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Analysis for a Molten Carbonate Fuel Cell *

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Abstract

In this paper we analyze a planar model for a molten carbonate electrode of a fuel cell. The model consists of two coupled second-order ordinary differential equations, one for the concentration of the reactant gas and one for the potential. Restricting ourselves to the case of a positive reaction order in the Butler-Volmer equation, we consider existence, uniqueness, various monotonicity properties, and an explicit approximate solution for the model. We also present an iteration scheme to obtain solutions, and we conclude with a few numerical examples.

1 Introduction.

Fuel Cells convert chemical energy in gases such as H_2, CH_4 and O_2 into electrical energy through electrochemical reactions. These cells tend to be highly efficient and are thus attractive ecological alternatives for generating electrical power. The electrodes in a typical fuel cell (the anode and the cathode) have a porous structure to obtain a large reactive area per unit of geometric area and hence a high current density. In this paper we consider a simple, dual-porosity, agglomerate-type model for the porous anode and cathode of a molten carbonate fuel cell. The model, first introduced by Giner & Hunter (1969) and later extended by Yuh & Selman (1984), is based on a phenomenological treatment of mass transport, electrode kinetics and ionic conduction, combined with structural assumptions. The aim of the model is to predict and optimize electrode performance in a small differential-conversion cell.

The electrode structure is represented schematically in Figure 2. It is assumed to consist of an array of porous slabs with a microporous structure, separated by void regions (macro pores). In each slab, catalyst particles form agglomerates (metal matrices) which, under working conditions, are saturated with electrolyte. Throughout this paper, each slab is assumed to be a homogeneously distributed continuum of catalyst particles and electrolyte. When

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current is drawn from the electrodes, reactant gas diffuses horizontally across the void regions, arrives at the vertical surface of a slab, and dissolves in the electrolyte contained in the agglomerate. After diffusing a certain distance, the gas reacts electrochemically at available sites on the catalyst particles. These electrochemical reactions create an ionic current which flows through the electrolyte in the vertical z-direction of the slab, and an electron current which flows through the electrode material in the opposite direction.

Yuh & Selman consider a cylindrical geometry with micropore cylinders instead of slabs. This leads to radial diffusion through the pores. The corresponding analysis is similar but much less explicit in that the ordinary differential equations that arise cannot be directly integrated. We shall consider this case in a future study. The specific system of equations to be considered in this work are as follows:

$$(P)\begin{cases} (a) & u_{xx} = \alpha u^p f(v(z)) \quad 0 < x < 1, \quad 0 < z < 1, \\ (b) & u_x(0; v(z)) = 0 \quad 0 < z < 1, \\ (c) & u(1; v(z)) = 1 \quad 0 < z < 1, \\ (d) & v_{zz} = \beta u_x(1; v(z)) \quad 0 < z < 1, \\ (e) & v(1) = V > 0 \\ (f) & v_z(0) = 0. \end{cases} \tag{1.1}$$

For compact notation, the variables x and z are used as subscripts to denote differentiation. The derivation of this system from physical assumptions is given in Section 2. As discussed in that section, u is a dimensionless concentration, v, a dimensionless potential, and V, a reference potential. The exponent p is the *reaction order*. In general it can be positive, negative or zero. In this paper, however, we restrict ourselves to the case where $p > 0$ since this case is of most practical importance for molten carbonate fuel cells. The function $f(\cdot)$ in (1.1a) is defined by

$$f(v) := e^{\alpha_a v} - e^{-\alpha_c v} \tag{1.2}$$

where α_a and α_c are dimensionless constants (discussed below). Note that f is a smooth, strictly increasing function satisfying $f(0) = 0$. Finally α and β are dimensionless, lumped parameters (both positive).

In (1.1a-c), the variable $v(z)$ appears only as a parameter. Therefore $u(\cdot; v(z))$ for any $z \in [0, 1]$ will have the smoothness of solutions of the auxiliary boundary value problem

$$(P_1)\begin{cases} (a) & w'' = \lambda w^p \quad (w \geq 0) \quad 0 < x < 1, \\ (b) & w'(0) = 0, \\ (c) & w(1) = 1. \end{cases} \tag{1.3}$$

Comparing (1.1a) and (1.3a), one observes that $\lambda > (<)0$ corresponds to points $z \in [0, 1]$ where $v(z) > (<)0$. If Problem (P_1) has a solution w, then

$$\lambda > (<)0 \Longleftrightarrow w'(1) > (<)0. \tag{1.4}$$

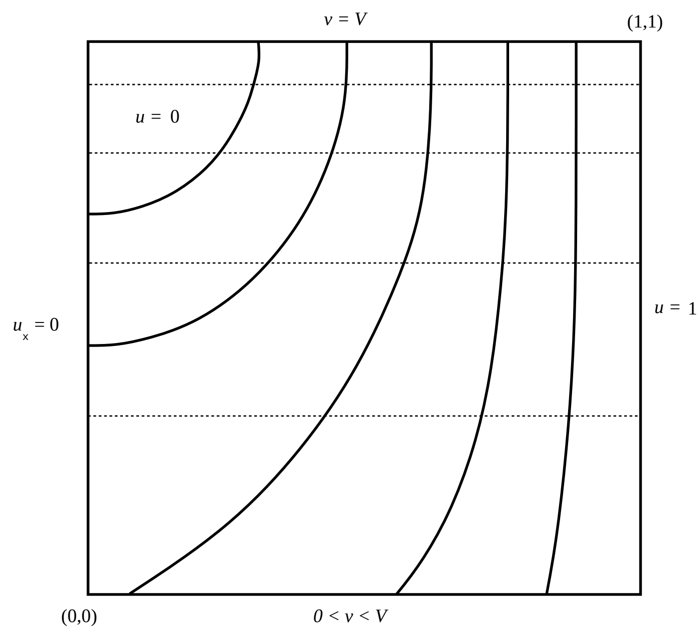

Figure 1: Schematic contour plot of the the solution (u, v). Note that v (dashed lines) is a function only of z, while u (solid lines) depends on both x and z.

Let (u, v) be a solution of Problem (P). Then using observation (1.4), one derives that

$$v > (<)0 \Longleftrightarrow v_{zz} > (<)0. \tag{1.5}$$

From this second observation and the boundary condition (1.1e), if follows that there *cannot* be a point $z_0 \in [0, 1]$ where $v(z_0) < 0$ and $v_z(z_0) = 0$, which implies that

$$v(z) \geq 0 \quad \text{and} \quad v_z(z) \geq 0 \qquad \forall z \in [0, 1]. \tag{1.6}$$

Later (in Section 5) a stronger result is proven, viz.

$$v(z) > 0 \quad \forall z \in [0, 1] \quad \text{and} \quad v_z(z) > 0 \quad \forall z \in (0, 1]. \tag{1.7}$$

These results are displayed in Figure 1 in a typical schematic contour plot of (u, v) on $[0, 1] \times [0, 1]$.

In Section 3 the solutions of Problem (P_1) are described for all $p > 0$. Because of (1.6), only the case $\lambda \geq 0$ will be considered. We show for $p \geq 1$ and $\lambda \geq 0$, or for $0 < p < 1$ and $0 \leq \lambda < \lambda(p) := 2(p+1)/(1-p)^2$, that all solutions are positive. For $0 < p < 1$ and $\lambda \geq \lambda(p)$, the solutions become zero in part of the domain, i.e., so-called *deadcore* solutions arise. Such a deadcore is also displayed in Figure 1. There the upper boundary potential, V, is sufficiently large so that $u \equiv 0$ in the region near $(0, 1)$. For $p < 0$, Problem (P_1) has been studied by Levine (1989) who presents a general survey of results for this parameter range. He shows that a bifurcation occurs for each $p < 0$ and that for $-1 < p < 0$, non-classical deadcore solutions exist for $\lambda \geq \lambda(p)$.

In Section 4 several monotonicity results are proven, and then these results are used to prove uniqueness for Problem (P). In addition this section contains an explicit approximation for the potential v which is valid when the concentration u has a deadcore. In Section 5 the existence of smooth solutions is established for all parameter values using a Schauder fixed-point argument. Finally Section 6 presents an alternative existence proof using a monotone iteration scheme and gives some computational results. As is the case for the approximation, however, this iteration scheme does not work for all parameter values.

2 Physical Derivation.

In this section, we discuss the physical basis of the fuel cell model under study. To set up the mathematical model, the following assumptions are made:

1. The electrode consists of a number of porous slabs containing catalyst particles, and the agglomerate (metal matrix) is flooded with electrolyte. As shown in Figure 2, each slab has constant thickness $2L$ and height H with $L/H \ll 1$. Each slab is assumed uniform in the direction perpendicular to Figure 2 making a two-dimensional description possible. (To simplify notation, the perpendicular width of the slab is taken to be unity.)

2. The electrolyte and the catalyst in the agglomerate slabs are homogeneously mixed and form a quasicontinuum.

3. Only one reactant gas (dissolved oxygen) is present. In this respect the present work follows Giner & Hunter. Yuh & Selman extended the model to allow for more reacting species.

4. The Butler-Volmer equation as expressed in (2.1) below is a suitable representation of the electrode kinetics. In particular, the local current density is directly proportional to a power p (positive in this paper) of the local reactant concentration. The transfer coefficients α_a and α_c are constant.

5. The current flows in the slab only in the z-direction and is uniformly distributed over each cross-section. Hence the potential gradient with respect to x can be disregarded. We also disregard the concentration gradient in the z-direction for the transport equation.

6. The system is isothermal, isobaric and at steady state.

7. All physical parameters here are constant.

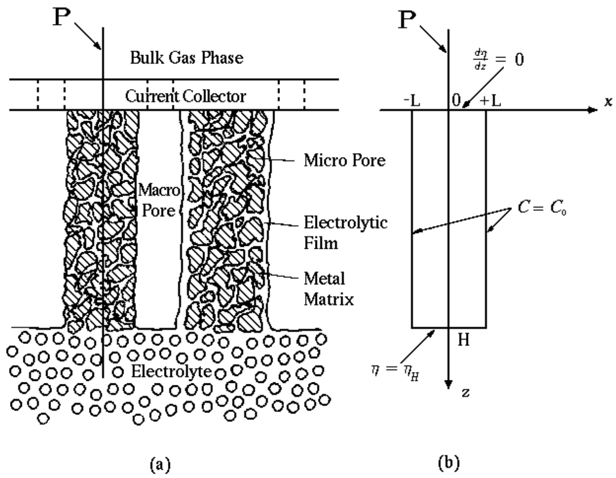

Figure 2: Schematic representation of the model.

Let $i = i(x, z)$ be the local current density, i.e., the current per unit area into the slab at the point (x, z). This current density is given by the Butler-Volmer equation:

$$i = i_0 \left(\frac{C(x,z)}{C_0} \right)^p [\exp(\alpha_a \eta(z) F/RT) - \ \exp(-\alpha_c \eta(z) F/RT)] \tag{2.1}$$

where the various quantities are

$C(x,z)$	:	concentration of dissolved oxygen,
C_0	:	reference concentration,
p	:	reaction order,
α_i	:	transfer coefficients for $i = a, c$ (both positive and both of order unity),
F	:	Faraday constant (9.65×10^4 Coulombs/mole),
R	:	gas constant (8.32 joules/mole K),
T	:	temperature,
$\eta(z)$	:	overpotential as a function of height z.

Steady state species balance incorporating diffusion and reaction is given by

$$D\frac{\partial^2 C}{\partial x^2} = \frac{s\tilde{A}i}{nF}, \quad -L < x < L, \quad 0 < z < H \tag{2.2}$$

where

D	:	effective diffusivity of the reactant gas in the electrolyte affected by the microporosity and the tortuosity,
$\tilde{A}$	:	specific surface area,
s	:	stoichiometric constant,
n	:	number of electrons involved in the electrode reactions.

One more equation is needed to determine the overpotential. It comes from the current balance equation. By Ohm's law,

$$\frac{d\eta}{dz} = -\frac{j(z)}{2L\kappa} \tag{2.3}$$

where

$j(z)$	:	total *ionic* current at height z,
κ	:	effective electrolytic conductivity.

Current balance then yields

$$-\frac{dj}{dz}(z) = \int_{-L}^{+L} \tilde{A} i(x,z)dx \tag{2.4}$$

and consequently

$$\frac{d^2\eta}{dz^2} = \frac{\tilde{A}}{2L\kappa}\int_{-L}^{+L} i(x,z)dx, \quad 0 < z < H. \tag{2.5}$$

Now combining (2.2) and (2.5), and noting that the problem is symmetric about $x = 0$, one obtains

$$\frac{d^2\eta}{dz^2} = \frac{DnF}{sL\kappa}\frac{\partial C}{\partial x}(L,z), \quad 0 < z < H. \tag{2.6}$$

The problem at hand then is to solve the coupled set of equations (2.1), (2.2) and (2.6) subject to the boundary conditions

$$C(\pm L, z) = C_0, \quad 0 < z < H, \tag{2.7}$$

and

$$\begin{array}{ll} (a) & \eta(H) = \eta_H > 0, \\ (b) & \frac{d\eta}{dz}(0) = 0 \end{array} \tag{2.8}$$

where η_H is the prescribed potential (or polarization).

Next we scale the problem by defining dimensionless variables and parameters: Let

$$u \equiv \frac{C}{C_0}, \quad x^* \equiv \frac{x}{L}, \quad z^* \equiv \frac{z}{H}$$

and

$$v \equiv \frac{F\eta}{RT}, \quad V \equiv \frac{F\eta_H}{RT}.$$

Also define the lumped parameters

$$\alpha \equiv \frac{L^2 i_0 s\tilde{A}}{DC_0 nF}, \quad \beta \equiv \frac{DnF^2C_0H^2}{RTsL^2\kappa}. \tag{2.9}$$

Writing (2.1), (2.2), (2.6)-(2.8) in terms of these dimensionless variables and parameters and dropping the asterisks leads to the compact system of equations (1.1). Some typical values for the constants in (2.9) are given by Giner and Hunter. For $H = 10^{-2}$ cm, $L = 10^{-4}$ cm and $i_o = 10^{-8}A/\mathrm{cm}^2$, those values imply that $\alpha \simeq 10^{-2}$ and $\beta \simeq 10^{-1}$. For the scaled potential, $V \simeq 10$ when $\eta_H = 300$ mV.

3 Preliminaries: the problem auxiliary (P_1).

In this section we consider solutions of Problem (P_1) for $p > 0$ and $\lambda \geq 0$. The case $\lambda = 0$ implies the trivial solution $w(x) \equiv 1$ for $0 \leq x \leq 1$. We therefore concentrate on solutions for which $\lambda > 0$. From the differential equation and the left boundary condition (1.3a,b), it follows that w is smooth (at least C^2) and satisfies

$$w'' > 0 \text{ and } w' > 0 \text{ on } \{x \in (0,1) : w(x) > 0\}. \tag{3.1}$$

There are two types of solutions of interest: positive solutions and deadcore solutions where $w = 0$ in part of the domain [see for example Bandle, Sperb & Stakgold (1984)]. In view of (3.1), the corresponding deadcore, i.e. the set where $w = 0$, must be an interval of the form $[0, x_0]$ with $x_0 \in [0, 1)$.

Assume now that w is any solution. Multiplying (1.3a) by w' and integrating yields

$$\frac{1}{2}(w')^2 = \frac{\lambda}{p+1}\left(w^{p+1} - w_0^{p+1}\right) \tag{3.2}$$

with $w_0 = w(0) > 0$ for positive solutions and $w_0 = 0$ for deadcore solutions. Rearranging and integrating once more leads to the expression

$$\int_{w(x)}^{1} \frac{ds}{\{s^{p+1} - w_0^{p+1}\}^{1/2}} = \sqrt{\frac{2\lambda}{p+1}}(1-x) \quad \text{for } 0 \leq x \leq 1. \tag{3.3}$$

Explicitly evaluating this integral with $w_0 = 0$ yields the following form for the deadcore solutions provided that $0 < p < 1$ and $\lambda \geq \lambda(p) := 2(p+1)/(1-p)^2$:

$$w(x) = \begin{cases} 0 & 0 \leq x \leq x_0 \\ \left(1 - \frac{1-p}{2}\sqrt{\frac{2\lambda}{p+1}}(1-x)\right)^{\frac{2}{1-p}} & x_0 < x \leq 1 \end{cases} \tag{3.4}$$

where

$$x_0 = 1 - \frac{2}{1-p}\sqrt{\frac{p+1}{2\lambda}}.$$

To find the positive solutions, consider (3.3) at $x = 0$. Define

$$F_p(w_0) := \int_{w_0}^{1} \frac{ds}{\{s^{p+1} - w_0^{p+1}\}^{1/2}} = \sqrt{\frac{2\lambda}{p+1}}. \tag{3.5}$$

Whenever one can solve this equation for a positive w_0, then using that value of w_0, expression (3.3) defines a solution of Problem (P_1). Thus we need to investigate the function $F_p(w_0)$ for $0 < w_0 \le 1$. For this analysis, it is convenient to write $F_p(w_0)$ as

$$F_p(w_0) = w_0^{\frac{1-p}{2}} \int_1^{w_0^{-1}} \frac{ds}{\{s^{p+1} - 1\}^{1/2}}. \tag{3.6}$$

First we consider the behavior as $w_0 \downarrow 0$. If $p > 1$ the integral converges but $w_0^{\frac{1-p}{2}} \to \infty$, and if $p = 1$ the integral diverges. Hence

$$\lim_{w_0 \downarrow 0} F_p(w_0) = +\infty \quad \forall p \ge 1. \tag{3.7}$$

If $0 < p < 1$ the integral diverges, but now $w_0^{\frac{1-p}{2}} \to 0$. Using the l'Hôpital rule, one finds

$$\begin{aligned} \lim_{w_0 \downarrow 0} F_p(w_0) &= \lim_{w_0 \downarrow 0} \frac{1}{w_0^{\frac{p-1}{2}}{}_0} \int_1^{w_0^{-1}} \frac{ds}{\{s^{p+1} - 1\}^{1/2}} \\ &= \frac{2}{1-p} \lim_{w_0 \downarrow 0} \frac{1}{\{1 - w_0^{p+1}\}^{1/2}} = \frac{2}{1-p}. \end{aligned} \tag{3.8}$$

Turning our attention to other facts regarding F_p, from (3.6) we see that $F_p \in C^\infty((0,1))$, and differentiation yields

$$F_p'(w_0) = \frac{1}{w_0}\{\frac{1-p}{2} F_p(w_0) - \frac{1}{\{1 - w_0^{p+1}\}^{1/2}}\}, \quad 0 < w_0 < 1. \tag{3.9}$$

Using

$$\lim_{w_0 \uparrow 1} F_p(w_0) = 0 \quad \forall p > 0 \tag{3.10}$$

in (3.9), one arrives at

$$\lim_{w_0 \uparrow 1} F_p'(w_0) = -\infty \quad \forall p > 0. \tag{3.11}$$

Moreover for $p \ge 1$, (3.9) implies

$$F_p'(w_0) < -\frac{1}{w_0\{1 - w_0^{p+1}\}^{1/2}} < 0, \quad 0 < w_0 < 1. \tag{3.12}$$

Combining (3.7), (3.10) and (3.12), we find that for every $p \geq 1$ and for every $\lambda > 0$, equation (3.5) has a unique positive solution $w_0(\lambda; p)$. Setting $w_0 = w_0(\lambda; p)$ in expression (3.3) implies that Problem (P_1) has a unique positive solution for p and λ in these parameter ranges. Also the smoothness of F_p and (3.12) imply that $w_0(\cdot; p) \in C^\infty((0,\infty)) \cap C([0,\infty))$.

Finally, we finish the case $0 < p < 1$ by constructing an upper bound for F_p and using this bound to show again that $F_p' < 0$. Substituting the estimate

$$u^{p+1} - w_0^{p+1} > (u - w_0)^{p+1} \quad \text{for} \quad 0 < w_0 < u \leq 1$$

into (3.5) gives the desired upperbound:

$$F_p(w_0) < \int_{w_0}^{1} \frac{ds}{\{s - w_0\}^{\frac{p+1}{2}}} = \frac{2}{1-p}(1 - w_0)^{\frac{1-p}{2}}. \tag{3.13}$$

Hence from (3.9),

$$F_p'(w_0) < \frac{1}{w_0}\left\{(1 - w_0)^{\frac{1-p}{2}} - \frac{1}{\{1 - w_0^{p+1}\}^{1/2}}\right\} < 0 \tag{3.14}$$

for $0 < w_0 < 1$, and so F_p is also strictly decreasing when $0 < p < 1$. To illustrate this result, Figure 3 shows the function $F_{1/2}(w_0)$ for $0 \leq w_0 \leq 1$. It was constructed using a numerical integration routine from the computer algebra package *Mathematica*. Combined with (3.8) and (3.10), it follows from (3.14) that for every $0 < p < 1$ and $0 < \lambda < \lambda(p)$, equation (3.5) has again a unique positive solution $w_0(\lambda; p)$, leading to a unique positive solution of Problem (P_1) (again after setting $w_0 = w_0(\lambda; p)$ in expression (3.3)). And again the smoothness of F_p and (3.14) imply that $w_0(\cdot; p) \in C^\infty((0, \lambda(p))) \cap C([0, \lambda(p)])$.

Lemma 3.1 summarizes all of the results obtained so far in this section:

Lemma 3.1 For every $p > 0$ and $\lambda > 0$, Problem (P_1) has a unique solution $w(x; \lambda, p)$ which is strictly increasing and convex at points where $w > 0$. The solution is strictly positive ($w(0; \lambda, p) > 0$) if $p \geq 1$, or if $0 < p < 1$ and $0 < \lambda < \lambda(p)$. Deadcore solutions with $w(0; \lambda, p) = 0$ arise in the case $0 < p < 1$ and $\lambda \geq \lambda(p)$. The later solutions can be written explicitly and are given by (3.4).

Because the derivative of u with respect to x, at $x = 1$, is used in the right hand side of equation (1.1d), it is necessary to investigate for every $p > 0$ the function $\Phi_p : [0,\infty) \to [0,\infty)$ defined through Problem (P_1) by

$$\Phi_p(\lambda) := w'(1; \lambda, p), \quad \lambda \geq 0. \tag{3.15}$$

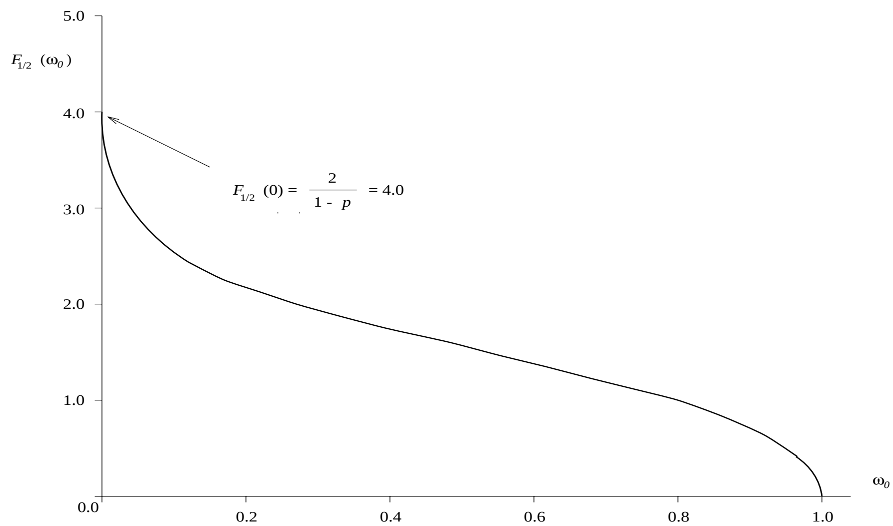

Figure 3: Numerical evaluation of the function $F_{1/2}(w_0)$, $0 \le w_0 \le 1$.

Proposition 3.2 For every $p > 0$,

(i) Φ_p is strictly increasing on $[0, \infty)$;

(ii) $\Phi_p(\lambda) \le \sqrt{\frac{2\lambda}{p+1}}$ for all $\lambda \ge 0$ and $\lim\limits_{\lambda\to\infty} \frac{1}{\sqrt{\lambda}} \Phi_p(\lambda) = \sqrt{\frac{2}{p+1}}$. In particular $\Phi_p(\lambda) = \sqrt{\frac{2\lambda}{p+1}}$ for $0 < p < 1$ and $\lambda \ge \lambda(p)$;

(iii) $\Phi_p \in C^1([0, \infty))$.

Proof. Using expression (3.2), one can write

$$\Phi_p(\lambda) = \sqrt{\frac{2\lambda}{p+1}} \{1 - w_0^{p+1}(\lambda; p)\}^{1/2}. \tag{3.16}$$

The properties of the function F_p discussed above imply that $w_0(0; p) = 1$ for all $p > 0$ and

$w_0(\cdot; p)$ is strictly decreasing on $\begin{cases} [0, \infty) & \text{with} \quad w_0(\infty; p) = 0 \quad \text{if} \quad p \ge 1. \\ [0, \lambda(p)] & \text{with} \quad w_0(\lambda(p), p) = 0 \quad \text{if} \quad 0 < p < 1. \end{cases}$

Moreover, $w_0(\lambda; p) = w(0; \lambda, p) = 0$ for $0 < p < 1$ and $\lambda \ge \lambda(p)$. These observations, applied to $w_0(\lambda; p)$ in (3.16), prove (i) and (ii). To prove (iii), we first note that the smoothness properties of $w_0(\lambda;p)$ imply

$$\Phi_p \in C([0,\infty)) \cap C^\infty((0,\infty)) \quad \text{for} \quad p \geq 1$$

and

$$\Phi_p \in C([0,\infty)) \cap C^\infty((0,\infty)\backslash\{\lambda(p)\}) \quad \text{for} \quad 0 < p < 1.$$

Thus it remains to verify differentiability at 0^+ and at $\lambda(p)$. To this end, we write (3.5) as

$$\{F_p(w_0(\lambda;p))\}^2 = \frac{2\lambda}{p+1}, \quad \text{with} \quad 0 < w_0(\lambda;p) < 1.$$

Differentiation with respect to λ gives

$$F_p(w_0)F_p'(w_0)\frac{dw_0(\lambda;p)}{d\lambda} = \frac{1}{p+1}. \tag{3.17}$$

From (3.9) we obtain

$$F_p(w_0)F_p'(w_0) = \frac{1-p}{2w_0}F_p^2(w_0) - \frac{F_p(w_0)}{w_0\{1-w_0^{p+1}\}^{1/2}}.$$

But using l'Hôpital and again (3.9) yields

$$\lim_{w_0\uparrow 1}\frac{F_p(w_0)}{\{1-w_0^{p+1}\}^{1/2}} = \lim_{w_0\uparrow 1}\frac{-2F_p'(w_0)\{1-w_0^{p+1}\}^{1/2}}{(p+1)w_0^p} = \frac{2}{1+p}.$$

Hence

$$\lim_{w_0\uparrow 1} F_p(w_0)F_p'(w_0) = -\frac{2}{1+p},$$

and thus

$$\lim_{\lambda\downarrow 0}\frac{dw_0(\lambda;p)}{d\lambda} = \frac{dw_0(0^+;p)}{d\lambda} = -\frac{1}{2}.$$

This implies

$$\begin{aligned}\lim_{\lambda\downarrow 0}\Phi_p'(\lambda) &= \lim_{\lambda\downarrow 0}\Bigg[\tfrac{1}{\sqrt{2(p+1)}}\left\{\tfrac{1-w_0^{p+1}(\lambda;p)}{\lambda}\right\}^{1/2} - \\ &\qquad \sqrt{\tfrac{p+1}{2}}\left\{\tfrac{\lambda}{1-w_0^{p+1}(\lambda;p)}\right\}^{1/2} w_0^p(\lambda;p)\tfrac{dw_0(\lambda;p)}{d\lambda}\Bigg] \\ &= 1 \quad (= \Phi_p'(0^+)).\end{aligned} \tag{3.18}$$

To prove that Φ_p is differentiable at $\lambda = \lambda(p)$ (for $0 < p < 1$), we use again (3.9) which we now write as

$$F_p'(w_0) = \frac{1-p}{2}\left\{\frac{F_p(w_0)-F_p(0)}{w_0}\right\} + \frac{1}{w_0}\left\{1 - \frac{1}{\{1-w_0^{p+1}\}^{1/2}}\right\}. \tag{3.19}$$

From this expression, it follows that either $\lim_{w_0\downarrow 0} F_p'(w_0) = 0$ or that this limit does not exist. Differentiating (3.9) yields

$$w_0 F_p''(w_0) = \left\{ \frac{1-p}{2} - 1 \right\} F_p'(w_0) - \frac{p+1}{2} w_0^p \left\{ 1 - w_0^{p+1} \right\}^{-3/2}. \tag{3.20}$$

From (3.14)

$$F_p'(w_0) < \frac{1}{w_0} \left\{ 1 - \frac{1-p}{2} w_0 - 1 \right\} = -\frac{1-p}{2}.$$

Substitution into (3.20) yields

$$w_0 F_p''(w_0) > \left(\frac{1+p}{2} \right) \left(\frac{1-p}{2} \right) - \frac{p+1}{2} w_0^p \left\{ 1 - w_0^{p+1} \right\}^{-3/2} > 0$$

with $w_0 \in (0, \delta)$ for some $\delta > 0$. Thus

$$F_p'(w_0) \text{ decreases monotonically as } w_0 \downarrow 0.$$

Then in view of (3.19), the only possibility is that

$$\lim_{w_0\downarrow 0} F_p'(w_0) = -\infty \quad \text{for } 0 < p < 1. \tag{3.21}$$

Combining (3.17), (3.21) and (3.8) yields

$$\lim_{\lambda\uparrow\lambda(p)} \frac{dw_0(\lambda; p)}{d\lambda} = 0.$$

which implies, from (3.16), the desired differentiability of Φ_p at $\lambda(p)$. □

4 Uniqueness, monotonicity and an approximate solution.

Assume for some

$$v \in C^2([0,1])$$

and

$$u(\cdot; v(z)) \in C^2([0,1]) \quad \text{for all} \quad 0 \le z \le 1$$

that (u, v) is a solution of Problem (P). Here we demonstrate that such a solution is unique and that it satisfies certain monotonicity properties. In addition for the deadcore case where u can be written explicitly, we construct an explicit approximation for v. The crucial property used in the monotonicity proofs is the monotonicity of the function Φ_p (see Proposition 3.2 (i)). The basic tool is the following comparison lemma.

Lemma 4.1 For $i = 1, 2$, let $w_i \in C^2([0,1])$ satisfy

$$\begin{cases} w_i'' = g_i(w_i) & 0 < z < 1, \\ w_i'(0) = 0, & w_i(1) = 1, \end{cases}$$

where the functions g_i are nondecreasing and $g_1 \geq g_2$ on $\mathbb{R}$. Then $w_1 \leq w_2$ on $[0,1]$.

Proof. Subtract the two equations and multiply the difference by $(w_1 - w_2)_+ = \max\{(w_1 - w_2), 0\}$. Integrating the result by parts gives

$$\int_{\{w_1 > w_2\}} \Big[\{(w_1 - w_2)'\}^2 + \{g_1(w_1) - g_1(w_2)\}(w_1 - w_2) + \{g_1(w_2) - g_2(w_2)\}(w_1 - w_2) \Big] dz = 0.$$

Since all three terms are nonnegative on $\{w_1 > w_2\}$, we must have

$$\{w_1 > w_2\} = \emptyset \quad \text{or} \quad w_1 \leq w_2 \quad \text{on } [0,1].$$

□

To use this lemma, we define (see also (3.15))

$$\Psi(v) := \beta \Phi_p(\alpha f(v)) \quad (v \geq 0) \tag{4.1}$$

and write (1.1 $d-f$) as

$$(P_2) \begin{cases} v'' = \Psi(v) & 0 < z < 1, \\ v'(0) = 0, \\ v(1) = V. \end{cases}$$

Problem (P_2) is in fact equivalent to Problem (P), and we can prove

Theorem 4.2 Problem (P) has at most one solution (u, v).

Proof. Suppose on the contrary that there are two pairs (u_1, v_1) and (u_2, v_2) that satisfy Problem (P). Since

$$u_{ix}(1; v_i(z)) = \Psi(v_i(z)) \quad \text{for} \quad 0 \leq z \leq 1,$$

we note that both v_1 and v_2 are solutions of Problem (P_2). Applying Lemma 4.1 gives directly $v_1 = v_2 (=: v)$ on $[0,1]$ and consequently using Lemma 3.1, $u_1(\cdot; v(z)) = u_2(\cdot; v(z))$ on $[0,1]$ for every $z \in [0,1]$. □

Next we consider the monotone dependence of the solutions with respect to the parameters α, β, p and V from in Problem (P).

Theorem 4.3 For $i = 1, 2$, let (u_i, v_i) denote the solution of Problem (P) corresponding to the parameter set $\{\alpha_i, \beta_i, p_i, V_i\}$. In each of the following statements we vary only one parameter; the remaining three are fixed. Then we have

(i) $0 < \alpha_1 < \alpha_2 < \infty$ implies $v_1 \geq v_2$ on $[0, 1]$;

(ii) $0 < \beta_1 < \beta_2 < \infty$ implies $v_1 \geq v_2$ on $[0, 1]$ and $u_1(\cdot; v_1(z)) \leq u_2(\cdot; v_2(z))$ on $[0, 1]$ for each $0 \leq z \leq 1$;

(iii) $0 < p_1 < p_2 < \infty$ implies $v_1 \leq v_2$ on $[0, 1]$;

(iv) $0 < V_1 < V_2 < \infty$ implies $v_1 < v_2$ on $[0, 1]$ and $u_1(\cdot; v_1(z)) \geq u_2(\cdot; v_2(z))$ on $[0, 1]$ for each $0 \leq z \leq 1$.

Proof.

(i) Let
$$\Psi_i(v) := \beta\Phi_p(\alpha_i f(v)) \text{ for } v \geq 0 \text{ and } i = 1, 2.$$
The monotonicity of Φ_p and $f(v) \geq 0$ imply $\Psi_1(v) \leq \Psi_2(v)$ for all $v \geq 0$. Since both v_1 and v_2 satisfy Problem (P_2), with in the right hand side Ψ_1 and Ψ_2 respectively, we obtain $v_1 \geq v_2$ on $[0, 1]$ after applying Lemma 4.1. In this case we have no information about sign $(\alpha_1 f(v_1(z)) - \alpha_2 f(v_2(z)))$, except near $z = 0$. Therefore no statement can be given about sign $(u_1 - u_2)$ which holds for all $z \in [0, 1]$.

(ii) Let
$$\Psi_i(v) := \beta_i\Phi_p(\alpha f(v)) \text{ for } v \geq 0 \text{ and } i = 1, 2.$$
As under (i) one shows that $v_1 \geq v_2$ on $[0, 1]$. Here we know that $\alpha f(v_1(z)) \geq \alpha f(v_2(z))$ and consequently $u_1(\cdot; v_1(z)) \leq u_2(\cdot; v_2(z))$ on $[0, 1]$ for each $z \in [0, 1]$ (again applying Lemma 4.1, now to the boundary value problem $(1.1a - c)$).

(iii) Let
$$\Psi_i(v) := \beta\Phi_{p_i}(\alpha f(v)) \text{ for } v \geq 0 \text{ and } i = 1, 2.$$
First we apply Lemma 4.1 to Problem (P_1). This gives $w(\cdot; \lambda, p_1) \leq w(\cdot; \lambda, p_2)$ on $[0, 1]$ and therefore $w'(1; \lambda, p_1) \geq w'(1; \lambda, p_2)$. From this $\Psi_1(v) \geq \Psi_2(v)$ follows. Then proceed as under (i).

(iv) The inequality $v_1 \leq v_2$ on $[0, 1]$ follows from a similar argument as used in the proof of Lemma 4.1. To prove strict inequality we argue by contradiction. Suppose there exists $z_0 \in [0, 1]$ where $v_1(z_0) = v_2(z_0)(=: a)$. Because $v_1 \leq v_2$ we also must have $v_1'(z_0) = v_2'(z_0)(=: b)$. The smoothness of Ψ guarantees that the initial value problem
$$\begin{cases} v'' = \Psi(v) & z > z_0 \\ v(z_0) = a \quad , & v'(z_0) = b \end{cases}$$

has a unique solution. This contradicts $v_1(1) = V_1 < V_2 = v_2(1)$. The inequality for the concentrations u_i follows as under (ii). □

A small modification of the above arguments shows that many of the inequalities are strict. We have

Corollary 4.4

(i) $0 < \alpha_1 < \alpha_2 < \infty$ implies $v_1 > v_2$ on $[0, 1)$ and $v_1'(1) < v_2'(1)$,

(ii) $0 < \beta_1 < \beta_2 < \infty$ implies $v_1 > v_2$ on $[0, 1)$ and $v_1'(1) < v_2'(1)$,

(iii) $0 < p_1 < p_2 < \infty$ implies $v_1 < v_2$ on $[0, 1)$ and $v_1'(1) > v_2'(1)$.

Finally in the deadcore case, we derive an explicit set of bounds on the function $v(z)$. In principal, these bounds could be used to construct an existence proof for this case, but instead a different, more general approach will be used to prove existence in the next section. The bounds are interesting in their own right, however, because they give an explicit approximate solution which is accurate for a significant parameter range. Using the explicit deadcore solution for u given for the auxiliary problem in (3.4), Eqn. (1.1d) becomes

$$v_{zz} = \beta \left(\frac{2\alpha f(v(z))}{p+1} \right)^{1/2} \qquad 0 < z < 1. \tag{4.2}$$

where again $f(v) := e^{\alpha_a v} - e^{-\alpha_c v}$. Since v is an increasing function, and since the value of v at the top, V, may be 10 or larger while $\alpha_i \simeq 1$, it is reasonable to construct bounds on v_{zz} by replacing $e^{-\alpha_c v}$ with either $e^{-\alpha_c v(0)}$ or $e^{-\alpha_c V}$. These bounds can then be integrated twice to obtain the following result:

Theorem 4.5 For deadcore solutions, the potential satisfies

$$v_0 - \frac{4}{\alpha_a} \ln \left[\cos(\frac{c_0 \alpha_a}{4} e^{\alpha_a v_0/4} z) \right] \le v(z) \le v_0 - \frac{4}{\alpha_a} \ln \left[\cos(\frac{C \alpha_a}{4} e^{\alpha_a v_0/4} z) \right]$$

where $v_0 \equiv v(0)$ and $c_0 \equiv c(v_0) \le C \equiv c(V)$ with

$$c(\cdot) := 2\sqrt{\beta/\alpha_a} \left(\frac{2\alpha}{p+1} \right)^{1/4} \left(1 - e^{-(\alpha_a + \alpha_c)(\cdot)} \right)^{1/4} .$$

In addition, setting $z = 1$, one finds that v_0 satisfies

$$V + \frac{4}{\alpha_a} \ln \left[\cos(\frac{C \alpha_a}{4} e^{\alpha_a v_0/4}) \right] \le v_0 \le V + \frac{4}{\alpha_a} \ln \left[\cos(\frac{c_0 \alpha_a}{4} e^{\alpha_a v_0/4}) \right]$$

To see that either bound in Theorem 4.5 is in fact a good approximation, consider the typical parameter values discussed in Section 2: $V = 10$, $\alpha_a =$

$\alpha_c = 1$, $p = 1/2$, $\alpha = 0.01$ and $\beta = 0.1$. These values satisfy for all $z \in [0,1]$ the requirement discussed in Section 3 for the formation of a deadcore in u, viz.

$$\frac{2(p+1)}{(1-p)^2} \leq \alpha f(v(z)).$$

Plugging these parameter values into a numerical package (*Maple V* was used here), one finds that v_0 lies in the range $9.347056686 \leq v_0 \leq 9.347056688$, and that $c_0 = 0.2149139860$ and $C = 0.2149139862$. And indeed this sort of accuracy should be expected as long as the value of v_0 does not become to close to zero.

5 Existence.

In Section 3 we discussed the solvability of Problem (P_1) for any given $\lambda \geq 0$ and $p > 0$. From the results obtained there, it follows that the boundary value problem (1.1a-c) has a unique solution $u(\cdot; v(z))$ for any $z \in [0,1]$ and any $v : [0,1] \to [0,\infty)$. Moreover the function $\Psi : [0,\infty) \to [0,\infty)$, defined by (4.1) and (3.15), i.e.

$$\Psi(v(z)) = \beta\Phi_p(\alpha f(v(z))) = \beta u_x(1; v(z)) \quad \text{for } v \geq 0,$$

satisfies

$$\begin{aligned}
&\Psi \in C^1([0,\infty)),\\
&\Psi(0) = 0,\\
&\Psi'(v(z)) > 0 \text{ for all } v \geq 0.
\end{aligned}$$

It remains to find a nonnegative potential v which satisfies the boundary value problem (1.1d-f) for any $V > 0$. For the deadcore case, the classical bounds given in Theorem 4.5 essentially prove the existence of such a potential. For the general problem, however, where no explicit formula for the concentration u is available, such bounds are more difficult to arrive at. Therefore we turn to a functional-analytic approach using a Schauder fixed-point argument to prove a general existence result.

For this purpose, we introduce the function

$$h(z) := V - v(z) \quad \text{for } 0 \leq z \leq 1 \tag{5.1}$$

which should satisfy

$$(\tilde{P}_2) \left\{ \begin{array}{ll} -h'' = \Psi(V-h) \quad 0 < z < 1 & , \\ h'(0) = 0, \quad h(1) = 0 & . \end{array} \right.$$

Because of the homogeneous boundary conditions, we can use the Green's function

$$G(z;s) = \left\{ \begin{array}{ll} 1-s & 0 \leq z \leq s \\ 1-z & s < z \leq 1 \end{array} \right.$$

to recast Problem $(\tilde{P}_2)$ as a fixed-point problem:

$$(FP)\begin{cases} \text{Find } h:[0,1]\to[0,V] \text{ such that for all } 0\le z\le 1 \\ h(z)=\int_0^1 G(z;s)\Psi(V-h(s))ds \quad (=: Th(z)). \end{cases} \tag{5.2}$$

To show the existence of a solution of Problem (FP), we use the following lemma (for a proof see Gilbarg & Trudinger (1977)):

Lemma 5.1 (Schauder). Let Σ be a closed, convex set in a Banach space B and let $J:\Sigma\to\Sigma$ be continuous with $J(\Sigma)$ precompact. Then J has a fixed-point, i.e. $Jx=x$ for some $x\in\Sigma$.

Let

$$\Sigma=\{h\in C([0,1]):0\le h\le V\},$$

and define the map $T_0:\Sigma\to\Sigma$ by

$$T_0h(z):=\min\{V,Th(z)\} \text{ for } h\in\Sigma \text{ and } z\in[0,1]. \tag{5.3}$$

Below we prove two propositions which allow us to apply Lemma 5.1.

Proposition 5.2 T_0 is continuous.

Proof. Let $r,t\in\Sigma$. Then

$$|(T_0r-T_0t)(z)|=\begin{cases} 0 & z\in\{Tr\ge V\} & \cap & \{Tt\ge V\} \\ V-Tt(z)\le(Tr-Tt)(z) & z\in\{Tr\ge V\} & \cap & \{Tt<V\} \\ V-Tr(z)\le(Tt-Tr)(z) & z\in\{Tr<V\} & \cap & \{Tt\ge V\} \\ |(Tr-Tt)(z)| & z\in\{Tr<V\} & \cap & \{Tt<V\} \end{cases}$$

Hence for all $0\le z\le 1$

$$\begin{aligned} |(T_0r-T_0t)(z)| &\le |(Tr-Tt)(z)| \\ &\le \int_0^1 G(z;s)|\Psi(V-r(s))-\Psi(V-t(s))|ds \\ &\le C\,\|r-t\|_\infty \end{aligned}$$

where $C:=\max\limits_{0\le\zeta\le V}|\Psi'(\zeta)|$. Consequently

$$\|T_0r-T_0t\|_\infty\le C\|r-t\|_\infty.$$

□

Proposition 5.3 $T_0(\Sigma)$ is precompact.

Proof. Let $0 \le a < b \le 1$ and $h \in \Sigma$. Then

$$\begin{aligned} Th(a) - Th(b) &= \textstyle\int_0^1 \{G(a;s) - G(b;s)\}\Psi(V - h(s))ds \\ &= (b-a)\textstyle\int_0^a \Psi(V - h(s))ds + \int_a^b (b-s)\Psi(V-h(s))ds. \end{aligned}$$

Hence

$$0 \le Th(a) - Th(b) \le \frac{1}{2}\Psi(V)(b^2 - a^2). \tag{5.4}$$

This implies that for the operator T_0,

$$0 \le T_0h(a) - T_0h(b) = \begin{cases} Th(a) - Th(b) & \text{if} \quad Th(a) < V \\ V - Th(b) & \text{if} \quad Th(a) \ge V,\ Th(b) < V \\ 0 & \text{if} \quad Th(b) \ge V, \end{cases}$$

and again we have

$$0 \le T_0h(a) - T_0h(b) \le Th(a) - Th(b). \tag{5.5}$$

Combining (5.4) and (5.5) gives that

$$\{T_0h\}_{h\in\Sigma} \text{ is equicontinuous and bounded.}$$

The precompactness now follows from the Arzela-Ascoli theorem. $\square$.

Hence there exists $\hat{h} \in \Sigma$ such that

$$\hat{h} = T_0\hat{h}\ , \quad \text{where} \quad \hat{h} \quad \text{is monotonically decreasing on } [0,1]. \tag{5.6}$$

Next we must show that $\hat{h}(z) < V$ for $0 \le z < 1$. Suppose not. Then for some $0 \le z_0 < 1$,

$$\hat{h}(z) = \begin{cases} V & \text{for} \quad 0 \le z \le z_0 \\ \in (0,V) & \text{for} \quad z_0 < z < 1 \\ 0 & \text{for} \quad z = 1. \end{cases}$$

Clearly

$$\hat{h}(z) = T\hat{h}(z) \quad \text{for} \quad z_0 \le z \le 1,$$

and thus

$$T\hat{h}(z_0) = V.$$

If $z_0 > 0$, then for $0 \le z \le z_0$ by continuity

$$\begin{aligned} T\hat{h}(z) &= \textstyle\int_{z_0}^1 G(z;s)\Psi(V - \hat{h}(s))ds \\ &= \textstyle\int_{z_0}^1 (1-s)\Psi(V - \hat{h}(s))ds = \text{ constant } = V. \end{aligned} \tag{5.6}$$

Hence $\hat{h}$ satisfies

$$\hat{h}(z) = T\hat{h}(z) \quad \text{for all} \quad 0 \le z \le 1.$$

This means that $\hat{h} \in C^2([0,1])$ also satisfies the differential equation

$$-\hat{h}'' = \Psi(V - \hat{h}) \quad \text{on} \quad (0,1) \tag{5.7}$$

and the conditions

$$\hat{h}(z_0) = V \quad \text{and} \quad \hat{h}'(z_0) = 0 \;\; (z_0 \geq 0). \tag{5.8}$$

The smoothness of Ψ implies that the initial value problem (5.7), (5.8) has $\hat{h}(z) \equiv V$, $0 \leq z \leq 1$, as its unique solution. However, this contradicts the boundary condition $\hat{h}(1) = 0$. Hence

$$0 \leq \hat{h}(z) < V \quad \text{for} \quad 0 \leq z \leq 1.$$

Introducing the potential $\bar{v} = V - \hat{h}$, we have shown

Theorem 5.4 Given any α, β, p and $V > 0$, there exist unique functions $\bar{v} \in C^2([0,1])$ and $\bar{u}(\cdot; \bar{v}(z)) \in C^2([0,1])$ for each $0 \leq z \leq 1$ which solve Problem (P). The potential satisfies

$$0 < \bar{v} \leq V \text{ and } \bar{v}_{zz} > 0 \text{ on } [0,1]$$

and consequently

$$\bar{v}_z > 0 \text{ on } (0,1].$$

6 Iteration procedure.

Section 5 demonstrates the existence of solutions for Problem (P) for any combination of the positive parameters α, β, p and V using a Schauder argument. In this section, an alternative, more constructive existence proof is given in which the solution is obtained by successive iterations. This method, however, only converges when the parameters α and β are sufficiently small.

The Method. Define sequences $\{v_n = v_n(z)\}_{n=0}^{\infty}$ and $\{u_n = u_n(x,z)\}_{n=1}^{\infty}$ with $x,z \in [0,1]$ in the following three-step iteration:

1. Let $v_0 := V$ on $[0,1]$.
2. With v_n given, let u_n be the solution of

$$\left.\begin{array}{ll} u_{n_{xx}} = \alpha f(v_n(z)) u_n^p & 0 < x < 1 \\ u_n(1,z) = 1 & \\ u_{n_x}(0,z) = 0. & \end{array}\right\} 0 \leq z \leq 1$$

3. With u_n given, let h_{n+1} be the solution of

$$\begin{aligned}&h_{n+1_{zz}} = \beta u_{n_x}(1,z) \quad 0 < z < 1\\ &h_{n+1_z}(0) = 0\\ &h_{n+1}(1) = V,\end{aligned}$$

and set $v_{n+1}(z) = \max\{h_{n+1}(z), 0\}$, $0 \le z \le 1$.

The following inequalities then hold:

Proposition 6.1

$$v_0 \ge v_2 \ge v_4 \ge \cdots\cdots \ge v_5 \ge v_3 \ge v_1 \ge 0 \quad \text{on} \quad [0,1]$$

and

$$u_0 \le u_2 \le u_4 \le \cdots\cdots \le u_5 \le u_3 \le u_1 \quad \text{on} \quad [0,1]\times[0,1].$$

Proof. The proof is by induction. Let $\mathbb{M} := \{n \in \mathbb{N}_0 | n \text{ is even}\}$. For $n \in \mathbb{M}$, consider the following statement:

$$(U_n)\begin{cases} v_{n+1} \le v_{n+3} \le v_{n+2} \le v_n & \text{on} \quad [0,1]\\ u_{n+1} \ge u_{n+3} \ge u_{n+2} \ge u_n & \text{on} \quad [0,1]\times[0,1].\end{cases}$$

We have to prove

(i) U_0 is true;

(ii) $U_n \Longrightarrow U_{n+2}$ for arbitrary $n \in \mathbb{M}$.

(i) Since $v_0 = V$, we obtain for u_0 the problem:

$$\begin{aligned}&u_{0_{xx}} = \alpha f(V) u_0^p\\ &u_{0_x}(0,z) = 0, \quad u_0(1,z) = 1,\end{aligned}$$

and for h_1:

$$\begin{aligned}&h_{1_{zz}} = \beta u_{0_x}(1,z) > 0\\ &h_{1_z}(0) = 0, \quad h_1(1) = V.\end{aligned}$$

Thus $v_1 = \max\{h_1, 0\} \le v_0$ on $[0,1]$. Consequently $f(v_1) \le f(v_0)$, and as in Lemma 4.1, this implies

$$u_1 \ge u_0 \quad \text{on} \quad [0,1]\times[0,1].$$

From the boundary condition at $x = 1$, it follows that

$$0 \le u_{1_x}(1,z) \le u_{0_x}(1,z) \quad \text{for} \quad 0 \le z \le 1,$$

and thus $h_2 \geq h_1$ on $[0,1]$. Therefore

$$V = v_0 \geq v_2 \geq v_1 \geq 0 \quad \text{on} \quad [0,1]. \tag{6.1}$$

Again as in Lemma 4.1, this gives

$$u_0 \leq u_2 \leq u_1 \quad \text{on} \quad [0,1] \times [0,1],$$

and thus

$$u_{0_x}(1,z) \geq u_{2_x}(1,z) \geq u_{1_x}(1,z) \geq 0 \quad \text{for} \quad 0 \leq z \leq 1$$

which means that $h_1 \leq h_3 \leq h_2$ on $[0,1]$. Together with (6.1), this implies the desired inequalities for the potentials. The corresponding inequalities for the concentrations follow after again applying Lemma 4.1.

(ii) Suppose U_n holds for some $n \in \mathbb{M}$. Then

$$u_{n+2} \leq u_{n+3} \leq u_{n+1} \quad \text{on } [0,1] \quad \times [0,1]$$

which gives

$$u_{n+2_x}(1,z) \geq u_{n+3_x}(1,z) \geq u_{n+1_x}(1,z) \text{ for } z \in [0,1].$$

This means

$$h_{n+3} \leq h_{n+4} \leq h_{n+2} \quad \text{on} \quad [0,1],$$

and thus

$$v_{n+3} \leq v_{n+4} \leq v_{n+2} \quad \text{on} \quad [0,1]. \tag{6.2}$$

As above this implies

$$u_{n+3} \geq u_{n+4} \geq u_{n+2} \quad \text{on} \quad [0,1] \times [0,1]. \tag{6.3}$$

Now repeating the arguments gives

$$v_{n+4} \geq v_{n+5} \geq v_{n+3} \quad \text{on} \quad [0,1] \tag{6.4}$$

and

$$u_{n+4} \leq u_{n+5} \leq u_{n+3} \quad \text{on} \quad [0,1] \times [0,1]. \tag{6.5}$$

The combination of (6.2)-(6.5) gives the statement U_{n+2}. □

The inequalities from Proposition 6.1 and its proof imply the existence of lower and upper potentials $\underline{v}$, $\bar{v}$ (or $\underline{h}$, $\bar{h}$) and concentrations $\underline{u}$, $\bar{u}$ such that

$$h_n \downarrow \bar{h},\ v_n \downarrow \bar{v} \text{ and } u_n \uparrow \underline{u} \text{ pointwise on } [0,1] \text{ as } n \to \infty \text{ through even values,}$$

and

$h_n \uparrow \underline{h},\ v_n \uparrow \underline{v}$ and $u_n \downarrow \bar{u}$ pointwise on $[0,1]$ as $n \to \infty$ through odd values.

Here

$$\bar{h} \geq \underline{h},\ \bar{v} = \max\{0, \bar{h}\},\ \underline{v} = \max\{0, \underline{h}\} \text{ and } \bar{u} \geq \underline{u}. \tag{6.6}$$

Using the integral representation, as in (5.2), for the solutions u_n and h_{n+1}, one finds immediately that the limit functions are classical solutions of the boundary value problems:

(i) Letting n (even) $\to \infty$ in step 2:

$$\begin{cases} \underline{u}_{xx} = \alpha f(\bar{v})\underline{u}^p & 0 < x < 1 \\ \underline{u}_x(0,z) = 0,\ \underline{u}(1,z) = 1, & \end{cases} \quad 0 \leq z \leq 1 \tag{6.7}$$

(ii) Letting n (even) $\to \infty$ in step 3:

$$\begin{cases} \underline{h}_{zz} = \beta \underline{u}_x(1,z) & 0 < z < 1 \\ \underline{h}_z(0) = 0,\ \underline{h}(1) = V, & \end{cases} \tag{6.8}$$

(iii) Letting n (odd) $\to \infty$ in step 2:

$$\begin{cases} \bar{u}_{xx} = \alpha f(\underline{v})\bar{u}^p & 0 < x < 1 \\ \underline{u}_x(0,z) = 0,\ \bar{u}(1,z) = 1, & \end{cases} \quad 0 \leq z \leq 1 \tag{6.9}$$

(iv) Letting n (odd) $\to \infty$ in step 3:

$$\begin{cases} \bar{h}_{zz} = \beta \bar{u}_x(1,z) & 0 < z < 1 \\ \bar{h}_z(0) = 0,\ \bar{h}(1) = V. & \end{cases} \tag{6.10}$$

Next we show that at least for a specified parameter range, the upper and lower solutions are identical.

Theorem 6.2 If $0 < \alpha\beta \max_{0 \leq s \leq V} f'(s) < 2$, then the iteration process converges: i.e.

$$u := \bar{u} = \underline{u} \text{ on } [0,1] \times [0,1] \quad \text{and} \quad v := \bar{v} = \underline{v} \text{ on } [0,1].$$

Moreover (u, v) satisfy Problem (P).

Proof. Integrating equation (6.9) with respect to x from $x = 0$ to $x = 1$ and substituting the result into equation (6.10) gives

$$\bar{h}_{zz} = \alpha\beta f(\underline{v}(z)) \int_0^1 \bar{u}^p(x,z)dx,\ 0 < z < 1. \tag{6.11}$$

Similarly one finds

$$\underline{h}_{zz} = \alpha\beta f(\bar{v}(z)) \int_0^1 \underline{u}^p(x,z)dx,\ 0 < z < 1. \tag{6.12}$$

Hence

$$\begin{aligned}(\bar{h} - \underline{h})_{zz} \quad &+ \quad \alpha\beta\{f(\bar{v}(z)) - f(\underline{v}(z))\} \textstyle\int_0^1 \bar{u}^p(x,z)dz \\ &= \quad \alpha\beta f(\bar{v}(z)) \textstyle\int_0^1 \{\bar{u}^p(x,z) - \underline{u}^p(x,z)\}dx \geq 0.\end{aligned} \tag{6.13}$$

Multiplying this equation by $\phi := \bar{h} - \underline{h}$ and integrating the result by parts with respect to z leads to

$$-\int_0^1 \{\phi_z\}^2 dz + \alpha\beta \int_0^1 [\phi(z)\{f(\bar{v}(z)) - f(\underline{v}(z))\} \int_0^1 \bar{u}^p(x,z)dx]dz \geq 0. \tag{6.14}$$

Set $M := \max\limits_{0 \leq s \leq V} f'(s)$. Then using $f(\bar{v}) - f(\underline{v}) \leq M(\bar{v} - \underline{v})$ and $0 \leq \bar{u} \leq 1$ in (6.14), we obtain the estimate

$$-\int_0^1 \{\phi_z\}^2 dz + \alpha\beta M \int_0^1 \phi(z)\{\bar{v}(z) - \underline{v}(z)\}dz \geq 0.$$

Further we observe that $\phi(z)\{\bar{v}(z) - \underline{v}(z)\} \leq \phi^2(z)$ for all $0 \leq z \leq 1$. Thus we arrive at the inequality

$$-\int_0^1 \{\phi_z\}^2 dz + \alpha\beta M \int_0^1 \phi^2 dz \geq 0. \tag{6.15}$$

Using

$$\int_0^1 \phi^2 dz \leq \frac{1}{2} \int_0^1 \{\phi_z\}^2 dz, \tag{6.16}$$

yields

$$\left\{-1 + \frac{1}{2}\alpha\beta M\right\} \int_0^1 \{\phi_z\}^2 dz \geq 0.$$

From this expression and (6.16) it follows that

$$\begin{aligned}\alpha\beta M < 2 \quad &\Longrightarrow \quad \phi = 0 \text{ on } [0,1] \Longrightarrow \bar{h} = \underline{h} (=: h) \Longrightarrow \bar{v} = \underline{v} (=: v) \text{ on } [0,1] \\ &\Longrightarrow \quad (\text{ from (6.7) and (6.9)})\ \bar{u} = \underline{u} (=: u) \text{ on } [0,1] \times [0,1].\end{aligned}$$

Next we show $0 < h = v$ on $[0,1]$. Suppose not. Then there exists $z_0 \in [0,1]$ such that $h(z) \leq 0$ (with $v(z) = 0$) on $[0,z_0]$ and $h(z) > 0$ (with $h(z) = v(z)$) on $(z_0,1]$. Equation (6.7) then implies $u(x,z) = 1$ for $(x,z) \in [0,1] \times [0,z_0]$. But this means that $h_{zz} = h_z = 0$ on $[0,z_0]$. Consequently $v_z(z_0) = 0$. Thus the function v satisfies

$$\begin{aligned}&v_{zz} = \Psi(v),\ \text{for } z_0 < z < 1, \\ &v(1) = V, \\ &v(z_0) = v_z(z_0) = 0.\end{aligned}$$

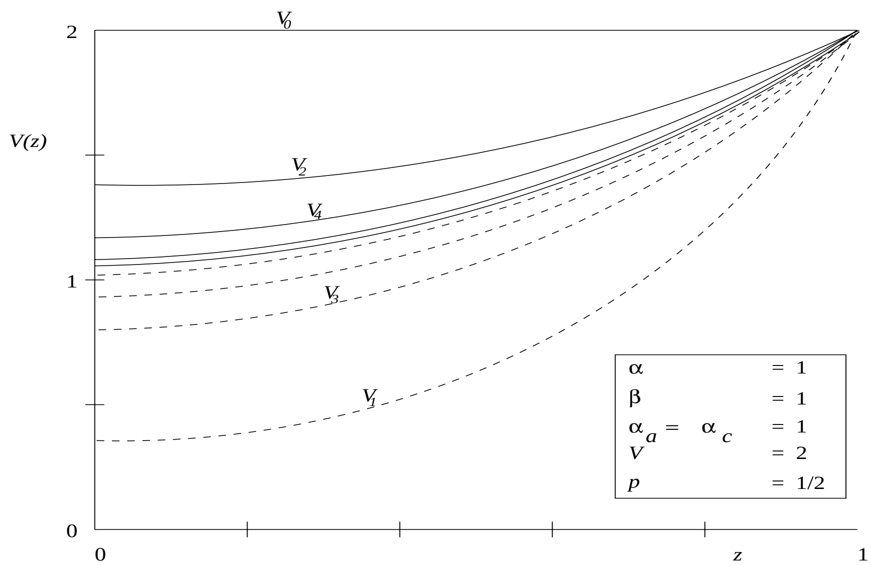

Figure 4: Computational results in case of convergence.

This gives a contradiction, again with a local uniqueness argument. Therefore we conclude that $h = v > 0$ on $[0, 1]$ and that (u, v) solves Problem (P). □

To illustrate the iteration method, we present computations for which we owe thanks to Jacqueline Prins. In Figure 4 we have chosen α,β and V so that numerically the method converges. Note that because the condition from Theorem 6.2 that $\alpha\beta \max f'(s) < 2$ is not sharp, it is not strictly required. In fact, in Figure 4 we have $\alpha\beta f'(V) = 7.524$. (We use here $f'(V) = \max f'(s)$ if $\alpha_a = \alpha_c$.)

As a second illustration, in Figure 5 we have selected values of the parameters so that no convergence occurs. Hence $\bar{v} > \underline{v}$ on $[0, 1)$. The actual solution v (which exists by Theorem 5.3) is denoted by the middle dashed-curve. It was computed using a shooting procedure for Problem (P_2). The details of this procedure will be given elsewhere.

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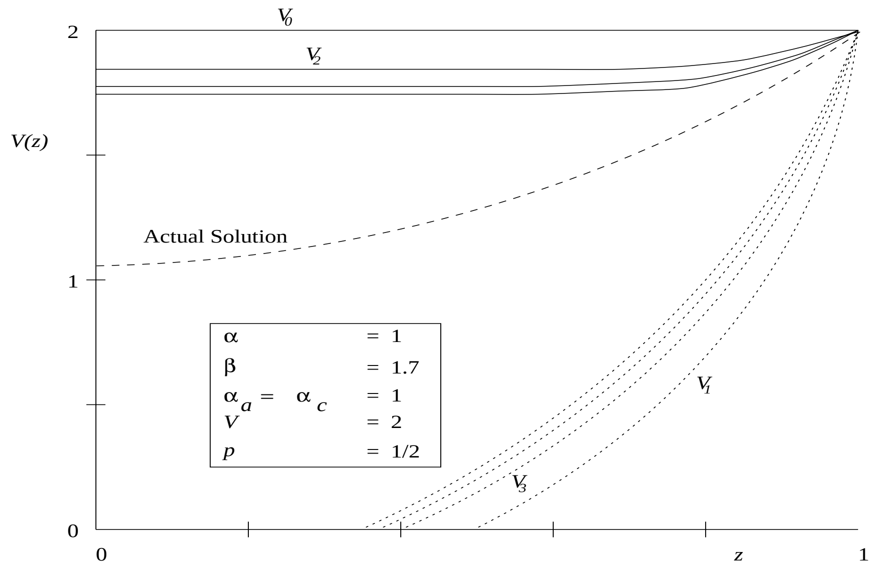

Figure 5: Computational results in case of non-convergence.

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