Weierstraß–Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

A special reaction–diffusion system

The pseudo–steady–state case

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submitted: 30th November 2001

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Preprint No. 703
Berlin 2001

2000 *Mathematics Subject Classification.* 35K45, 35K57, 80A30, 92E20..

Key words and phrases. Initial boundary value problems, reaction–diffusion equations, chemical reactions, chemical kinetics..

Edited by
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E-Mail (X.400): c=de;a=d400-gw;p=WIAS-BERLIN;s=preprint
E-Mail (Internet): preprint@wias-berlin.de
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Abstract

A system of reaction–diffusion equations modelling the diffusion of iodine and its reaction with radicals in a thin layer of radiation–activated polyethylene is considered. A reduced model, the pseudo–steady–state case, is investigated.

1. Introduction

By the influence of radiation of ultraviolet light of appropriate wavelength free radicals of high reactivity are induced within a thin polyethylene layer. To determine the concentration of the radicals their reaction with iodine diffusing through the layer is considered. The resulting iodide within the layer can be determined –up to a certain depth– by XPS (X–ray Photoelectron Spectroscopy). For a quantitative study we consider a mathematical model proposed by R. Wilken from the Fraunhofer Institute for Applied Polymer Research at Teltow–Seehof (Germany). The model is based on the assumption that one reactant – iodine – is transported by diffusion and reacts according to the laws of classical reaction kinetics with the immobile radicals forming immobile iodide. So the model consists of a coupled system of a reaction–diffusion equation and an ordinary differential equation. The model allows to study the influence of different parameters like diffusion constant, reaction rate constants, initial and boundary values of the concentrations involved.

For high reactivity of the free radicals scaling arguments show that it is useful to deal with the so–called pseudo–steady–state case. In this paper we consider this reduced problem.

2. The model equations

The species involved in the model are I – iodine, R – radicals, S – iodide. The experimental situation allows to consider the problem as spatially one–dimensional. So we are interested in the concentrations

$$I = I(t,x), \quad R = R(t,x), \quad S = S(t,x)$$

on

$$G = \{(t,x) :\ 0 < t < T,\ 0 < x < a\}$$

for some $T > 0$ which satisfy there the model equations

$$\frac{\partial I}{\partial t} = D\frac{\partial^2 I}{\partial x^2} - c_1 IR, \tag{2.1}$$

$$\frac{dR}{dt} = -c_1 IR - c_2 R, \tag{2.2}$$

$$\frac{dS}{dt} = c_1 IR. \tag{2.3}$$

with a given diffusion constant D and given constant reaction rates c_1, c_2. For the concentration I of iodine we prescribe boundary conditions

$$I(t,0) = I_0, \quad \frac{\partial I}{\partial x}(t,a) = 0, \quad 0 < t \le T, \tag{2.4}$$

with a given constant $I_0 > 0$. For all concentrations I, R, S initial conditions are prescribed by

$$I(0,x) = 0, \quad R(0,x) = R_0(x), \quad S(0,x) = 0, \quad 0 \le x \le a, \tag{2.5}$$

with a given initial concentration of free radicals $R_0(x) > 0$. In the actual models only constant initial values or decaying initial values

$$R_0(x) = R_0 \quad \text{or} \quad R_0(x) = R_0 \exp(-x/\mu)$$

were considered. Here $R_0 > 0$ is a given constant and the extinction coefficient $\mu > 0$ characterizes the decay of the radiation effects with increasing depth.

Remark 2.1. It makes sense to consider the equations (2.1) (2.2) on the half strip $G = \{(t,x) : \ 0 < t < T, \ 0 < x < \infty\}$, modifying the initial and boundary conditions appropriately. Especially, the Neumann boundary condition at $x = a$ is dropped.

Remark 2.2. Initial and boundary conditions for the iodine concentration I are discontinuous at the point $(t = 0, x = 0)$ – a situation quite common for evolution equations. A smoother situation can be obtained with a boundary condition for I at $x = 0$ of the form

$$I(t,0) = I_0(1 - \exp(-\kappa t))$$

with a given constant $\kappa > 0$. Here we assume that the dosage of the iodine at $x = 0$ takes some time to reach its peak level I_0 – a plausible assumption.
The boundary condition at $x = a$ is the usual boundary condition at an impenetrable wall.

The iodide concentration S doesn't appear in the first two equations (2.1) (2.2), so the system decouples and S could be eliminated. Nevertheless, we keep it because the essential quantity to be compared with measurements is the weighted spatial mean

$$h(t) = \frac{1}{\lambda}\int_0^b S(t,x)\exp(-x/\lambda)dx, \quad 0 \le t \le T.$$

Here $0 < b < a$ is a given depth and $\lambda > 0$, both quantities characterize the measurement by XPS.

The model equations can be solved numerically using standard methods (finite differences) for given constants $D, c_1, c_2, I_0, R_0, \kappa, \lambda, \mu$. Of greater interest as this direct problem are inverse problems linked with the model: How can we get information about the constants involved from the comparison measurement – calculation ?

Remark 2.3. A similar problem is considered in [F]. A somewhat different system of model equations has been treated in [GZ], see also [GS1], [GS2].

Remark 2.4. The special case of system (2.1) (2.2) for $c_2 = 0$ with the initial–boundary conditions

$$I(t,0) = I_0, \quad I(0,x) = 0, \quad R(0,x) = R_0$$

on the half strip $G = \{(t,x) : \; 0 < t < T, \; 0 < x < \infty\}$ has been considered in [HHP1], generalizations to more general reaction kinetics (not covering our case) in [HHP2], [HHP3]. Similar problems arise in combustion theory, see [LS], [B], [LMS], [DS], [L] .

3. Scaling of the model equations

The dimension of a physical quantity q in the sense of dimensional analysis is denoted by $[q]$. Using the fundamental dimensions T, L, M for time, length, mass we then have for the dimensions of the quantities appearing in the model equations

$$[t] = T, [x] = L, [D] = L^2T^{-1}, [I] = [I_0] = [R] = [R_0] = ML^{-3},$$
$$[c_1] = L^3M^{-1}T^{-1}, [c_2] = T^{-1}.$$

Natural dimensionless independent variables can be introduced by

$$\xi = \frac{x}{b}, \quad \tau = \frac{Dt}{b^2}$$

where we took the depth b as length unit. (Another natural choice for the finite strip of thickness a would be taking a as length unit.) With new dependent variables J, P defined by

$$I(t,x) = I\left(\frac{b^2\tau}{D}, b\xi\right) = J(\tau,\xi) \quad R(t,x) = R\left(\frac{b^2\tau}{D}, b\xi\right) = P(\tau,\xi),$$

the model equations (2.1) (2.2) are transformed into

$$\frac{\partial J}{\partial \tau} = \frac{\partial^2 J}{\partial \xi^2} - b_1 JP, \quad \frac{dP}{d\tau} = -b_1 JP - b_2 P, \qquad b_1 = \frac{b^2 c_1}{D}, \quad b_2 = \frac{b^2 c_2}{D}.$$

Introducing dimensionless concentrations by

$$u = \frac{J}{I_0}, \quad v = \frac{P}{R_1}$$

with the boundary value I_0 and an appropriate R_1 as reference concentrations the final dimensionless form of the model equations becomes

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} - A_1 uv, \quad \frac{dv}{d\tau} = -A_2 uv - b_2 v, \qquad A_1 = b_1 R_1, \quad A_2 = b_1 I_0. \tag{3.1}$$

The coefficients A_1, A_2, b_2 are dimensionless. Introducing the new unknown w by

$$v = \exp(-b_2 \tau) w$$

transforms the model equations to

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} - A_1 e^{-b_2 t} uw, \quad \frac{dw}{d\tau} = -A_2\, uw. \tag{3.2}$$

The new length scale $\eta = \sqrt{A_1}\xi$ and the new unknown functions

$$U(\tau, \eta) = u\left(\tau, \frac{\eta}{\sqrt{A_1}}\right) = u(\tau, \xi), \quad V(\tau, \eta) = v\left(\tau, \frac{\eta}{\sqrt{A_1}}\right) = v(\tau, \xi)$$

transform (3.1) into

$$\frac{1}{A_1}\frac{\partial U}{\partial \tau} = \frac{\partial^2 U}{\partial \eta^2} - UV, \quad \frac{dV}{d\tau} = -A_2 UV - b_2 V. \tag{3.3}$$

Correspondingly, with the new unknown function

$$W(\tau, \eta) = w\left(\tau, \frac{\eta}{\sqrt{A_1}}\right) = w(\tau, \xi)$$

the equations (3.2) get the form

$$\frac{1}{A_1}\frac{\partial U}{\partial \tau} = \frac{\partial^2 U}{\partial \eta^2} - e^{-b_2 t}\, UW, \quad \frac{dW}{d\tau} = -A_2\, UW. \tag{3.4}$$

In the case of fast reacting radicals one has $A_1 \gg 1$. This motivates to suppress the time derivative in the first equation of (3.1) and to consider the so–called *pseudo–steady–state case*

$$\frac{\partial^2 U}{\partial \eta^2} - UV = 0, \quad \frac{dV}{d\tau} = -A_2 UV - b_2 V. \tag{3.5}$$

Similar considerations for system (3.3) give

$$\frac{\partial^2 U}{\partial \eta^2} - e^{-b_2 t}\, UW = 0, \quad \frac{dW}{d\tau} = -A_2\, UW. \tag{3.6}$$

Remark 3.1. Dropping the time derivative is a common procedure in chemical engineering literature. It changes the parabolic equation of system (3.2) to an elliptic equation for which an initial condition cannot be imposed. We are in the situation of singular perturbation. The justification for this procedure has been studied – for a somewhat different situation – in [DS].

4. The pseudo–steady–state system

We write $A = A_2 > 0$, $B = b_2 > 0$, $\overline{G} = [0,T] \times [0,\infty)$ and consider the system

$$\frac{\partial^2 U}{\partial \eta^2} - UV = 0, \quad \frac{dV}{d\tau} = -AUV - BV \tag{4.1}$$

on the half strip $G = \{(\tau,\eta) :\ 0 < \tau < T,\ 0 < \eta < \infty\}$ for some $T > 0$ with the boundary conditions

$$U(\tau,0) = 1, \quad \lim_{\eta\to\infty} U(\tau,\eta) = 0, \quad 0 \le \tau \le T \tag{4.2}$$

and the initial condition

$$V(0,\eta) = V_0(\eta) > 0, \quad 0 \le \eta < \infty. \tag{4.3}$$

In the first equation of (4.2) the time τ appears as a parameter, whereas in the second equation the spatial variable η appears as a parameter. Formal integration of the second equation of (4.1) gives

$$V(\tau,\eta) = V_0(\eta) e^{-B\tau} \exp\left(-A\int_0^\tau U(s,\eta)ds\right).$$

By inserting this in the first equation of (4.1) we obtain a non–local parameter dependent (parameter τ) two–point boundary value problem for U :

$$\frac{\partial^2 U}{\partial \eta^2} = V_0(\eta) e^{-B\tau} U(\tau,\eta) \exp\left(-A\int_0^\tau U(s,\eta)ds\right) \tag{4.4}$$

with the boundary conditions (4.2). At the initial time $\tau = 0$ we obtain for $U_0 = U(0,\cdot)$ the linear boundary value problem

$$\frac{\partial^2 U_0}{\partial \eta^2} = V_0(\eta)U_0(\eta), \quad U_0(0) = 1, \quad \lim_{\eta\to\infty} U_0(\eta) = 0.$$

For the special case $V_0(\eta) = V_0 = const. > 0$ the solution is $U_0(\eta) = \exp(-\sqrt{V_0}\eta)$.

Our main result is the following theorem. (For the notation see the Appendix.)

Theorem 4.1. *The system* (4.1), (4.2), (4.3) *with* $V(0,\eta) = V_0 = const. > 0$ *has for any* $T > 0$ *a unique classical solution* (U,V) *with*

$$U > 0, V > 0 \quad on \quad \overline{G}, \quad U \in C([0,T], C^2(\overline{\mathbb{R}_+})), \quad V \in C^1([0,T], C(\overline{\mathbb{R}_+})).$$

Proof. *Existence.* We define a sequence $\{U^{(n)}, V^{(n)}\}$, $n = 1, 2, \dots$ as follows. For $n = 1$ we take for $(U^{(1)}, V^{(1)})$ the solution of

$$\begin{aligned} U^{(1)}_{\eta\eta} &= V_0 U^{(1)} \text{ in } G, \quad U^{(1)}(\tau, 0) = 1, \quad \lim_{\eta\to\infty} U^{(1)}(\tau,\eta) = 0, \quad 0 \le \tau \le T, \\ V^{(1)}_{\tau} &= -(A\,U^{(1)} + B)V^{(1)} \text{ in } \overline{G}, \quad V^{(1)}(0,\eta) = V_0 > 0 \text{ for } \eta \ge 0. \end{aligned}$$

The solution is

$$U^{(1)}(\tau,\eta) = \exp(-\sqrt{V_0}\eta), \quad V^{(1)}(\tau,\eta) = V_0 \exp\left[-\left(B + A\exp\left(-\sqrt{V_0}\eta\right)\right)\tau\right].$$

Obviously, we have $U^{(1)} \in C([0,T], C^2(\overline{\mathbb{R}_+}))$, $V^{(1)} \in C^1([0,T], C(\overline{\mathbb{R}_+}))$. For $n \ge 2$ we define $(U^{(n)}, V^{(n)})$ as the solution of

$$\begin{aligned} U^{(n)}_{\eta\eta} &= V^{(n-1)} U^{(n)} \text{ in } G, \quad U^{(n)}(\tau, 0) = 1, \quad \lim_{\eta\to\infty} U^{(n)}(\tau,\eta) = 0, \quad 0 \le \tau \le T, \\ V^{(n)}_{\tau} &= -(A\,U^{(n)} + B)V^{(n)} \text{ in } \overline{G}, \quad V^{(n)}(0,\eta) = V_0 > 0 \text{ for } \eta \ge 0. \end{aligned}$$

We show by induction that $(U^{(n)}, V^{(n)})$ are well defined and have all necessary properties. The case $n = 1$ is already done. From Lemma 5.4, Lemma 5.6 of the Appendix follows that for fixed τ with $0 \le \tau \le T$ there exists

$$U^{(n)}(\tau,\cdot) \in C^2(\overline{\mathbb{R}_+}), \quad U^{(n)}(\tau,\cdot) > 0,$$

because of

$$V^{(n-1)} \in C^1([0,T], C(\overline{\mathbb{R}_+})), \quad V^{(n-1)} > 0 \text{ in } \overline{G},$$

by induction assumption. By well–known theorems on the parameter dependence of solutions of ordinary differential equations (see e.g. [A], [H]) we get $U^{(n)} \in C([0,T], C^2(\overline{\mathbb{R}_+}))$. By the same arguments we obtain from the integral representation

$$V^{(n)}(\tau,\eta) = V_0 \exp\left(-B\tau - A\int_0^\tau U^{(n)}(s,\eta)\,ds\right) \tag{4.5}$$

of the solution $V^{(n)}$ of the linear equation

$$V^{(n)}_\tau = -(A\,U^{(n)} + B)V^{(n)}, \quad V^{(n)}(0,\eta) = V_0$$

that

$$V^{(n)} \in C^1([0,T], C(\overline{\mathbb{R}_+})), \quad V^{(n)} > 0 \text{ in } \overline{G}.$$

Next we show by induction that for $n \ge 1$

$$1 \ge U^{(n+1)} \ge U^{(n)} > 0 \quad \text{and} \quad 0 < V^{(n+1)} \le V^{(n)} \le V_0 \text{ in } \overline{G}. \tag{4.6}$$

From $V^{(1)} \le V_0$ we obtain with the comparison assertion of Lemma 5.7

$$1 \ge U^{(2)} \ge U^{(1)} > 0 \quad \text{in } \overline{G}.$$

From formula (4.5) follows $0 < V^{(2)} \leq V^{(1)}$. Repeating these arguments gives (4.6).

From these monotonicity properties of the sequences $\{U^{(n)}\}, \{V^{(n)}\}, \quad n = 1, 2, \ldots$ follows that there are functions U, V defined on $\overline{G}$ such that

$$U^{(n)}(\tau, \eta) \longrightarrow U(\tau, \eta), \quad V^{(n)}(\tau, \eta) \longrightarrow V(\tau, \eta) \text{ for } n \longrightarrow \infty \text{ pointwise in } \overline{G}.$$

From Lebesgue's Theorem on dominated convergence (we have $0 < U^{(n)} \leq 1$ for all n) we get from the integral representation (4.5) by taking $n \longrightarrow \infty$

$$V(\tau, \eta) = V_0 \exp\left(-B\tau - A \int_0^\tau U(s, \eta)\, ds\right). \tag{4.7}$$

To conclude similarly for U , we use the representation (5.5)

$$U^{(n)}(\tau, \eta) = 1 - \int_0^\eta \left(\int_\xi^\infty V^{(n-1)}(\tau, r) U^{(n)}(\tau, r)\, dr\right) d\xi.$$

From the integral representation (4.5) we get

$$V^{(n-1)}(\tau, r) \geq V_0 \exp(-(A+B)\tau) \geq V_0 \exp(-(A+B)T) = C(T)$$

and with the comparison assertion of Lemma 5.7 for the equation $U^{(n)}_{\eta\eta} = V^{(n-1)} U^{(n)}$ we get

$$U^{(n)}(\tau, r) \leq \exp\left(-r\sqrt{C(T)}\right).$$

So we find

$$V^{(n-1)}(\tau, r) U^{(n)}(\tau, r) \leq V_0 \exp\left(-r\sqrt{C(T)}\right),$$

where the right–hand side is obviously integrable on $\{(r, \xi) | 0 \leq \xi \leq \eta, \xi \leq r < \infty\}$. Again by Lebesgue's Theorem on dominated convergence we can interchange the limit $n \longrightarrow \infty$ and the integration and we obtain

$$U(\tau, \eta) = 1 - \int_0^\eta \left(\int_\xi^\infty V(\tau, r) U(\tau, r)\, dr\right) d\xi. \tag{4.8}$$

Differentiation of (4.7), (4.8) shows that (U, V) is the solution.

Uniqueness. Assume that there are two solutions $(U^{(i)}, V^{(i)}),\ i = 1, 2;$ with the properties found in the existence part. Subtracting the corresponding equations we get for the differences

$$u = U^{(1)} - U^{(2)}, \quad v = V^{(1)} - V^{(2)}$$

the equations

$$\begin{aligned} v_\tau &= -(B + A\,U^{(1)})\, v - A\,V^{(2)} u, \qquad v(0, \eta) = 0 \text{ for } \eta \geq 0 \\ u_{\eta\eta} &= U^{(1)} v + V^{(2)} u, \quad u(\tau, 0) = 0, \quad \lim_{\eta \to \infty} u(\tau, \eta) = 0, \quad 0 \leq \tau \leq T. \end{aligned}$$

We apply an L^1 technique (see e.g. [DS]). We multiply the first equation by $sgn(v)$, the second equation by $sgn(u)$ and integrate over the strip $[0,\tau]\times[0,\infty),\ 0\le\tau\le T$,where

$$sgn(a)=\begin{cases}-1: & a<0\\ \ \ 0: & a=0\\ +1: & a>0\end{cases}$$

As the result of these manipulations we obtain

$$\begin{aligned}\int_0^\tau\int_0^\infty v_\tau\, sgn(v)\, d\sigma d\eta = &-\int_0^\tau\int_0^\infty (B+AU^{(1)})|v|\, d\sigma d\eta\\ &-A\int_0^\tau\int_0^\infty V^{(2)}u\, sgn(v)\, d\sigma d\eta\end{aligned}$$

and

$$\int_0^\tau\int_0^\infty u_{\eta\eta}\, sgn(u)\, d\sigma d\eta=\int_0^\tau\int_0^\infty U^{(1)}v\, sgn(u)\, d\sigma d\eta+\int_0^\tau\int_0^\infty V^{(2)}|u|\, d\sigma d\eta.$$

Taking into account the initial and boundary conditions one can show that

$$\int_0^\tau\int_0^\infty v_\tau\, sgn(v)\, d\sigma d\eta=\int_0^\infty |v(\tau,\eta)|\, d\eta$$

and

$$\int_0^\tau\int_0^\infty u_{\eta\eta}\, sgn(u)\, d\sigma d\eta\le 0.$$

Using this in the equalities above we have because of $V^{(2)}\ge 0,\ U^{(1)}\ge 0$ the estimate

$$0\le\int_0^\tau\int_0^\infty V^{(2)}|u|\, d\sigma d\eta\le\int_0^\tau\int_0^\infty U^{(1)}|v|\, d\sigma d\eta$$

from which we obtain

$$\int_0^\infty |v(\tau,\eta)|\, d\eta\le A\int_0^\tau\int_0^\infty U^{(1)}|v|\, d\sigma d\eta\le A\int_0^\tau\int_0^\infty |v(\tau,\eta)|\, d\sigma d\eta.$$

Gronwall's lemma gives $v=0$ in $[0,\tau]\times[0,\infty),\ 0\le\tau\le T$, the maximum principle gives $u=0$ there. □

Remark 4.1. The Theorem can also be proved for a nonconstant initial value $V_0\in C(\overline{\mathbb{R}_+})$ with $V_0(\eta)>0$ for $\eta\ge 0$.

5. Appendix

Here we prove some auxiliary results for the linear two–point boundary value problem on a finite interval and on the half line. The dependence on the (time) parameter τ is omitted. Our notation and reasoning follow closely [Br].

As usual we denote for the interval I $(I=(0,L), \quad L>0, \text{ or } I=(0,\infty))$ by $C(I)$ ($C^k(I)$, respectively) the set of continuous functions on I (the set of k times continuously differentiable functions on I , respectively). Correspondingly, $C_c(I)$ are the continuous functions with compact support in I , $C_c^k(I)=C_c(I)\cap C^k(I)$. We denote by $C(\overline{I})$ the Banach space of continuous functions on $\overline{I}=[0,L]$ and by $C^k(\overline{I})$ the Banach space of functions from $C^k(I)$ which can be extended continuously to $\overline{I}$.

By $L_2(I)$ we denote the usual Hilbert space of square integrable functions with the scalar product

$$(f,g)=\int_I f(\eta)g(\eta)d\eta \quad \text{and the norm} \quad \|f\|^2=\int_I |f(\eta)|^2 d\eta.$$

The Sobolev space $H^1(I)=W^{1,2}(I)$ is the space of square integrable functions on I with square integrable first (generalized) derivative. Scalar product and norm are defined by

$$(f,g)_{H^1}=(f,g)+(f_\eta,g_\eta), \quad \|f\|^2_{H^1}=\|f\|^2+\|f_\eta\|^2.$$

For $m\geq 2$ we define $H^m(I)=W^{m,2}(I)$ recursively by

$$H^m(I)=\{f\in H^{m-1}(I), \quad f_\eta\in H^{m-1}(I)\}$$

and denote by $H^1_0(I)$ the closure of $C_c(I)$ in $H^1(I)$. For I bounded holds Friedrichs inequality

$$\|f\|\leq C\|f_\eta\| \quad \forall f\in H^1_0(I)$$

with an appropriate constant C depending in $|I|$. This fact allows to use on $H^1_0(I)$

$$\|f\|_{H^1_0}=\|f_\eta\|$$

as an equivalent norm to the H^1–norm. As usual, we denote by $H^{-1}=(H^1_0)^*$ the dual space of $H^1_0(I)$ and the dual pairing between $F\in H^{-1}$ and $g\in H^1_0(I)$ by $\langle F,g\rangle$.

Consider on $I=(0,L), \quad L>0$ the boundary–value problem

$$U_{\eta\eta}=p(\eta)U, \quad U(0)=1, \;\; U(L)=0 \tag{5.1}$$

where $p\in C(\overline{I})$, $p(\eta)>0 \quad \forall\, \eta\in\overline{I}$. So we have bounds

$$0<c_0\leq p(\eta)\leq C_0 \quad \text{for} \quad 0\leq\eta\leq L.$$

We homogenize the boundary conditions by introducing $U=W+h$ where $h\in C^2(\overline{I})$ with

$$0\leq h(\eta)\leq 1, \quad h(\eta)=1 \;\text{ for }\; 0\leq\eta\leq L/3, \quad h(\eta)=0 \;\text{ for }\; \eta>2L/3.$$

This transforms (5.1) into

$$W_{\eta\eta}-p(\eta)W=f(\eta) \;\text{ on }\; I, \quad W(0)=W(L)=0, \tag{5.2}$$

where $f : \eta \longmapsto f(\eta) = p(\eta)h(\eta) - h_{\eta\eta}(\eta)$. By construction $f \in C(\overline{I})$. We show existence and uniqueness of classical solutions to (5.2) (and, consequently, to (5.1)) via the well–known Lax–Milgram Lemma (see e.g. [Br]) and regularity assertions.

Definition 5.1. A weak solution of (5.2) is a function $W \in H_0^1(I)$ which satisfies

$$\int_I \{W_\eta g_\eta + p(\eta)Wg + fg\}d\eta = 0 \quad \forall g \in H_0^1(I).$$

Lemma 5.2. *The problem* (5.2) *has a unique solution* $W \in C^2(\overline{I})$.

Proof. Consider on $H_0^1(I)$ the bilinear form

$$a(W,g) = \int_I \{W_\eta g_\eta + p(\eta)Wg\}d\eta.$$

By Friedrichs inequality this form is continuous because of

$$|a(W,g)| \leq (1 + C_0 C)\|W\|_{H_0^1}\|g\|_{H_0^1} \quad \forall W, g \in H_0^1(I)$$

and coercive

$$a(W,W) \geq \|W\|_{H_0^1}^2 \quad \forall W \in H_0^1(I)$$

because of $p > 0$ on $\overline{I}$. The linear form

$$F : g \longmapsto -\int_I fg d\eta$$

is continuous on $H_0^1(I)$ because of $f \in C(\overline{I})$, i.e., $F \in H^{-1}$ (again by Friedrichs inequality). We apply the Lax–Milgram Lemma to find a unique function $W \in H_0^1(I)$ satisfying

$$a(W,g) = \langle F, g\rangle \quad \text{for all} \quad g \in H_0^1(I).$$

Obviously, W is the unique weak solution of (5.2). To show the regularity of this solution we remark that $pW + f \in L_2(I)$ and that the estimate

$$\left|\int_I W_\eta g_\eta d\eta\right| = \left|\int_I (pW+f)g d\eta\right| \leq \|pW+f\|\,\|g\| \quad \forall\, g \in C_c^1(I)$$

holds. This is equivalent to $W_\eta \in H^1(I)$, i.e., $W \in H^2(I)$. Since, moreover, we have $f, p \in C(\overline{I})$ it follows $(W_\eta)_\eta \in C(\overline{I})$ and consequently $W_\eta \in C^1(\overline{I})$ or $W \in C^2(\overline{I})$. A weak solution W with this properties is obviously classical solution. □

Lemma 5.3. *The problem* (5.1) *has a unique classical solution* $U \in C^2(\overline{I})$. *The solution satisfies*

$$0 \leq U(\eta) \leq 1 \quad \forall\, \eta \in \overline{I}.$$

Proof. Playing back the homogenization, the existence and uniqueness assertion follows from Lemma 5.2. To prove the maximum and minimum property, we argue as usual.
If we had $U(\eta_1) < 0$ in $\eta_1 \in I$ then there would exist $\eta_0 \in I$ such that

$$U(\eta_0) = \inf_{0 \le \eta \le L} U(\eta) < 0, \quad U_\eta(\eta_0) = 0, \quad U_{\eta\eta}(\eta_0) \ge 0.$$

Because of $p(\eta) > 0$ in $\overline{I}$ we have a contradiction with the equation (5.1). Thus $U(\eta) \ge 0$ in $\overline{I}$.
If we had $U(\eta_1) > 1$ in $\eta_1 \in I$ then there would exist $\eta_0 \in I$ such that

$$U(\eta_0) = \sup_{0 \le \eta \le L} U(\eta) > 1, \quad U_\eta(\eta_0) = 0, \quad U_{\eta\eta}(\eta_0) \le 0.$$

Again we have (using the positivity of p in $\overline{I}$) a contradiction with (5.1), and consequently $U(\eta) \le 1$ in $\overline{I}$.□

Remark 5.1. The bounds for the solution U are nothing but maximum principle for the boundary–value problem (5.1).

In the following we prove results analogous to Lemma 5.3 for the half line $\mathbb{R}_+$ of positive reals, we denote $\overline{\mathbb{R}_+} = \{\eta : 0 \le \eta < \infty\}$. The proof uses results for finite intervals and a diagonalization procedure as in [GLO]. As usual, we denote by $BC(\overline{\mathbb{R}_+})$ ($BC^2(\overline{\mathbb{R}_+})$, respectively) the space of continuous and bounded functions on $\overline{\mathbb{R}_+}$ (with first and second derivatives continuous and bounded there, respectively).

Lemma 5.4. *The boundary value problem*

$$u_{\eta\eta} = p(\eta)u \quad \textit{on } \mathbb{R}_+, \quad u(0) = 1, \ \lim_{\eta\to\infty} u(\eta) = 0 \tag{5.3}$$

with $p \in BC(\overline{\mathbb{R}_+})$, $p(\eta) > 0$ *on* $\overline{\mathbb{R}_+}$, *has a unique classical solution* $u \in BC^2(\overline{\mathbb{R}_+})$ *satisfying*

$$0 \le u(\eta) \le 1 \quad \forall\, \eta \in \overline{\mathbb{R}_+}.$$

Proof. Consider the sequence of functions $\{U^{(k)}\}$, $k = 1, 2, ...;$ defined as follows: $U^{(k)}$ is solution of (5.1) on $\overline{I_k} = [0, kL]$, i.e.,

$$U^{(k)}_{\eta\eta} = p(\eta)U^{(k)}, \quad U^{(k)}(0) = 1, \ U^{(k)}(kL) = 0.$$

Denote

$$P = \sup_{0 \le \eta < \infty} p(\eta).$$

By Lemma 5.3 we have

$$M_0^{(k)} = \sup_{0 \le \eta \le kL} |U^{(k)}(\eta)| = 1, \quad M_2^{(k)} = \sup_{0 \le \eta \le kL} |U^{(k)}_{\eta\eta}(\eta)| \le P, \quad k = 1, 2... ,$$

and, as the following Lemma 5.5 shows, there is a uniform bound for the first derivative

$$M_1^{(k)} = \sup_{0\le\eta\le kL} |U_\eta^{(k)}(\eta)|$$

which does not depend on k .

Define the sequence $\{W^{(k)}\},\ k=1,2,...;$ of functions on $\overline{\mathbb{R}_+}$ by

$$W^{(k)}(\eta) = \begin{cases} U^{(k)}(\eta) & \text{for } 0\le\eta\le kL \\ 0 & \text{for } \eta\ge kL. \end{cases}$$

Obviously, each $W^{(k)}$ is continuous on $\overline{\mathbb{R}_+}$ and twice continuously differentiable there, with the possible exception at $\eta = kL$. The sequence $\{W^{(k)}\},\ k=1,2,...;$ is equibounded and equicontinuous on $[0,L]$. By the Arzelà–Ascoli theorem there is a subsequence $\widetilde{\mathbb{N}_1}$ of the sequence $\mathbb{N}$ of natural numbers and a function $z_1\in C^1(\overline{I_1})$ such that

$$W^{(n)} \longrightarrow z_1,\quad W_\eta^{(n)} \longrightarrow z_{1\eta}\quad \text{uniformly on } \overline{I_1}=[0,L] \text{ for } n\longrightarrow\infty,\quad n\in\widetilde{\mathbb{N}_1}.$$

Take $\mathbb{N}_1 = \widetilde{\mathbb{N}_1}\setminus\{1\}$. Again by the Arzelà–Ascoli theorem there is a subsequence $\widetilde{\mathbb{N}_2}\subset\mathbb{N}_1$ and a function $z_2\in C^1(\overline{I_2})$ such that

$$W^{(n)} \longrightarrow z_2,\quad W_\eta^{(n)} \longrightarrow z_{2\eta}\quad \text{uniformly on } \overline{I_2}=[0,2L] \text{ for } n\longrightarrow\infty,\quad n\in\widetilde{\mathbb{N}_2}.$$

Because of $\widetilde{\mathbb{N}_2}\subset\mathbb{N}_1$ we have $z_2=z_1$ on $[0,L]$. Take $\mathbb{N}_2=\widetilde{\mathbb{N}_2}\setminus\{2\}$ and go on by induction. One obtains for $k=1,2,...$ a subsequence $\mathbb{N}_k$ of the naturals with $\mathbb{N}_k\subset\mathbb{N}_{k-1}$ and a function $z_k\in C^1(\overline{I_k})$ such that

$$W^{(n)} \longrightarrow z_k,\quad W_\eta^{(n)} \longrightarrow z_{k\eta}\quad \text{uniformly on } \overline{I_k}=[0,kL] \text{ for } n\longrightarrow\infty,\quad n\in\mathbb{N}_k$$

with the property $z_k=z_{k-1}$ on $[0,(k-1)L]$.

Now we construct the solution u as follows. Fix $\eta\in\overline{\mathbb{R}_+}$ and let k be a positive integer satisfying $\eta\le k$. Define $u(\eta)=z_k(\eta)$. By construction, u is well defined and $u\in C^1(\overline{\mathbb{R}_+})$. It holds, by Lemma 5.3 and the construction above

$$W_\eta^{(n)}(\eta) - W_\eta^{(n)}(0) = \int_0^\eta p(s)W^{(n)}(s)ds \quad \text{for } n\in\mathbb{N}_k.$$

Since $W^{(n)}\longrightarrow z_k$ and $W_\eta^{(n)}\longrightarrow z_{k\eta}$ uniformly on $\overline{I_k}=[0,kL]$ for $n\longrightarrow\infty$, $n\in\mathbb{N}_k$, we get

$$z_{k\eta}(\eta)-z_{k\eta}(0)=\int_0^\eta p(s)z_k(s)ds \quad \text{or} \quad u_\eta(\eta)-u_\eta(0)=\int_0^\eta p(s)u(s)ds.$$

So we have $u_\eta\in C^1(\overline{\mathbb{R}_+})$ and the differential equation $u_{\eta\eta}=p(\eta)u$ holds. Obviously, the boundary condition $u(0)=1$ is satisfied and $u,u_\eta,u_{\eta\eta}$ are continuous and bounded, i.e., $u\in BC^2(\overline{\mathbb{R}_+})$. The maximum principle and the resulting estimate of the solution are shown as in Lemma 5.3. Uniqueness of the solution follows from the maximum principle. □

Lemma 5.5. *There is a uniform bound for the first derivative*

$$M_1^{(k)} = \sup_{0 \le \eta \le kL} |U_\eta^{(k)}(\eta)|$$

which does not depend on k *.*

Proof. Because of $p(\eta) > 0$, $U^{(k)}(\eta) \ge 0$ on $[0, kL]$ we have $U_{\eta\eta}^{(k)}(\eta) \ge 0$ on $[0, kL]$, i.e., the function $\eta \mapsto U^{(k)}(\eta)$ is convex on $[0, kL]$. Consequently, the graph

$$G = \{(\eta, U^{(k)}(\eta)),\ \eta \in [0, kL]\}$$

lies above the tangent passing through the point $(kL, 0)$. From this geometrical condition follows

$$-U_\eta^{(k)} \le \frac{1}{kL} \le \frac{1}{L}.$$

Moreover, we have $U_\eta^{(k)}(kL) \le 0$. Otherwise we had $U_\eta^{(k)}(kL) > 0$ and by continuity there were a $\eta_1 \in (0, kL)$ for which

$$U^{(k)}(\eta_1) = -\int_{\eta_1}^{kL} U_\eta^{(k)}(\eta) d\eta < 0$$

– a contradiction with Lemma 5.3. So we can conclude $|U^{(k)}(kL)| \le 1/L$. From

$$U_\eta^{(k)}(\eta) = U_\eta^{(k)}(kL) - \int_\eta^{kL} U_{\eta\eta}^{(k)}(\sigma) d\sigma, \quad \eta \in [0, kL]$$

with $U_{\eta\eta}^{(k)}(\eta) \ge 0$ on $[0, kL]$ follows

$$U_\eta^{(k)}(\eta) \le 0 \text{ on } [0, kL]. \tag{5.4}$$

Now we have for arbitrary $\alpha > 0$ the estimate (omitting arguments)

$$0 \le U_{\eta\eta}^{(k)} = p(\eta) U^k \le \alpha (U_\eta^{(k)})^2 + P$$

or

$$0 \ \le \ \frac{U_{\eta\eta}^{(k)}}{\alpha (U_\eta^{(k)})^2 + P} \ \le \ 1.$$

With (5.4) we get

$$0 \ \ge \ \frac{2\alpha U_{\eta\eta}^{(k)} U_\eta^{(k)}}{\alpha (U_\eta^{(k)})^2 + P} \ \ge \ 2\alpha U_\eta^{(k)} \qquad \text{or} \qquad \frac{d}{d\eta} \log\left\{\alpha (U_\eta^{(k)})^2 + P\right\} \ \ge \ 2\alpha U_\eta^{(k)}.$$

Integrating this inequality gives for any η_0 with $0 \le \eta_0 \le kL$

$$\int_{\eta_0}^{kL} \frac{d}{d\eta} \log\left\{\alpha (U_\eta^{(k)})^2 + P\right\} d\eta \ge 2\alpha \int_{\eta_0}^{kL} U_\eta^{(k)} d\eta$$

from which, taking into account $U^{(k)}(kL) = 0$, $U^{(k)}(\eta_0) \le 1$ and $U_\eta^{(k)}(kL)^2 \le 1/L^2$, follows

$$\log\left\{\alpha(U_\eta^{(k)}(\eta_0))^2 + P\right\} \le 2\alpha + \log\left\{\frac{\alpha}{L^2} + P\right\}.$$

So we obtain

$$\alpha(U_\eta^{(k)}(\eta_0))^2 + P \le \left\{\frac{\alpha}{L^2} + P\right\}\exp(2\alpha)$$

and, finally,

$$|U_\eta^{(k)}(\eta_0)| \le \left[\frac{\exp(2\alpha)}{L^2} + \frac{P}{\alpha}(\exp(2\alpha) - 1)\right]^{1/2}.$$

This is a bound for the first derivatives

$$M_1^{(k)} = \sup_{0\le\eta\le kL} |U_\eta^{(k)}(\eta)| \le C(P,\alpha)$$

which does not depend on k . □

We note some further properties of the solution of the boundary value problem (5.3).

Lemma 5.6. *For the solution* u *of* (5.3) *holds*

$$u_\eta(\eta) \le 0, \quad \lim_{\eta\to\infty} u_\eta(\eta) = 0, \quad u_\eta(0) = -\int_0^\infty p(y)u(y)dy, \quad u(\eta) > 0 \;\; \textit{for} \;\; \eta \ge 0.$$

We have the representation

$$u(\eta) = 1 - \int_0^\eta \left(\int_\xi^\infty p(r)u(r)\,dr\right) d\xi \tag{5.5}$$

Proof. Assume that there exists $\eta_0 \in \overline{\mathbb{R}_+}$ with $u_\eta(\eta_0) > 0$. Because of the continuity of u_η there is an $\eta_1 > \eta_0$ with $u(\eta_1) > u(\eta_0)$. From $u(\eta) \longrightarrow 0$ for $\eta \longrightarrow 0$ and the continuity of u follows the existence of an $\eta_2 > \eta_1$ with $u(\eta_2) = u(\eta_0)$. By Rolle's theorem there exists a χ with $\eta_0 < \chi < \eta_2$ and $u_\eta(\chi) = 0$. Now we have

$$u_\eta(\chi) = u_\eta(\eta_0) + \int_{\eta_0}^\chi u_{\eta\eta}d\eta = u_\eta(\eta_0) + \int_{\eta_0}^\chi p(\eta)u(\eta)d\eta > 0$$

since p, u are nonnegative. This contradiction proves the first assertion.

To prove the second assertion we remark that from $u_\eta \le 0$, $u_{\eta\eta} \ge 0$ on $\overline{\mathbb{R}_+}$ follows that $u_\eta(\eta)$ is nondecreasing and bounded as $\eta \uparrow \infty$. Hence there exists $\lim_{\eta\to\infty} u_\eta(\eta)$. If we had

$$\lim_{\eta\to\infty} u_\eta(\eta) = -\delta, \quad (\delta > 0),$$

there would exist an $\eta_0 > 0$ with

$$u_\eta(\eta) \le -\delta/2 \quad \text{for} \quad \eta \ge \eta_0.$$

Then we have for $y > \eta_0$

$$u(y) = u(\eta_0) + \int_{\eta_0}^{y} u_\eta d\eta \leq u(\eta_0) - \frac{\delta}{2}(y - \eta_0).$$

For sufficiently large y we could get $u(y) < 0$ which contradicts $0 \leq u(y) \leq 1$. So we obtain the assertion $\lim_{\eta \to \infty} u_\eta(\eta) = 0$.

Integrating the differential equation gives

$$u_\eta(\eta) - u_\eta(0) = \int_0^{\eta} u_{\eta\eta} dy = \int_0^{\eta} p(y)u(y)dy.$$

Using the just proved result the third assertion follows.

To show the positivity of u for $\eta \geq 0$ we conclude as follows. We have $u(0) = 1$, and if there were an $\eta_0 > 0$ with $u(\eta_0) = 0$, we could assume (because of the continuity of u) that $u(\eta) > 0$ for $0 \leq \eta < \eta_0$. We must have $u_\eta(\eta_0) = 0$, because (first assertion) $u_\eta(\eta) \leq 0$ and the assumption $u_\eta(\eta_0) < 0$ leads to a contradiction with $u(\eta) \geq 0$ for $\eta \geq 0$. Applying the classical uniqueness theorem to the initial value problem

$$u_{\eta\eta} = p(\eta)u, \quad u(\eta_0) = 0, \quad u_\eta(\eta_0) = 0,$$

we have $u(\eta) = 0$ in an neighbourhood $\eta_1 < \eta_0 < \eta_2$. This contradicts the construction of η_0 .

To prove (5.5) we note that

$$u_\eta(\xi) - u_\eta(N) = -\int_{\xi}^{N} u_{\eta\eta}(r)\, dr = -\int_{\xi}^{N} p(r)u(r)\, dr.$$

Using the second assertion we obtain by taking $N \longrightarrow \infty$

$$u_\eta(\xi) = -\int_{\xi}^{\infty} p(r)u(r)\, dr.$$

Integrating once more gives (5.5). □

Lemma 5.7. *Let be u, w solutions of the boundary value problems*

$$u_{\eta\eta} = p(\eta)u \quad \text{on } \mathbb{R}_+, \quad u(0) = 1, \quad \lim_{\eta \to \infty} u(\eta) = 0,$$

$$w_{\eta\eta} = q(\eta)w \quad \text{on } \mathbb{R}_+, \quad w(0) = 1, \quad \lim_{\eta \to \infty} w(\eta) = 0,$$

with $p, q \in BC(\overline{\mathbb{R}_+})$. Assume

$$p(\eta) \geq q(\eta) > 0 \quad \text{for} \quad 0 \leq \eta < \infty.$$

Then holds

$$u(\eta) \leq w(\eta), \quad 0 \leq \eta < \infty.$$

Proof. For u, w we have all the properties formulated in Lemma 5.4, Lemma 5.6. From the differential equations we get

$$wu_{\eta\eta} - uw_{\eta\eta} = (p(\eta) - q(\eta))uw$$

or

$$\frac{\partial}{\partial\eta}(wu_\eta - uw_\eta) = \frac{\partial}{\partial\eta}\left(w^2\frac{\partial}{\partial\eta}\left(\frac{u}{w}\right)\right) = (p-q)uw.$$

Integration gives

$$w^2\frac{\partial}{\partial\eta}\left(\frac{u}{w}\right) = -\int_\eta^\infty (p-q)uw\,dy \le 0$$

because of $p \ge q$, $u \ge 0$, $w \ge 0$. This shows that u/w is nonincreasing, hence

$$\frac{u(\eta)}{w(\eta)} \le \frac{u(0)}{w(0)} = 1$$

and the result follows. □

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