \omega_1(0) = 0 = \omega_1'(1); \\ \omega_2'' - \bar{u}\omega_2 = \gamma_2; & \omega_2(0) = 0 = \omega_2'(1). \end{cases} \quad (4.5)$$

It is easily seen that each \mathbf{S}_j is a well-defined compact operator: $\mathcal{Y} := \text{Lip}^* \rightarrow \mathcal{Y}$ (For \mathbf{S}_2 this uses positivity of \bar{u} ; for \mathbf{S}_1 the non-negativity of \bar{w}). Now define

$$F(\bar{\gamma}, \Delta) = \begin{pmatrix} \gamma_1 - \Delta - \bar{u}\mathbf{S}_2\gamma_2 - (\mathbf{S}_1\gamma_1)(\mathbf{S}_2\gamma_2) \\ \gamma_2 + \Delta - \bar{w}\mathbf{S}_1\gamma_1 - (\mathbf{S}_1\gamma_1)(\mathbf{S}_2\gamma_2) \end{pmatrix}, \quad \text{where } \bar{\gamma} = \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix}. \quad (4.6)$$

It is easy to verify that $F(\bar{0}, 0) = 0$ and to compute the Frechet derivative at $(\bar{0}, 0)$:

$$\mathbf{A} := \left. \frac{\partial F}{\partial \bar{\gamma}} \right|_{(\bar{0}, 0)} = \begin{pmatrix} 1 & -\bar{u}\mathbf{S}_2 \\ -\bar{w}\mathbf{S}_1 & 1 \end{pmatrix}.$$

For future reference, we note that if we set $\Delta = K - \bar{K}$ and

$$\begin{aligned} \omega_1 &:= u - \bar{u}, & \gamma_1 &:= \Delta + \bar{u}\omega_2 - \omega_1\omega_2 \\ \omega_2 &:= w - \bar{w}, & \gamma_2 &:= -\Delta + \bar{w}\omega_1 - \omega_1\omega_2 \end{aligned}$$

then it is again easy to verify from the equations that we have

$$F(\bar{\gamma}, \Delta) = 0. \quad (4.7)$$

with $u - \bar{u} = \mathbf{S}_1\gamma_1$ and $w - \bar{w} = \mathbf{S}_2\gamma_2$.

Lemma 4.5. $\mathcal{N}(\mathbf{A})$ is trivial.

Proof. Suppose $\bar{\gamma} = \begin{pmatrix} a \\ b \end{pmatrix}$ is in $\mathcal{N}(\mathbf{A})$ and set $\phi := \mathbf{S}_1 a$, $\psi := \mathbf{S}_2 b$ so, from the definition of \mathbf{A} ,

$$a - \bar{u}\psi = 0, \quad b - \bar{w}\phi = 0,$$

and, by (4.5),

$$\phi'' - \bar{w}\phi = a = \bar{u}\psi, \quad \psi'' - \bar{u}\psi = b = \bar{w}\phi,$$

Then $(\phi - \psi)'' = 0$ so, as (4.5) gives $\phi'(1) = 0 = \psi'(1)$, we have $\psi - \phi = \text{const} =: c$ and $\bar{u}\psi = \bar{u}\phi + c\bar{u}$. Thus,

$$\phi'' - (\bar{u} + \bar{w})\phi = c\bar{u} \quad \text{with } \phi(0) = 0 = \phi'(0) \quad \text{and } \phi'(1) \geq 0.$$

Multiplying by $\phi_- := \min\{0, \phi\} \leq 0$, we get

$$0 \leq \left[\int_0^1 (\phi'_-)^2 dx + \int_0^1 (\bar{u} + \bar{w})\phi_-^2 dx \right] = -c \int_0^1 \bar{u}\phi_- dx$$

whence either $c \geq 0$, or $\phi_- \equiv 0$. Similarly, multiplying by $\phi_+ := \max\{0, \phi\} \geq 0$, we get

$$0 \leq \left[\int_0^1 (\phi'_+)^2 dx + \int_0^1 (\bar{u} + \bar{w})\phi_+^2 dx \right] = -c \int_0^1 \bar{u}\phi_+ dx,$$

whence $c \leq 0$, or $\phi_+ \equiv 0$.

Case 1. $[c = 0 \text{ so } \phi \equiv \psi]$. Then $\phi'' - (\bar{u} + \bar{w})\phi = 0$ with $\phi(0) = 0 = \phi'(0)$, whence $\phi \equiv 0$ and $\psi \equiv 0$, so $a = 0 = b$.

Case 2. $[c > 0]$. Note that if $c > 0$, then we have shown $\phi_+ \equiv 0$, i.e., $\phi \leq 0$. We know from [5] that $\bar{u} > 0$ in some neighborhood of 0; let $c\bar{u} \geq 2\delta > 0$ on some $[0, \varepsilon]$. By continuity,

since $\phi(0) = 0$, we have $|\phi| \leq \delta'$ on $[0, \varepsilon]$ (with $\varepsilon = \varepsilon(\delta') > 0$ for arbitrary δ' , and we now take $\delta' = \delta/\tilde{M}$, where $0 \leq \bar{u} + \bar{w} \leq \tilde{M}$). Then $\phi'' = c\bar{u} + (\bar{u} + \bar{w})\phi \geq 2\delta - \tilde{M}\delta' = \delta > 0$ on $[0, \varepsilon]$, whence

$$\phi'(x) = \phi'(0) + \int_0^x \phi'' d\xi \geq \delta x$$

on $[0, \varepsilon]$, so $\phi(x) \geq \delta x^2/2 > 0$, which is contradicting with $\phi \leq 0$. Thus we cannot have $c > 0$.

Case 3. $[c < 0]$. Much as in Case 2, if $c < 0$, then $\phi_- \equiv 0$, so $\phi \geq 0$ and $c\bar{u} \leq -2\delta < 0$ on $[0, \varepsilon]$ with $|\phi| \leq \delta' = \delta/\tilde{M}$ on $[0, \varepsilon]$. As above, we now get $\phi'' \leq -\delta$, so $\phi'(x) \leq -\delta x$, so $\phi(x) \leq -\delta x^2/2$, which is contradicting with $\phi \geq 0$. Thus we cannot have $c < 0$ either.

This leaves only Case 1, and so proves Lemma 4.5. \square

Completion of the proof of the Theorem. We note that \mathbf{A} has the form “identity + compact” on $\mathcal{Y} = \text{Lip}^*$ with $\mathcal{N}(A)$ trivial and so is boundedly invertible there. By the Implicit Function Theorem (IFT) in \mathcal{Y} , it then follows that there is a unique local C^1 solution $\Gamma : \Delta \mapsto \bar{\gamma}$ of (4.7) in a neighborhood of 0 in \mathcal{Y} — i.e., $F(\bar{\gamma}, \Delta) = 0$ for $\bar{\gamma} = \Gamma(\Delta)$ with $\Gamma(\Delta) = O(\|\Delta\|_{\mathcal{Y}})$ so, using Lemma 4.4, we have $\gamma_1 = O(\epsilon^{1/3})$ and $\gamma_2 = O(\epsilon^{1/3})$ in the sense of \mathcal{Y} .

Setting $\omega_3 := v - \bar{v}$, we note that $\omega_3'' = \Delta$ with $\omega_3'(0) = 0 = \omega_3(1)$; thus, since Lemma 4.4 gives $\Delta = O(\epsilon^{1/3})$ in the sense of \mathcal{Y} , we immediately have $v - \bar{v} = O(\epsilon^{1/3})$ in the sense of $\mathcal{Y}_2 = \{f : f'' \in \mathcal{Y}\}$. Next, since $\mathbf{S}_1, \mathbf{S}_2$ are continuous from \mathcal{Y} to \mathcal{Y}_2 , we see from the above that also $u - \bar{u} = \mathbf{S}_1\gamma_1 = O(\epsilon^{1/3})$ and $w - \bar{w} = \mathbf{S}_2\gamma_2 = O(\epsilon^{1/3})$ in the sense of \mathcal{Y}_2 . Since \mathcal{Y}_2 embeds continuously (indeed, compactly) in $C[0, 1]$, we note that this sense of the error will certainly imply $O(\epsilon^{1/3})$ approximation also in the sense of sup norm. \blacksquare

5. Further remarks

Let us now consider another qualitatively different setting for the asymptotics. First, note that if $\alpha = 0$ in the time-dependent system with $u(0, \cdot) = 0$ (for any fixed λ — one can then let $\lambda \rightarrow \infty$) we have $u \equiv 0$ for all t, x and this goes to the steady state (independent of λ)

$$\bar{u} \equiv 0, \quad \bar{v} \equiv \beta, \quad \bar{w} \equiv w^* := \int_0^1 w(0, x) dx.$$

Note that this is *not* of the form “(3.6) with $x^* = 0$ ” and that w^* is here given by the initial data but is indeterminate from the steady state system alone (since no reactions occur in the absence of the reactant A , we simply have a spatial redistribution of the initial concentration $w(0, x)$ of reactant C over the domain).

On the other hand, if we take $\lambda \rightarrow \infty$ first and *then* let $\alpha \rightarrow 0$, it was observed in Seidman and Kalachev [5] that we will get $w^* \rightarrow \infty$, and so, *no limit solution at all*.

However, suppose we let $\alpha \rightarrow 0$, $\lambda \rightarrow \infty$ simultaneously, in a related fashion — say we consider

$$\alpha := \tilde{\alpha}\lambda^{-\nu} = \tilde{\alpha}\epsilon^{\nu},$$

for some fixed $\tilde{\alpha}, \nu > 0$. Numerical experiments suggest that we would then also get no limit solution. Heuristically this can be explained as follows. The first reaction, transforming the

substances A and B into C , is very fast. If the concentration α of reactant A on the boundary $x = 0$ is small (in our case, asymptotically small), all the molecules of A will be used up for production of C and there will be no molecules of A left to participate in the second “slow” reaction $A + C \rightarrow \text{product}$. This will lead to continuous growth of the concentration of C , with different positive values of ν giving different rates of growth. [Note that in the case of $\alpha = O(1)$, there are enough molecules of A to deplete the concentration of B in some region of the domain $[0, 1]$, where now $v = 0$ so the first reaction cannot consume any more molecules of A at its fast rate. This reaction still takes place, but now its rate is diffusion limited: determined by the rate at which molecules of B diffuse into the depleted region. The diffusion in our system is “slow”, and thus the production of C is comparatively slow. At some point all the additional molecules of C produced by the first reaction will be consumed by the second reaction. This process eventually leads to a limit solution of the non-stationary problem.]

Let us now show how the asymptotic algorithm reflects these changes in the behavior of the solution (2.1), (1.2) in this setting for the particular choice $\nu = 1/2$ so $\alpha = \sqrt{\epsilon}\tilde{\alpha}$, where $\epsilon = 1/\lambda \ll 1$. Then we expect the asymptotic solution to be in the form

$$u(x, \epsilon) = \bar{u}_0(x) + \sqrt{\epsilon}\bar{u}_1(x) + \dots + P_0u(\zeta) + \sqrt{\epsilon}P_1u(\zeta) + \dots,$$

with similar expressions for v and w . Here \bar{u}_i are the regular terms of the asymptotic expansion, $P_i(\zeta)$ are the boundary functions in the vicinity of the boundary $x = 0$ and $\zeta = x/\sqrt{\epsilon}$ is the stretched variable. Substituting this form of the asymptotic solution into the equation (2.1) and boundary conditions (1.2), and equating terms of like powers of ϵ separately for different types of functions, we obtain the problems for the terms of the asymptotic series.

For the regular functions of zeroth order, we have, as in the previous setting,

$$\bar{u}_0\bar{v}_0 = 0,$$

and we expect that since $\alpha = O(\sqrt{\epsilon})$, the boundary conditions for \bar{u}_0 are homogeneous, so

$$\bar{u}_0(x) \equiv 0,$$

while the function $\bar{v}_0(x)$ (as yet unknown) cannot vanish identically since it satisfies a non-homogeneous boundary condition at $x = 1$.

For the regular functions of the order $O(\sqrt{\epsilon})$, we similarly obtain $\bar{u}_1(x) \equiv 0$ but \bar{v}_1 is still unknown. For the regular functions of the order $O(\epsilon)$, we write

$$\bar{u}_{0xx} = 0 = \bar{u}_0\bar{v}_2 + 2\bar{u}_1\bar{v}_1 + \bar{u}_2\bar{v}_0 + \bar{u}_0\bar{w}_0,$$

$$\bar{v}_{0xx} = \bar{u}_0\bar{v}_2 + 2\bar{u}_1\bar{v}_1 + \bar{u}_2\bar{v}_0,$$

$$\bar{w}_{0xx} = -\bar{u}_0\bar{v}_2 - 2\bar{u}_1\bar{v}_1 - \bar{u}_2\bar{v}_0 + \bar{u}_0\bar{w}_0,$$

whence

$$\bar{u}_2 = 0, \quad \bar{v}_{0xx} = 0, \quad \bar{w}_{0xx} = 0.$$

This gives $\bar{v}_0 = ax + b$ and $\bar{w}_0 = cx + d$, where the constants a, b, c and d must be obtained from the additional conditions

$$\begin{aligned} \bar{v}_{0x}(0) + (P_1v)_\zeta(0) &= 0, & \bar{v}_0(1) &= \beta, \\ \bar{w}_{0x}(0) + (P_1w)_\zeta(0) &= 0, & \bar{w}_{0x}(1) &= 0. \end{aligned} \tag{5.1}$$

We must also take into account the conditions which involve boundary functions of the zeroth order as well as P_1u :

$$\begin{aligned} \bar{u}_0(0) + P_0u(0) &= 0, \quad \text{so} \quad P_0u(0) = 0, \\ (P_0v)_\zeta(0) &= 0, \quad (P_0w)_\zeta(0) = 0, \end{aligned} \quad (5.2)$$

$$\bar{u}_1(0) + P_1u(0) = P_1u(0) = \tilde{\alpha}. \quad (5.3)$$

To define $\bar{v}_{0x}(0)$ and $\bar{w}_{0x}(0)$ completely, we first solve the problems for the boundary functions of orders $O(1)$ and $O(\sqrt{\epsilon})$. In the leading order, we have

$$(P_0u)_{\zeta\zeta} = P_0u \cdot [\bar{v}_0(0) + P_0u],$$

with similar equations for P_0v and P_0w . With homogeneous conditions and the decay conditions at infinity, these equations (5.2) have only trivial solutions.

For the $O(\sqrt{\epsilon})$ boundary functions we obtain:

$$(P_1v)_{\zeta\zeta} = P_1u \cdot \bar{v}_0(0) = (P_1u)_{\zeta\zeta} = -(P_1w)_{\zeta\zeta}$$

from which, together with the conditions at infinity, we easily see that

$$P_1u = P_1v = -P_1w.$$

The equation for P_1u , with conditions (5.3) and $P_1u(\infty) = 0$, has a solution

$$P_1u(\zeta) = \tilde{\alpha}e^{-\sqrt{\bar{v}_0(0)}\zeta},$$

where $\bar{v}_0(0)$ is still unknown. Since $P_1v(\zeta) = P_1u(\zeta)$, we can substitute this expression into the first condition of (5.1) (for the v -functions at $x = 0$) to get

$$\bar{v}_{0x}(0) - \tilde{\alpha}\sqrt{\bar{v}_0(0)} = 0$$

and, taking into account the form of $\bar{v}_0(x)$, we obtain $a - \tilde{\alpha}\sqrt{b} = 0$ or $b = a^2/\tilde{\alpha}^2$. Since $\bar{v}_0(1) = a + b = \beta$, this gives

$$a^2 + \tilde{\alpha}^2a - \tilde{\alpha}^2\beta = 0 \quad \text{so} \quad a = -\frac{\tilde{\alpha}^2}{2} \left[-1 + \sqrt{1 + \beta/\tilde{\alpha}^2} \right];$$

since a must be non-negative.

There is then no solution of the stationary problem for \bar{w}_0 : $\bar{w}_0(x) = cx + d$, since we come to a contradiction when attempting to define the constants in the expression for \bar{w}_0 from corresponding boundary conditions. Indeed, $\bar{w}_{0x}(x) = c$, and on the one hand $\bar{w}_{0x}(0) = c = -\tilde{\alpha}\sqrt{\bar{v}_0(0)} = -\tilde{\alpha}\sqrt{b} \neq 0$ (b now is a known constant), while on the other hand $\bar{w}_{0x}(1) = c = 0$ (which follows from (5.1)).

Numerical computations for the original non-stationary problem (see (1.1)) with large λ and small α confirm the absence of a stationary solution. Asymptotic algorithm applied to the non-stationary problem with $\lambda = 1/\epsilon$ and $\alpha = \sqrt{\epsilon}\tilde{\alpha}$ will lead for $\bar{w}_0(x, t)$ to the equation $\bar{w}_{0t} = \bar{w}_{0xx}$ with boundary conditions $\bar{w}_{0x}(0, t) = ta\sqrt{b} < 0$ and $\bar{w}_{0x}(1, t) = 0$. It can be easily shown that this problem for $\bar{w}_0(x, t)$ has a solution growing in t for every $x \in [0, 1]$.

It can also be checked that the behavior of $\bar{w}_0(x, t)$ is similar to that of the function $w(x, t)$, determined numerically as the solution of the non-stationary problem.

6. Conclusion

In this paper a particular asymptotic algorithm (the so-called, *boundary function method*) is applied to construct a formal asymptotic expansion of the solution of original problem (2.1), (1.2). The theorem on estimation of the remainder is proved for the leading order approximation. In contrast to the treatment in Seidman and Kalachev [5], where the *passage to the limit* type of result was presented without establishment of the rate of convergence, here we explicitly determined the rate of convergence to the leading order approximation as the small parameter ϵ goes to 0.

The problem (2.1), (1.2) has many important applications in chemical engineering modeling. Somewhat related problems (so-called, problems with exchange of stabilities) were considered using different techniques (upper and lower solutions) in Butuzov et al. [1], [2].

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