

Flow and reactive transport in porous media induced by well injection: Similarity solution

C. J. VAN DUIJN

*Delft University of Technology, Department of Mathematics, PO Box 5031,
NL 2600 GA Delft, The Netherlands*

PETER KNABNER

*Erlangen University, Institute for Applied Mathematics,
Martensstrasse 3, D 91058 Erlangen, Germany*

[Received 29 August 1992 and in revised form 15 November 1993]

The authors study concentration profiles of solutes undergoing equilibrium absorption in the vicinity of a water well. For the case of a contamination event, the limit problem of vanishing well radius, which is of self-similar nature, is analysed in detail. Existence, uniqueness, and qualitative properties of solutions of the corresponding ordinary differential equations are shown. Some numerical examples are also presented.

1. Introduction

Many situations arise in which hazardous chemicals, introduced into the sub-surface, affect the quality of our drinking water supplies. Therefore it is of importance to understand and estimate the movement of such chemicals dissolved in the groundwater.

In this paper we consider the problem where chemicals are being injected into the soil by localized sources. Such a source can be a long thin pipe buried into the soil, leading for homogeneous soils to a description in terms of two space dimensions, or some small localized source in the three-dimensional space. By considering the appropriate half-space problem, situations describing localized surface injection can also be considered (see Fig. 1). However, we shall always select the domain

$$\Omega_\varepsilon := \{x \in \mathbb{R}^N : |x| > \varepsilon\}, \quad (1.1)$$

for $N = 2$ and $N = 3$ to model the porous medium, e.g. the soil or aquifer. Here x [m] is a point in space and $\partial\Omega_\varepsilon = \{x \in \mathbb{R}^N : |x| = \varepsilon\}$ models the surface of the well, i.e. the source with radius $\varepsilon > 0$.

The water flow regime is characterized by the water flux vector q [m/s] and the water content Θ [m³/m³] satisfying the conservation equation

$$\partial_t \Theta = -\nabla \cdot q \quad \text{for } x \in \Omega_\varepsilon, \quad t > 0, \quad (1.2)$$

where t [s] denotes time.

The chemicals under discussion, such as organic herbicides or heavy metals, undergo various reactions. Adsorption on to the solid soil particles as a

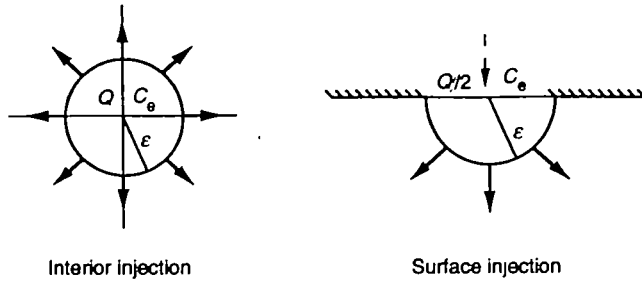


FIG. 1. Injection of contaminant into the soil ($N = 2$).

retention/release reaction is often the most important factor with respect to the mobility of the chemical. Taking adsorption into account, the mass balance equation reads

$$\partial_t(\Theta C + \rho S) + \nabla \cdot (Cq - \Theta D \nabla C) = 0 \quad \text{for } x \in \Omega_e, \quad t > 0. \tag{1.3}$$

Here C [mol/m³] denotes the concentration of dissolved chemical (per unit volume of fluid), S [mol/kg] the concentration of adsorbed chemical (per unit mass of porous skeleton), ρ [kg/m³] is the bulk density of the soil, and D [m²/s] a matrix, the sum of the molecular diffusion and mechanical dispersion (see e.g. Bear, 1972).

Often the adsorption reaction is fast compared with the water flow, so that a quasistationary approach is feasible, describing the reaction to be in equilibrium, i.e.

$$S = \psi(C), \tag{1.4}$$

where ψ , called the adsorption isotherm, can be derived from laboratory batch experiments. Typical examples of isotherms are (see e.g. Freeze & Cherry, 1979):

$$\left. \begin{aligned} \psi(C) &= k_1 C^p, & (k_1 > 0, \quad 0 < p < 1) & \quad \text{(Freundlich),} \\ \psi(C) &= \frac{k_2 C}{1 + k_3 C} & (k_2, k_3 > 0) & \quad \text{(Langmuir).} \end{aligned} \right\} \tag{1.5}$$

The example of the Freundlich isotherm shows that (1.3) is not only a nonlinear diffusion–convection equation in general, but may even be degenerate, since ψ need not be differentiable at $C = 0$. We will include these cases in our subsequent analysis.

As a result of the injection of water at $\partial\Omega_e$, the normal mass flux is given as a convective flux with the concentration C_e of the chemical dissolved in the injected water, i.e.

$$(Cq - \Theta D \nabla C) \cdot \nu = C_e q \cdot \nu \quad \text{for } x \in \partial\Omega_e, \quad t > 0, \tag{1.6}$$

where ν is the unit outward normal of Ω_e . Here $\nu = -e_x$, with $e_x := x/|x|$ being the unit vector in the radial direction.

Equations (1.3), (1.4), (1.6) have to be supplemented with an initial condition

$$C(\cdot, 0) = C_0 \quad \text{in } \Omega_e. \tag{1.7}$$

Throughout this paper we shall consider C_e and C_0 to be constant. The description of a contamination event leads to the property

$$C_e > C_0. \tag{1.8}$$

One could also think of the reverse case

$$C_0 > C_e, \tag{1.9}$$

corresponding, for example, to a remedial event by flushing with clean water. As the analysis of both cases is substantially different, we will restrict ourselves here to (1.8) and postpone the investigation of (1.9).

Our concern is a detailed analysis of the concentration profiles in the vicinity of the well. To this end we assume some further simplifications. We consider the porous medium to be homogeneous and either saturated or the water flow to be stationary. This leads to

$$\rho > 0 \quad \text{and} \quad \Theta > 0 \quad \text{are constants,} \tag{1.10}$$

and thus from (1.2)

$$\nabla \cdot \mathbf{q} = 0 \quad \text{for } x \in \Omega_\varepsilon, \quad t > 0. \tag{1.11}$$

If we assume the normal water flux at the well surface $\partial\Omega_\varepsilon$ to be uniform with a prescribed total rate Q [m^N/s], possibly depending on time, then

$$\mathbf{q}(x, t) = \frac{Q(t)}{\omega_N r^{N-1}} \mathbf{e}_x, \tag{1.12}$$

where $r = |x|$ is the radial coordinate and ω_N the surface area of the unit ball in \mathbb{R}^N , i.e. $\omega_N = 2(N - 1)\pi$.

We are in particular interested in the dynamics near the well for small well radius ε . The conventional dispersion theories, relating D to \mathbf{q} , would lead to unbounded dispersion coefficients for $\varepsilon \rightarrow 0$ (cf. Bear, 1972). On the other hand, we consider a homogeneous medium and thus expect the dispersion and molecular diffusion coefficients to be of the same order of magnitude. We describe this situation by assuming

$$D > 0 \quad \text{is scalar and constant.} \tag{1.13}$$

We nondimensionalize the dependent variables in the following way. Set

$$u := \frac{C - C_0}{\delta C}, \quad \delta C := C_e - C_0, \tag{1.14}$$

$$\beta(u) := u + \frac{\rho}{\Theta \delta C} [\psi(\delta C u + C_0) - \psi(C_0)].$$

Then $u = u(x, t)$ satisfies

$$\left. \begin{aligned} \partial_t \beta(u) + \nabla \cdot \left(u \frac{\Lambda(t)}{|x|^{N-1}} \mathbf{e}_x - D \nabla u \right) &= 0 \quad \text{for } x \in \Omega_\varepsilon, \quad t > 0, \\ -D \nabla u \cdot \mathbf{v} &= \frac{\Lambda(t)}{\varepsilon^{N-1}} (u - 1) \quad \text{for } x \in \partial\Omega_\varepsilon, \quad t > 0, \\ u(x, 0) &= 0 \quad \text{for } x \in \Omega_\varepsilon. \end{aligned} \right\} \tag{1.15}$$

Here

$$\Lambda(t) := Q(t)/\omega_N \Theta. \tag{1.16}$$

Due to the radial symmetric flow field and the boundary conditions, we expect u also to be radial symmetric and to satisfy

$$(\bar{P}_\epsilon) \begin{cases} \partial_t \beta(u) + \frac{1}{r^{N-1}} \partial_r [\Lambda(t)u - Dr^{N-1} \partial_r u] = 0 & \text{for } r > \epsilon, t > 0, \\ D \partial_r u(\epsilon, t) = \frac{\Lambda(t)}{\epsilon^{N-1}} [u(\epsilon, t) - 1] & \text{for } t > 0, \\ u(r, 0) = 0 & \text{for } r > \epsilon. \end{cases} \tag{1.17}$$

To emphasize the role of ϵ , we denote its solutions by $u_\epsilon = u_\epsilon(r, t)$. With regard to β , we assume

$$\begin{aligned} H_{\beta 1}: & \beta \in C^\infty(0, \infty) \cap C([0, \infty)), \\ H_{\beta 2}: & \beta(0) = 0, \beta'(u) > 0, \text{ and } \beta''(u) \leq 0 \text{ for } u > 0. \end{aligned}$$

These properties are in particular implied when using examples (1.5) for ψ .

To study Problem (\bar{P}_ϵ) for small well radius ϵ , it is reasonable to consider the limit $\epsilon \rightarrow 0$. We conjecture the convergence, in a sense to be specified, of the solutions u_ϵ to the solution $u = u(r, t)$ of

$$(\bar{P}_0) \begin{cases} \partial_t \beta(u) + \frac{1}{r^{N-1}} \partial_r [\Lambda(t)u - Dr^{N-1} \partial_r u] = 0 & \text{for } r > 0, t > 0, \\ u(0, t) = 1 & \text{for } t > 0, \\ u(r, 0) = 0 & \text{for } r > 0. \end{cases} \tag{1.18}$$

This is made rigorous, including a rate of convergence, in van Duijn & Peletier (1994) for $N = 2$ and for the special case where the injection rate is constant. Note that only for special cases of injection rates $Q(t)$, the solution of (\bar{P}_0) exists in the form of a *self-similar solution*, i.e. only depending on the variable $\eta := rt^\alpha$ with

$$u(r, t) = f(\eta). \tag{1.19}$$

Inserting f into the differential equation and comparing terms, we see that for α the only possible choice is $\alpha = -\frac{1}{2}$ and for the injection rate

$$Q(t) = Q_1 t^{1/2} \tag{1.20}$$

for some $Q_1 > 0$.

The function $f = f(\eta)$, with $\eta = r/t^{1/2}$, then satisfies the boundary value problem

$$(SD) \begin{cases} \frac{1}{2} \eta^N [\beta(f)]' + (D\eta^{N-1} f' - af)' = 0 & \text{for } 0 < \eta < \infty, \\ f(0) = 1 \text{ and } f(\infty) = 0, \end{cases} \tag{1.21}$$

where primes denote ∂_η and

$$a := Q_1/\omega_N \Theta. \tag{1.22}$$

To study the existence of solutions of (SD) and their properties is the purpose of this paper. In particular, to investigate the limiting behaviour of the solution profiles for $D \rightarrow 0$, we use the form (SD), and also for the outline of a numerical

algorithm for the approximation of f . In those cases where we consider a fixed dispersion coefficient D , we prefer a fully dimensionless form for the boundary value problem. We use tD [m²] instead of t . Then in (1.15), D is replaced by 1 and $\Lambda(t)$ by $\lambda t^{N/2-1}$, where λ is a dimensionless parameter given by

$$\lambda := Q_1 / \omega_N \Theta D^{1/2N}. \tag{1.23}$$

Problems (\bar{P}_ϵ) and (\bar{P}_0) are then replaced by

$$(P_\epsilon) \begin{cases} \partial_t \beta(u_\epsilon) + \frac{1}{r^{N-1}} \partial_r (\lambda t^{1/2N-1} u_\epsilon - r^{N-1} \partial_r u_\epsilon) = 0 & \text{for } r > \epsilon, t > 0, \\ \partial_r u_\epsilon(\epsilon, t) = \frac{\lambda}{\epsilon^{N-1}} t^{1/2N-1} [u_\epsilon(\epsilon, t) - 1] & \text{for } t > 0, \\ u_\epsilon(r, 0) = 0 & \text{for } r > 0 \end{cases} \tag{1.24}$$

and by (P_0) , consisting of the first and third equation and the boundary condition $u(0, t) = 1$ for $t > 0$. Analogously the equation for the self-similar solution now reads

$$(S) \begin{cases} \frac{1}{2} \eta^N [\beta(f)]' + (\eta^{N-1} f' - \lambda f)' = 0 & \text{for } 0 < \eta < \infty, \\ f(0) = 1 \quad \text{and} \quad f(\infty) = 0. \end{cases} \tag{1.25}$$

The outline of the sections is as follows. In Section 2 the unique existence of a solution of Problem (S) and characteristic properties are investigated for $N = 2$. The existence proof uses a shooting argument (for a transformed equation), which is also the basis of the numerical algorithm described in Section 5. For the behaviour near $\eta = 0$, the value of the parameter λ turns out to be crucial. The behaviour near $\eta = \infty$ is determined by the singular character of the reaction, leading to sharp fronts exactly in the case $1/\beta \in L^1(0, \delta)$ for some $\delta > 0$. Analogous results are sketched in Section 4 for $N = 3$. Section 3 investigates the hyperbolic limit $D \rightarrow 0$ for the formulation of Problem (SD). Finally Section 5 deals with an numerical algorithm for (SD) and some examples.

2. The self-similar solution

In this section we study the existence, uniqueness, and qualitative properties of solutions of the boundary value problem (S). Except for some introductory observations, the cases $N = 2$ and $N = 3$ are treated separately. However, only for $N = 2$ are the details of the proofs given. The results for $N = 3$ are summarized in Section 4.

We start with the definition of a solution. For this we introduce the negative flux function

$$F(\eta) = \eta^{N-1} f'(\eta) - \lambda f(\eta) \quad \text{for } \eta > 0. \tag{2.1}$$

DEFINITION 2.1 A function $f : [0, \infty) \rightarrow [0, 1]$ is called a solution of Problem (S) if

- (i) F and $\beta(f)$ are absolutely continuous on $[0, \infty)$;
- (ii) $F' + \frac{1}{2} \eta^N [\beta(f)]' = 0$ a.e. on $(0, \infty)$; (2.2)
- (iii) $f(0) = 1$ and $f(\infty) = 0$. (2.3)

From this definition we deduce the following proposition.

PROPOSITION 2.2 Let f be a solution of Problem (S) and let $P = \{\eta > 0 : f(\eta) > 0\}$. Then

- (i) $f \in C^x(P)$;
- (ii) $f' < 0$ on P ;
- (iii) $F(\eta) \rightarrow 0$ as $\eta \rightarrow \infty$.

Proof. (i) The continuity of F and f implies $f \in C^1((0, \infty))$ and P open. Further, the boundary condition $f(0) = 1$ gives that P is nonempty. Thus each point $\eta_0 \in P$ has a neighbourhood $N \subset P$ such that f is strictly positive on N . This implies $\beta(f) \in C^1(N)$ and, from equation (2.2), also $F \in C^1(N)$. Using this in (2.1) results in $f \in C^2(N)$. Continuing this process leads to the desired result.

(ii) This follows from a local uniqueness argument as in Atkinson & Peletier (1971, 1974).

(iii) Let $f(\eta) > 0$ for all $\eta > 0$. Then the monotonicity of f , together with (2.1) and (2.2), yields

$$F(\eta) < 0 \quad \text{and} \quad F'(\eta) > 0 \quad \text{for all } \eta > 0.$$

Hence

$$\lim_{\eta \rightarrow \infty} F(\eta) = F_x \leq 0 \quad (\text{exists}). \quad (2.4)$$

We show that $F_x < 0$ leads to a contradiction. Expression (2.1) gives

$$\lim_{\eta \rightarrow \infty} \eta^{N-1} f'(\eta) \rightarrow F_x. \quad (2.5)$$

For $N = 2$, this contradicts directly the boundary condition $f(\infty) = 0$. For $N = 3$ we use (2.5) in equation (2.2) to find

$$\lim_{\eta \rightarrow \infty} \frac{F'(\eta)}{\eta} = -\frac{1}{2} \beta'(0^+) F_x.$$

Now $F_x < 0$ contradicts the asymptotic behaviour (2.4). \square

The monotonicity of f means that P consists of a single interval of the form

$$P = (0, L) \quad \text{with } L \leq \infty.$$

When $L = \infty$, we are dealing with a solution satisfying

$$f(\eta) > 0 \quad \text{and} \quad f'(\eta) < 0 \quad \text{for all } \eta > 0,$$

and when $L < \infty$ (possibly), we have a solution of the form

$$\begin{aligned} f(\eta) > 0 \quad \text{and} \quad f'(\eta) < 0 \quad \text{for } 0 < \eta < L, \\ f(L) = f'(L) = 0, \\ f(\eta) = 0 \quad \text{for } \eta > L. \end{aligned}$$

Whether $L < \infty$ or $L = \infty$ occurs depends on the properties of the nonlinear term $\beta(f)$ near $f = 0$. We will investigate this in the next section. Another point that

requires attention concerns the behaviour of the solution near the origin, because there the equation has a singularity. We consider in detail the case $N = 2$.

2.1 Structure of solution

Throughout this section, we suppose that f is a solution of Problem (S) for $N = 2$. With regard to the behaviour near $\eta = 0$, we have the following proposition.

PROPOSITION 2.3 $\lim_{\eta \downarrow 0} \eta^{1-\lambda} f'(\eta) = -A$ (exists with $0 < A < \infty$).

Proof. On the interval $(0, L)$, we may write the differential equation as

$$\frac{f''}{f'} = \frac{\lambda - 1}{\eta} - \frac{1}{2} \eta \beta'(f(\eta)).$$

Integrating this expression gives

$$\eta_2^{1-\lambda} f'(\eta_2) = \eta_1^{1-\lambda} f'(\eta_1) \exp\left(-\frac{1}{2} \int_{\eta_1}^{\eta_2} s \beta'(f(s)) ds\right) \text{ for } 0 < \eta_1 < \eta_2 < L,$$

which implies the existence of the limit (fix $\eta_2 > 0$ and let $\eta_1 \downarrow 0$). \square

Before we consider the behaviour of the solution near $\eta = L$, we first give the necessary and sufficient condition for which L is finite; see also van Duijn & Knabner (1991, 1992), where similar questions for travelling waves are considered.

PROPOSITION 2.4 $L < \infty \Leftrightarrow 1/\beta \in L^1(0, \delta)$ for some $\delta > 0$.

Proof. Suppose $1/\beta \in L^1(0, \delta)$ and $L = \infty$. Integrating equation (2.2) from $\eta > 0$ to ∞ gives

$$\eta f'(\eta) - \lambda f(\eta) = \frac{1}{2} \int_{\eta}^{\infty} s^2 [\beta(f(s))] ds.$$

Using the monotonicity of $\beta(f(\cdot))$, we estimate

$$\eta f'(\eta) - \lambda f(\eta) < -\frac{1}{2} \eta^2 \beta(f(\eta))$$

or

$$-\frac{f'(\eta)}{\beta(f(\eta))} > \frac{1}{2} \eta - \frac{\lambda f(\eta)}{\beta(f(\eta))} \frac{1}{\eta} \tag{2.6}$$

for every $\eta > 0$. Now fix $\eta_0 > 0$. Integrating (2.6) from η_0 to $\eta > \eta_0$ yields

$$\int_{f(\eta)}^{f(\eta_0)} \frac{1}{\beta(s)} ds > \frac{1}{4} (\eta^2 - \eta_0^2) - \int_{\eta_0}^{\eta} \frac{\lambda f(s)}{s \beta(f(s))} ds.$$

Since β is concave, we have

$$\int_{f(\eta)}^{f(\eta_0)} \frac{1}{\beta(s)} ds > \frac{1}{4} (\eta^2 - \eta_0^2) - \frac{\lambda f(\eta_0)}{\beta(f(\eta_0))} \ln(\eta/\eta_0).$$

Letting $\eta \rightarrow \infty$ contradicts the integrability of $1/\beta$. Next suppose $L < \infty$ and

$1/\beta \notin L^1(0, \delta)$. Now we integrate equation (2.2) from some $0 < \eta < L$ to L and obtain

$$\eta f'(\eta) - \lambda f(\eta) = \frac{1}{2} \int_{\eta}^L s^2 [\beta(f(s))]'. \quad (2.7)$$

In this expression, we estimate for every $0 < \eta < L$

$$\eta f'(\eta) - \lambda f(\eta) > -\frac{1}{2} L^2 \beta(f(\eta))$$

or

$$-\frac{f'(\eta)}{\beta(f(\eta))} < \frac{1}{2} \frac{L^2}{\eta} - \lambda \frac{f(\eta)}{\beta(f(\eta))}. \quad (2.8)$$

Now fix $0 < \eta_0 < L$. Integrating (2.8) from η_0 to $\eta_0 < \eta < L$ yields

$$\int_{f(\eta_0)}^{f(\eta)} \frac{1}{\beta(s)} ds < \frac{1}{2} L^2 \ln(\eta/\eta_0).$$

Letting $\eta \nearrow L$ in this expression, contradicts the nonintegrability of $1/\beta$. \square

To describe the behaviour of $f(\eta)$ near $\eta = L < \infty$, we introduce the function

$$\Phi(f) = \int_0^f \frac{1}{\beta(s)} ds.$$

Then we have the following proposition.

PROPOSITION 2.5 $\lim_{\eta \uparrow L} [\Phi(f(\eta))] = -\frac{1}{2}L$.

Proof. From (2.7) we obtain for every $0 < \eta < L$

$$\eta f'(\eta) - \lambda f(\eta) = -\frac{1}{2} \eta^2 \beta(f(\eta)) - \int_{\eta}^L s \beta(f(s)) ds,$$

or

$$[\Phi(f(\eta))] + \frac{1}{2} \eta = \lambda \frac{f(\eta)}{\eta \beta(f(\eta))} - \frac{1}{\eta \beta(f(\eta))} \int_{\eta}^L s \beta(f(s)) ds.$$

This equality implies

$$\lim_{\eta \uparrow L} [\Phi(f(\eta))] = -\frac{1}{2}L + \frac{\lambda}{L \beta'(0^+)}.$$

The concavity of β gives $\beta'(0^+) \leq \infty$. But $\beta'(0^+) < \infty$ implies $1/\beta \notin L^1(0, \delta)$, hence $\beta'(0^+) = \infty$, which yields the result. \square

Example 2.6. When considering a Freundlich isotherm we have (see also (1.5))

$$\beta(f) = f + Kf^p \quad \text{with } K > 0 \text{ and } 0 < p < 1.$$

Clearly $1/\beta \in L^1(0, \delta)$. For the behaviour of the solution near L , we find from

$$[\Phi(f(\eta))] = \frac{f'(\eta)}{f(\eta) + Kf^p(\eta)} = \frac{1}{1 - pf^{1-p}(\eta) + K} (f^{1-p})'(\eta) \quad \text{for } 0 < \eta < L$$

that

$$\lim_{\eta \uparrow L} (f^{1-p})'(\eta) = -\frac{1}{2}(1-p)KL.$$

In case of a Langmuir isotherm, we have

$$\beta(f) = f + \frac{K_1 f}{1 + K_2 f}.$$

Hence $\beta'(0^+) < \infty$ and consequently $L = \infty$. \square

2.2 Existence, uniqueness, and monotonicity

In view of the behaviour of the solution near $\eta = 0$, we introduce here the transformation

$$s = \frac{1}{\lambda} \eta^\lambda \quad \text{and} \quad g(s) = f(\eta).$$

Then by Proposition 2.3, g is differentiable up to $s = 0$. Using this we study for g the initial value problem

$$(IVP) \begin{cases} g'' + C(\lambda)s^{2\lambda-1}[\beta(g)]' = 0 & \text{for } s > 0, \\ g(0) = 1, \quad g'(0) = -A, \end{cases} \tag{2.9}$$

where $C(\lambda) = \frac{1}{2}\lambda^{2\lambda-1}$. For a given $A > 0$, we denote the solution by $g(s; A)$. The object here is to show that there exists a unique $A^* > 0$ such that either $g(A^*; s) > 0$ for all $s \geq 0$ with $g(A^*; \infty) = 0$ (if $L = \infty$), or $g(A^*; s) > 0$ for $0 \leq s < L^*$ with $g(A^*; L^*) = g'(A^*; L^*) = 0$ (if $L < \infty$). Here $L^* = \lambda^{-1}L^\lambda$. Extending g by zero in the latter case, it is then easily verified that the function

$$f(\eta) := g(A^*; \lambda^{-1}\eta^\lambda) \quad \text{for } \eta \geq 0$$

defines a solution in the sense of Definition 2.1.

To prove local existence for Problem (IVP), we first integrate (2.9) to obtain the integral representation

$$g(s) = 1 - A \int_0^s \exp\left(-C(\lambda) \int_0^z t^{2\lambda-1} \beta'(g(t)) dt\right) dz =: Tg(s) \tag{2.10}$$

Then, for $\delta > 0$ sufficiently small (depending on A), the operator T maps the set $X = \{u \in C([0, \delta]) : \frac{1}{2} \leq u \leq 1\}$ into itself and is a contraction. Consequently for any $A > 0$, equation (2.10) has a unique solution $g(A; \cdot) \in X$. Then one shows that in fact $g(A; \cdot) \in C^1([0, \delta]) \cap C^\infty((0, \delta))$ and that, on $(0, \delta)$, g satisfies equation (2.9) with $g'(A; \cdot) < 0$ and $g''(A; \cdot) > 0$. We can continue this solution for larger values of s as long as g remains positive. If the solution can be continued for all $s > 0$, then the monotonicity implies the existence of

$$\lim_{s \rightarrow \infty} g(A; s) =: g(A; \infty) \in (0, 1). \tag{2.11}$$

On the other hand, for A large, the solution may exist only on a finite interval $(0, L_A)$ where

$$g(A; L_A) = 0 \quad \text{and} \quad g'(A; L_A) < 0. \tag{2.12}$$

Let

$$S^+ = \{A > 0 : (2.11) \text{ holds}\} \quad \text{and} \quad S^- = \{A > 0 : (2.12) \text{ holds}\}.$$

Then we have the following lemma.

LEMMA 2.7 The sets S^+ and S^- are nonempty, open, and connected such that $\inf S^+ = 0$ and $\sup S^- = \infty$.

Proof. We first show that solutions $g(A; \cdot)$ of Problem (IVP) vary monotonically with the shooting parameter A . Let $0 < A_1 < A_2 < \infty$ and let $g_i = g(A_i; \cdot)$ for $i = 1, 2$. Clearly $g_1 > g_2$ in a right neighbourhood of $s = 0$. Now suppose there exists $\hat{s} > 0$ such that $g_1 > g_2$ on $(0, \hat{s})$ and $g_1(\hat{s}) = g_2(\hat{s})$. To obtain a contradiction, we subtract the equations for g_1 and g_2 , multiply the result by s , and integrate from $s = 0$ to $s = \hat{s}$. Then

$$\hat{s}(g_1 - g_2)'(\hat{s}) = \frac{2}{\lambda} C(\lambda) \int_0^{\hat{s}} s^{2\lambda-1} [\beta(g_1) - \beta(g_2)] ds.$$

This is not possible because both terms have opposite sign. Hence, if $A_* \in S^+$, then any $A < A_*$ belongs to S^+ and clearly $\inf S^+ = 0$. We construct a strictly positive lower bound on $[0, \infty)$ to show that S^+ is nonempty. This bound follows from (2.10) in which we use the observation that $\beta'(g(t)) > \beta'(1)$ for $t > 0$. Then

$$g(s) > 1 - A \int_0^s \exp[-\frac{1}{2}\lambda C(\lambda)\beta'(1)z^{2\lambda}] dz,$$

from which we deduce that

$$(0, 2^{1-\lambda}[\beta'(1)]^{\lambda/2}/\Gamma(\frac{1}{2}\lambda)) \subset S^+.$$

where Γ denotes the gamma function.

Next let $A^* \in S^-$. Because solutions do not intersect, we find for any $A > A^*$ that the corresponding solution becomes zero at $s = L_A < L_{A^*}$. If

$$g'(A; L_A) < 0, \tag{2.13}$$

then $A \in S^-$ also. Now, if $g'(A; L_A) = 0$, then extending g by zero would lead to a solution in the sense of Definition 2.1. Then we can apply the monotonicity argument from above to obtain a contradiction. Thus, for $A > A^*$, (2.13) is the only possibility.

To show that S^- is nonempty, we construct an upper bound which intersects the s -axis for A sufficiently large. We obtain this bound by introducing the scaling

$$t = As \quad \text{and} \quad h(A; t) = g(A; s),$$

and by considering for h the resulting problem

$$\left. \begin{aligned} h'' + C(\lambda)A^{-2\lambda}t^{2\lambda-1}[\beta(h)]' &= 0 \quad \text{for } t > 0, \\ h(0) &= 1, \quad h'(0) = -1. \end{aligned} \right\} \tag{2.14}$$

Clearly $h' < 0$ and $h'' > 0$ on the interval of existence and

$$h(A; t) \geq \max \{(1 - t), 0\} \tag{2.15}$$

for all $t \geq 0$ and for all $A > 0$. Integrating (2.14) twice gives

$$h(t) = 1 - t - C(\lambda)A^{-2\lambda} \int_0^t (t - z)z^{2\lambda-1}[\beta(h(z))]' dz.$$

For $t \geq \frac{1}{2}$ we estimate the integrand in this expression with (2.15), to obtain

$$(t - z)z^{2\lambda-1}[\beta(h(z))]' \geq \begin{cases} -(t - z)z^{2\lambda-1}\beta'(\frac{1}{2}) & \text{for } 0 < z \leq \frac{1}{2}, \\ t^{2\lambda}[\beta(h(z))]' & \text{if } \lambda \leq 2 \\ t(\frac{1}{2})^{2\lambda-1}[\beta(h(z))]' & \text{if } \lambda > 2 \end{cases} \text{ for } \frac{1}{2} \leq z \leq t.$$

This leads to

$$h(z) \leq 1 - t + \frac{1}{2}\lambda C(\lambda)A^{-2\lambda}\beta'(\frac{1}{2})(\frac{1}{2})^{2\lambda}t + C(\lambda)A^{-2\lambda}\beta(1)d(\lambda; t)t, \tag{2.16}$$

where

$$d(\lambda; t) = \begin{cases} t^{2\lambda-1} & \text{if } \lambda \leq 2, \\ (\frac{1}{2})^{2\lambda-1} & \text{if } \lambda > 2. \end{cases}$$

The right-hand side in (2.16) becomes negative for the appropriate choice of A (large) and $t > 1$. Hence, for all sufficiently large A , the solutions $g(A; s)$ vanish at $s = L_A$ where $g'(A; L_A) \leq 0$. Using again the monotonicity argument, one finds that there cannot exist two of such solutions which both have a zero derivative when they vanish. This proves that S^- is nonempty. The upper bound (2.16) also implies that $\sup S^- = \infty$.

Finally, the continuous dependence for Problem (IVP) means that both S^+ and S^- are open. \square

The properties of the sets S^+ and S^- imply that there exists $A^* \in (0, \infty)$ such that

$$\sup S^+ \leq A^* \leq \inf S^-.$$

Considering the solution $g(A^*; s)$, either we have

$$(I) \begin{cases} g(A^*; \cdot) > 0, & g'(A^*; \cdot) < 0, \\ g''(A^*; \cdot) > 0 & \text{on } (0, \infty), \end{cases}$$

or there exists $L^* > 0$ such that

$$(II) \begin{cases} g(A^*; \cdot) > 0 & \text{on } (0, L^*), \\ g(A^*; L^*) = g'(A^*, L^*) = 0. \end{cases}$$

Applying once more the monotonicity argument, it follows that the value of A^* is uniquely determined. Extending g by zero in case (II), we obtain the following theorem.

THEOREM 2.8 Problem (S) has a unique solution f , given by $f(\eta) = g(A^*; \eta^\lambda)$ for $\eta \geq 0$.

Problem (S) can be solved explicitly when $\lambda = 2$. We work out the details in the next example.

Example 2.9. Taking $\lambda = 2$ reduces equation (2.9) to

$$g'' + \frac{1}{2}[\beta(g)]' = 0 \quad \text{for } s > 0.$$

Integration gives

$$g' + \frac{1}{2}\beta(g) = -A + \frac{1}{2}\beta(1).$$

Choosing $A = \frac{1}{2}\beta(1)$, and using $\beta(0) = 0$, implies that g' vanishes whenever g vanishes. Hence we find the expressions

$$\int_{g(s)}^1 \frac{1}{\beta(t)} dt = \frac{1}{2}s \quad \text{and} \quad \int_{f(\eta)}^1 \frac{1}{\beta(t)} dt = \frac{1}{4}\eta^2. \quad \square$$

When the function β is differentiable up to $s = 0$, i.e. $\beta'(0^+) < \infty$, we have precise information about the asymptotic behaviour of $f(\eta)$ as $\eta \rightarrow \infty$.

THEOREM 2.10 Let β satisfy $H_{\beta 1,2}$ such that $\beta' \in C^\alpha([0, 1])$, with $\alpha \in (0, 1)$. Then, given any $\eta_0 > 0$, there exists constants K_1 and K_2 such that

$$K_1 \leq f(\eta) / \left(\int_{1/\lambda\eta^\lambda}^\infty e^{-\frac{1}{2}\lambda C(\lambda)\beta'(0)t^{2\lambda}} dt \right) \leq K_2$$

for all $\eta \geq \eta_0$.

Proof. We construct the estimates for the transformed function g . Equation (2.9) implies

$$-C(\lambda)s^{2\lambda-1}\beta'(0) \leq g''/g' = -C(\lambda)s^{2\lambda-1}\beta'(g) \leq -C(\lambda)s^{2\lambda-1}\beta'(1) \quad (2.17)$$

Integrating for given $s \geq s_0 > 0$, we get

$$-\frac{1}{2}\lambda C(\lambda)\beta'(0)(s^{2\lambda} - s_0^{2\lambda}) \leq \ln \frac{g'(s)}{g'(s_0)} \leq -\frac{1}{2}\lambda C(\lambda)\beta'(1)(s^{2\lambda} - s_0^{2\lambda}),$$

and once more gives

$$K_1 \int_1^\infty e^{-\frac{1}{2}\lambda C(\lambda)\beta'(0)t^{2\lambda}} dt \leq g(s) \leq K_2 \int_s^\infty e^{-\frac{1}{2}\lambda C(\lambda)\beta'(1)t^{2\lambda}} dt. \quad (2.18)$$

Next, we improve the upperbound by writing

$$g''/g' = -C(\lambda)\beta'(0)s^{2\lambda-1} + C(\lambda)s^{2\lambda-1}[\beta'(0) - \beta'(g)]. \quad (2.19)$$

Using the upper bound from (2.18) and the Hölder continuity of the derivative β' , it follows that the second term on the right in (2.19) is integrable on $[s_0, \infty)$. Hence

$$\ln \frac{g'(s)}{g'(s_0)} \leq -\frac{1}{2}\lambda C(\lambda)\beta'(0)(s^{2\lambda} - s_0^{2\lambda}) + C^* \quad (s \geq s_0)$$

for some $C^* > 0$. Integrating this expression once more gives the improves upper bound

$$g(s) \leq K_2 \int_s^\infty e^{\frac{1}{2}\lambda C(\lambda)\beta'(0)t^{2\lambda}} dt$$

for some $K_2 > 0$. Returning to the variable η proves the result. \square

For later use, in particular when studying the convergence of solutions of the time-dependent problem for singular reactions, we regularize the function β . We put

$$\beta_n(s) = \beta\left(s + \frac{1}{n}\right) - \beta\left(\frac{1}{n}\right) \quad (s \geq 0, n \in \mathbb{N}). \tag{2.20}$$

Then β_n again satisfies $H_{\beta,1,2}$ and in addition $\beta_n \in C^\infty([0, \infty))$. It leads to the regularized problems

$$(S_n) \begin{cases} f'' + \frac{1-\lambda}{\eta} f' + \frac{1}{2}\eta[\beta_n(f)]' = 0 & (\eta > 0), \\ f(0) = 1, \quad f(\infty) = 0. \end{cases}$$

By Theorem (2.8) Problem (S_n) has a unique solution f_n , which is positive, smooth, and strictly decreasing on $(0, \infty)$. Furthermore, each f_n satisfies the asymptotic behaviour from Theorem (2.10) with $\beta'(0)$ replaced by $\beta'_n(0) = \beta'(1/n)$. Furthermore, we have the following theorem.

THEOREM 2.11 Considering the approximations (2.20), we have $f_n(\eta) \rightarrow f(\eta)$ as $n \rightarrow \infty$, uniformly in $\eta \geq 0$.

Proof. For each $n \in \mathbb{N}$, the transformed functions g_n satisfy

$$\left. \begin{aligned} g'' + C(\lambda)s^{2\lambda-1}[\beta_n(g)]' &= 0 \quad \text{for } s > 0, \\ g(0) = 1, \quad g(\infty) &= 0. \end{aligned} \right\} \tag{2.21}$$

Setting $z_n = g_n + 1/n$ and using (2.20), we find that each z_n is a solution of

$$\begin{aligned} z'' + C(\lambda)s^{2\lambda-1}[\beta(z)]' &= 0 \quad \text{for } s > 0, \\ z(0) = 1 + 1/n, \quad z(\infty) &= 1/n. \end{aligned}$$

Applying the monotonicity argument again, we find

$$z_n \geq z_{n+1} \geq g \quad \text{on } [0, \infty), \quad \text{for all } n \in \mathbb{N}$$

Hence,

$$\lim_{n \rightarrow \infty} z_n \searrow z \geq g \quad \text{pointwise on } (0, \infty),$$

and thus

$$\lim_{n \rightarrow \infty} g_n \rightarrow z \geq g \quad \text{pointwise on } (0, \infty). \tag{2.22}$$

Next multiply equation (2.21) by s and integrate the result. For any $s > 0$ and $n \in \mathbb{N}$, there results

$$s g'_n(s) = g_n(s) - 1 - C(\lambda) s^{2\lambda} \beta_n(g_n(s)) + \frac{2}{\lambda} C(\lambda) \int_0^s t^{2\lambda-1} \beta_n(g_n(t)) dt. \quad (2.23)$$

Thus, for any given $K \Subset (0, \infty)$, there exists $M > 0$ such that

$$-M \leq g'_n < 0 \quad \text{on } K, \quad \text{for all } n \in \mathbb{N}.$$

By equicontinuity,

$$g_n \rightarrow z \quad \text{in } C(K),$$

along some subsequence $n \nearrow \infty$. In fact, since $g \leq z \leq 1$ on $[0, \infty)$, we obtain $z \in C([0, \infty))$ and $z(0) = 1$. The monotonicity of the sequence $\{z_n\}$ gives $z(\infty) = 0$ and

$$g_n \rightarrow z \quad \text{in } C([0, \infty)),$$

for the entire sequence $n \nearrow \infty$ (apply Dini's Theorem to $\{z_n\}$ and use the asymptotic behaviour (upper bound in (2.18)). Passing to the limit in expressing (2.23) gives $z \in C^1((0, \infty))$ and for all $s > 0$

$$s z'(s) = z(s) - 1 - C(\lambda) s^{2\lambda} \beta(z(s)) + \frac{2}{\lambda} C(\lambda) \int_0^s t^{2\lambda-1} \beta(z(t)) dt. \quad (2.24)$$

Since z decays exponentially fast at infinity, we obtain from (2.24) $\lim_{s \rightarrow \infty} s z'(s) = l$ (exists). Clearly $l = 0$ since $z(\infty) = 0$. Therefore

$$\frac{2}{\lambda} C(\lambda) \int_0^\infty t^{2\lambda-1} \beta(z(t)) dt = 1.$$

The same identity holds for g . Then we conclude from $z \geq g$ that in fact $z = g$ on $[0, \infty)$. This completes the proof of the theorem. \square

3. The hyperbolic limit

To study the limit $D \searrow 0$, we cannot use the scaling of the variables as was done to obtain Problem (S). Instead we return to the nondimensionless formulation leading to Problem (SD), which we give here for $N = 2$:

$$(SD) \begin{cases} (D\eta f' - af)' + \frac{1}{2}\eta^2[\beta(f)]' = 0 & \text{for } \eta > 0, \\ f(0) = 1, \quad f(\infty) = 0. \end{cases} \quad (3.1)$$

From the theory developed in Section 2, we conclude that, for each $D > 0$, this problem has a unique solution f_D which satisfies

(i) $0 \leq f_D \leq 1$ on $[0, \infty)$:

(ii) $\|f'_D\|_{L^1((0, \infty))} = 1$ (by the monotonicity of f_D); (3.2)

(iii) $\int_0^\infty \eta \beta(f_D(\eta)) d\eta = a$ (mass conservation). (3.3)

We use $W^{1,1}(K) \subseteq L^p(K)$ for $1 \leq p < \infty$ and for $K \subseteq (0, \infty)$, so that for a sequence $D \searrow 0$ there exists a function $\hat{f} \in L^\infty((0, \infty))$ such that

$$0 \leq \hat{f} \leq 1 \quad \text{a.e. on } [0, \infty),$$

and a subsequence, denoted again by $D \searrow 0$, along which

$$f_D \rightarrow \hat{f} \quad \text{in } L^p(K) \quad \text{and} \quad f_D \rightarrow \hat{f} \quad \text{a.e. on } (0, \infty).$$

The monotonicity of the functions in the approximating sequence implies that \hat{f} , possibly redefined on a set of measure zero, is monotone on $(0, \infty)$. Further it follows from (3.3) and $\hat{f} \geq 0$ that

$$\int_0^\infty \eta \beta(\hat{f}(\eta)) \, d\eta = a. \tag{3.4}$$

Hence $\hat{f}(\infty) = 0$. To obtain an equation for the limit \hat{f} , we introduce the weak form of (3.1), i.e.

$$\int_0^\infty [(D\eta f'_D - af_D)\varphi' + \beta(f_D)(\eta\varphi + \frac{1}{2}\eta^2\varphi')] \, d\eta = 0,$$

with $\varphi \in C_0^\infty((0, \infty))$. Passing to the limit in this expression gives

$$\int_0^\infty \{\eta\beta(\hat{f})\varphi + [\frac{1}{2}\eta^2\beta(\hat{f}) - a\hat{f}]\varphi'\} \, d\eta = 0$$

for all $\varphi \in C_0^\infty((0, \infty))$. Hence

$$\frac{1}{2}\eta^2\beta(\hat{f}) - a\hat{f} \quad \text{is locally absolutely continuous on } (0, \infty)$$

and

$$\frac{1}{2}\eta_2^2\beta(\hat{f}(\eta_2)) - a\hat{f}(\eta_2) - \frac{1}{2}\eta_1^2\beta(\hat{f}(\eta_1)) + a\hat{f}(\eta_1) = \int_{\eta_1}^{\eta_2} \eta\beta(\hat{f}(\eta)) \, d\eta \tag{3.5}$$

for any $0 < \eta_1 < \eta_2 < \infty$. Letting $\eta_2 \rightarrow \infty$ in this expression shows that

$$\lim_{\eta \rightarrow \infty} \eta^2\beta(\hat{f}(\eta)) = \ell \in \mathbb{R} \quad (\text{exists}).$$

Now suppose $\ell \neq 0$. Then

$$\eta\beta(\hat{f}(\eta)) \approx \ell/\eta \quad \text{as } \eta \rightarrow \infty,$$

contradicting the mass-conservation equation (3.4). Hence $\ell = 0$ and (3.5) gives, with $\eta_2 \rightarrow \infty$,

$$-\frac{1}{2}\eta^2\beta(\hat{f}(\eta)) + a\hat{f}(\eta) = \int_\eta^\infty s\beta(\hat{f}(s)) \, ds. \tag{3.6}$$

This shows that

$$\lim_{\eta \downarrow 0} \hat{f}(\eta) = 1. \tag{3.7}$$

Now suppose \hat{f} has a jump discontinuity for some $\eta_s > 0$, with

$$\hat{f}^{+(-)} = \lim_{\eta \uparrow (\downarrow) \eta_s} \hat{f}(\eta).$$

Then the continuity of the right-hand side in (3.6) gives the relation

$$\eta_s^2 = 2a \frac{\hat{f}^+ - \hat{f}^-}{\beta(\hat{f}^+) - \beta(\hat{f}^-)}, \quad (3.8)$$

which is the well-known Rankine–Hugoniot shock condition (see e.g. Whitham, 1974). The concavity of β , applied to condition (3.8), implies that there exists at most one value of η where a discontinuity or shock can occur. By the monotonicity of \hat{f} and (3.7), there are two possibilities. Either $\hat{f} \in C([0, \infty))$ or there exists $\eta_s > 0$ such that $\hat{f} \in C([0, \eta_s) \cup (\eta_s, \infty))$, with $\hat{f}^+ > \hat{f}^-$ at η_s . Now suppose that, for some interval $I \subset (0, \infty)$, we have

$$\hat{f} > 0 \text{ and strictly decreasing on } I, \quad \hat{f} \in C(I).$$

Then, from (3.6),

$$-\frac{1}{2}\eta^2\beta(\hat{f}) + a\hat{f} \in C^1(I)$$

and

$$[-\frac{1}{2}\eta^2\beta(\hat{f}) + a\hat{f}]' = -\eta\beta(\hat{f}) \text{ on } I.$$

Using once more the continuity of \hat{f} , we obtain, for each $\eta \in I$,

$$\lim_{\Delta \rightarrow 0} \frac{\hat{f}(\eta + \Delta) - \hat{f}(\eta)}{\Delta} \left(a - \frac{1}{2}\eta^2 \frac{\beta(\hat{f}(\eta + \Delta)) - \beta(\hat{f}(\eta))}{\hat{f}(\eta + \Delta) - \hat{f}(\eta)} \right) = 0. \quad (3.9)$$

The term between brackets converges, for $\Delta \rightarrow 0$, to $a - \frac{1}{2}\eta^2\beta'(\hat{f}(\eta))$. Note that this is a strictly decreasing function of η (since $\beta'' \leq 0$), taking on the value a at $\eta = 0$ and converging to $-\infty$ for $\eta \rightarrow \infty$. Hence there is a unique $\bar{\eta} > 0$ such that $a - \frac{1}{2}\bar{\eta}^2\beta'(\hat{f}(\bar{\eta})) = 0$. Using this observation in (3.9) gives

$$\hat{f} \text{ differentiable with } \hat{f}' = 0 \text{ on } I \setminus \{\bar{\eta}\}$$

and, since $\hat{f} \in C(I)$,

$$\hat{f} = \text{constant on } I,$$

contradicting the strict monotonicity of \hat{f} on I . This leaves the following as the only possibility for \hat{f} :

$$\hat{f}(\eta) = \begin{cases} 1 & \text{if } 0 \leq \eta < \eta_s \\ 0 & \text{if } \eta_s < \eta < \infty, \end{cases} \quad \text{with } \eta_s = \left(\frac{2a}{\beta(1)} \right)^{\frac{1}{2}}. \quad (3.10)$$

By the uniqueness of the limit function, the solutions f_D corresponding to the entire sequence $D \searrow 0$ converge to \hat{f} . Hence we have the following theorem.

THEOREM 3.1 Let f_D be the solution of Problem (SD) for $D > 0$. Then, along any sequence $D \searrow 0$,

$$f_D \rightarrow \hat{f} \quad \text{a.e. on } (0, \infty),$$

with \hat{f} given by (3.10).

Remark 3.2. For a singular reaction, leading to $f_D(\eta) > 0$ for $0 \leq \eta < L_D$ and $f_D(\eta) = 0$ for $\eta \geq L_D$, it follows from the mass-conservation equation (3.3) that $L_D > \eta_s$ for every $D > 0$.

4. Results for $N = 3$

We recall Problem (S) for $N = 3$:

$$(S) \begin{cases} (\eta^2 f' - \lambda f)' + \frac{1}{2} \eta^3 [\beta(f)]' = 0 & \text{for } \eta > 0, \\ f(0) = 1, \quad f(\infty) = 0. \end{cases} \tag{4.1}$$

Multiplying equation (4.1) by $\exp(\lambda/\eta)$ yields

$$[\eta^2 e^{\lambda/\eta} f']' + \frac{1}{2} \eta^3 e^{\lambda/\eta} [\beta(f(\eta))]' = 0, \tag{4.2}$$

from which we deduce for the behaviour near $\eta = 0$

$$\lim_{\eta \downarrow 0} \eta^2 e^{\lambda/\eta} f'(\eta) = -A \quad (\text{exists with } 0 < A < \infty).$$

consequently,

$$\lim_{\eta \downarrow 0} f'(\eta) = 0 \quad \text{for all } \lambda > 0. \tag{4.3}$$

As in the two-dimensional setting, we have here

$$f'(\eta) < 0 \quad \text{whenever } f(\eta) > 0,$$

which implies again that the set

$$P = \{\eta > 0 : f(\eta) > 0\}$$

is of the form

$$P = (0, L) \quad \text{with } L \leq \infty.$$

The characterization for finite L is as in Proposition 2.4, i.e.

$$L < \infty \iff 1/\beta \in L^1(0, \delta) \quad \text{for some } \delta > 0.$$

When $L < \infty$, the behaviour of $f(\eta)$ for η near L is given by Proposition 2.5.

To prove the existence result, we introduce the transformation

$$s = e^{-\lambda/\eta} \quad \text{and} \quad g(s) = f(\eta)$$

and study the initial value problem

$$(IVP) \begin{cases} g'' + \frac{1}{2} \lambda^2 \left(-\frac{1}{\ln s}\right)^3 \frac{1}{s} [\beta(g)]' = 0 & (0 < s < 1), \\ g(0) = 1, \quad g'(0) = -A. \end{cases}$$

Again we look for decreasing and concave solutions of this problem. By the

method of Section 2.2, we find that there exists a unique $A^* > 0$ and a unique solution $g(A^*; s)$ such that either

$$(I) \begin{cases} g(A^*; \cdot) > 0 & \text{on } (0, 1), \\ g(A^*; 1) = g'(A^*; 1) = 0, \end{cases}$$

or there exists $L^* \in (0, 1)$ such that

$$(II) \begin{cases} g(A^*; \cdot) > 0 & \text{on } (0, L^*), \\ g(A^*; L^*) = g'(A^*; L^*) = 0. \end{cases}$$

In the latter case, we extend the solution by zero on $(0, 1)$. As a result we find that

$$f(\eta) := g(A^*; e^{-\lambda/\eta}) \quad \text{for } \eta \geq 0,$$

is the unique solution of Problem (S).

Example 4.1. Let the adsorption isotherm ψ be linear. Then

$$\beta(f) = f + Kf \quad \text{with } K > 0,$$

and for Problem (IVP) we have

$$\begin{aligned} g'' + \frac{1}{2}\lambda^2(1+K)\left(-\frac{1}{\ln s}\right)^3 \frac{1}{s} g' &= 0 \quad (0 < s < 1), \\ g(0) = 1, \quad g'(0) &= -A. \end{aligned}$$

Integrating the equation twice yields

$$g(s) = 1 - A \int_0^s \exp\left[-\frac{1}{3}\lambda^2(1+K)\left(\frac{1}{\ln t}\right)^2\right] dt.$$

Taking

$$A^* = 1 / \int_0^1 \exp\left[-\frac{1}{3}\lambda^2(1+K)\left(\frac{1}{\ln t}\right)^2\right] dt,$$

gives a positive, decreasing, and concave solution on $(0, 1)$ which satisfies

$$g(A^*; 1) = g'(A^*; 1) = 0.$$

In terms of the original similarity variable, the solution reads

$$f(\eta) = 1 - A^* \int_0^{e^{-\lambda/\eta}} \exp\left[-\frac{1}{3}\lambda^2(1+K)\left(\frac{1}{\ln t}\right)^2\right] dt.$$

To study the hyperbolic limit $D \searrow 0$, we return to Problem (SD) for $N = 3$:

$$(SD) \begin{cases} (D\eta^2 f' - af)' + \frac{1}{2}\eta^3 [\beta(f)]' = 0 & \text{for } \eta > 0, \\ f(1) = 1, \quad f(\infty) = 0. \end{cases}$$

Note that the dependent variable η in Problems (SD) and (S) is different: $\eta = r/\sqrt{t}$ [$m/s^{1/2}$] in Problem (SD), whereas $\eta = r/\sqrt{(Dt)}$ [-] in Problem (S).

Any solution f_D of Problem (SD) satisfies the mass-conservation identity

$$\int_0^\infty \eta^2 \beta(f_D(\eta)) \, d\eta = \frac{2}{3}a. \tag{4.4}$$

Going through the procedure of Section 3, we obtain, for any sequence $D \searrow 0$,

$$f_D \rightarrow \hat{f} \quad \text{a.e. on } (0, \infty),$$

where

$$\hat{f}(\eta) = \begin{cases} 1 & \text{if } 0 \leq \eta < \eta_s, \\ 0 & \text{if } \eta_s < \eta < \infty, \end{cases} \quad \text{with } \eta_s = \left(\frac{2a}{\beta(1)}\right)^{\frac{1}{2}}. \tag{4.5}$$

5. Numerical approximation

In this section we describe an algorithm to approximate the solutions of Problem (SD) and indicate some examples. We consider here only $N=2$. Based on Section 4 an analogous algorithm for $N=3$ can be designed. The numerical procedure is strongly related to the existence proof from Section 2.2. It is shown there (by means of the transformation $s = \lambda^{-1}\eta^\lambda$) that the situation is as follows.

The solution of Problem (SD) is characterized by a value $A^* > 0$ such that

$$\lim_{\eta \downarrow 0} \eta^{1-\lambda} f'(\eta) = -A^*.$$

Setting

$$S^+ := [0, A^*) \quad \text{and} \quad S^- := (A^*, \infty),$$

we find that for $A \in S^+$ the solution of the initial value problem

$$(IVP_\eta) \begin{cases} \frac{1}{2} \eta^N [\beta(f)]' + (-af + D\eta^{N-1}f)' = 0, \\ f(0) = 1, \quad \lim_{\eta \downarrow 0} \eta^{1-\lambda} f'(\eta) = -A, \end{cases} \tag{5.1}$$

satisfies

$$\lim_{\eta \rightarrow \infty} f(\eta) > 0, \tag{5.2}$$

and for $A \in S^-$ the solution of (IVP_η) satisfies

$$f(\eta_\lambda) = 0, \quad f'(\eta_\lambda) < 0 \quad \text{for some } \eta_\lambda > 0. \tag{5.3}$$

This shows the convergence of the shooting algorithm (if performed exactly):

The shooting algorithm

(1) Choose $A_t^0 \in S^-, A_u^0 \in S^+, j := 0$.

(2) $A := \frac{1}{2}(A_t^j + A_u^j), j := j + 1$.

(3) Compute the solution of (IVP_η) .

(4) If $A \in S^+$,

$$A_u^j := A, \quad A_t^j := A_t^{j-1}, \quad \text{goto (2)}.$$

(5) If $A \in S^-$,

$$A_t^j := A, \quad A_u^j := A_u^{j-1}, \quad \text{goto (2)}.$$

(6) Stop.

This algorithm either finds the solution in finitely many steps or generates sequences $A'_j \in S^-$ and $A''_j \in S^+$, such that

$$|A'_j - A''_j| = 2^{-j} |A'_0 - A''_0| \rightarrow 0 \quad \text{for } j \rightarrow \infty,$$

and $A^* \in (A'_j, A''_j)$. Several steps of the algorithm cannot be performed exactly. To approximate the solution of (IVP_η) , we integrate the equation as in the proof of Proposition 2.3. This incorporates the shooting parameter A :

$$f'(\eta) = -A\eta^{a/D-1} \exp\left(-\frac{1}{2D} \int_0^\eta s\beta'(f(s)) ds\right), \quad f(0) = 1. \tag{5.4}$$

We approximate the solution of (5.4) by the third-order Adams–Bashforth method. The integrands are approximated by the trapezoidal rule. The procedure is started by extrapolation steps starting from $\eta = 0$, based on Proposition 2.3. The number of such steps is increased for $a/D < 1$ to deal with the singularity in (5.4). In this way we compute approximating values f_i for $f(\eta_i)$. (However, the examples given below all are computed with equidistant $\eta_i = ih$, for $i = 1, 2, \dots$ and $h > 0$.)

The occurrence of $f(\eta_i) = 0$ is tested by $|f_i| < \varepsilon_1$ for some control parameter $\varepsilon_1 > 0$ and correspondingly $f(\eta_i) > 0$ and $f(\eta_i) < 0$ have to be interpreted. The parameter A is considered to be in S^+ if, for some $i > \bar{l}$ ($\bar{l} \in \mathbb{N}$ is a given control parameter, sufficiently large), $f(\eta_i) > 0$ and $f(\eta_k)$ remains close to $f(\eta_i)$ for $\bar{l} \leq k \leq i$. To avoid misinterpretation, in particular for $a/D \gg 1$, when the self-similar solution is very flat in the vicinity of $\eta = 0$ (see Fig. 4), we also require $\eta_i \geq \eta_s$, where η_s is the position of the shock in the limit case $D = 0$ (see (3.10) and (4.5)).

To facilitate the detection of $A \in S^-$, β is extended monotonically for $f < 0$. The parameter A is considered to be in S^- , if for some i , say $i = \bar{l}$, $f(\eta_i) < 0$ and $f(\eta_i) > 0$ for all $i < \bar{l}$.

For $0 \leq \eta \leq \infty$, let $M(\eta)$ denote the mass for the given $\eta > 0$, scaled by $1/\omega_N$ (see also (3.3)):

$$M(\eta) := \int_0^\eta \beta(f(\eta)) \eta^{N-1} d\eta, \tag{5.6}$$

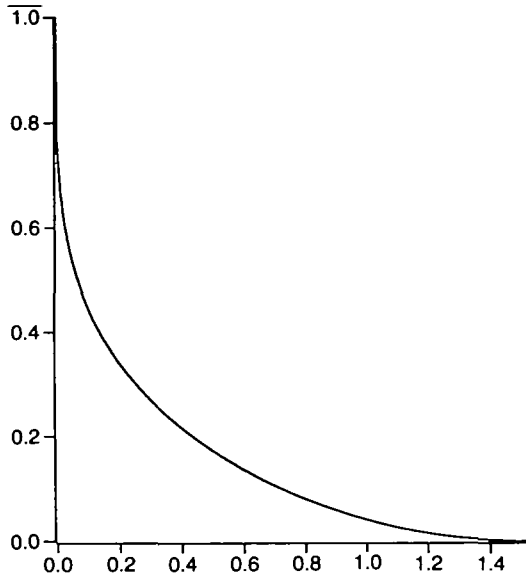
where

$$M(\infty) = 2a/N.$$

We approximate $M(\eta_i)$ by the trapezoidal rule as a measure of accuracy and use it in the case of singular reactions ($L < \infty$) to detect convergence and estimate the position of the front L .

This is done by the requirement $f(\eta_i) = 0$ and mass error $= 2a/N - M(\eta_i) < \varepsilon_2$, where $\varepsilon_2 > 0$ is a control parameter. In the case $L = \infty$, we use the requirement $f(\eta_i) = 0$ and $f'(\eta_i) = 0$. An alternative in the finite case would be the use of Proposition 2.5. The choice of the discretization parameter h determines the accuracy of a solution in terms of ε_1 and ε_2 .

The shooting algorithm could also be based on Problem (IVP). If we then interpret the numerical procedure in terms of the original variable η , this

FIG. 2. Self-similar solution for $a/D < 1$.

amounts to a grading of the mesh $\{\eta_i\}$. For $a/D < 1$, this way may be preferable, but not for $a/D \gg 1$.

In Figs. 2–4 we show the solution profiles for the following data:

$$\beta(u) := u + (\rho/\Theta)k_1(u)_+^p;$$

$$\rho = \Theta = 0.5, \quad k_1 = 3, \quad p = 0.5;$$

$(u)_+^p$ is regularized by a straight line in $[0, 10^{-14}]$;

$$Q_1 = 2.5.$$

$$\text{Fig. 2: } D = 3 \Rightarrow a/D = 0.2653;$$

$$\text{Fig. 3: } D = 0.15 \Rightarrow a/D = 5.3052;$$

$$\text{Fig. 4: } D = 0.009375 \Rightarrow a/D = 84.883;$$

$$h = 10^{-4}, \quad \varepsilon_1 = 10^{-8}, \quad \varepsilon_2 = 10^{-4}.$$

6. Concluding discussion

In this paper we studied the concentration profiles of a solute undergoing equilibrium adsorption in the vicinity of a water injecting well. We restricted ourselves to a contamination event, i.e. to a concentration C_e in the injected water higher than the initial concentration C_0 . The initial-boundary value problem, which may be expected to be the limit problem for a vanishing well radius, allows for self-similar solution, which have been considered in detail in this paper. Besides the singularity due to the specific flow regime, we also allow for a degeneration in the problem caused by an adsorption isotherm with unbounded slope near zero concentration, as the Freundlich isotherm.

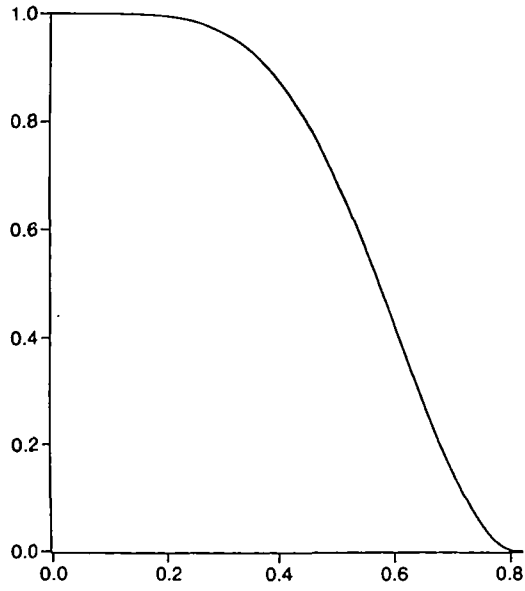


FIG. 3. Self-similar solution for $a/D > 1$.

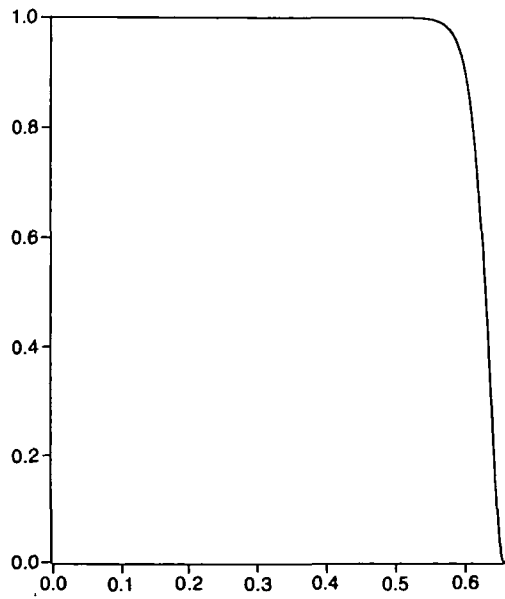


FIG. 4. Self-similar solution for $a/D \gg 1$.

Although we cannot determine a closed form for the self-similar solution, our analysis reveals most of its relevant properties. In addition, the existence proof by means of a shooting argument gives rise to simple numerical algorithm, requiring only the solution of an initial value problem for an ordinary differential equation. It turns out that the behaviour at the well is only determined by a dimensionless parameter λ measuring the relative strength of convection versus dispersion, and is not influenced by the isotherm. One may expect that the situation is different for the remedial event $C_0 < C_e$ not considered here. In particular, for two space dimensions and $\lambda < 1$, the solution develops a cusp at the well. This also shows the usefulness of the similarity solution in connection with the numerical approximation of reactive solute transport driven by complex flow regimes. The similarity solution may not only serve as an 'explicit solution' to validate numerical codes designed to cope with general geometries and flow regimes. As the numerical approximation in particular of the cusp case may be difficult, one can think of incorporating the similarity solution found here in general numerical codes to provide the approximate solution (or its first iterate) in the vicinity of wells.

The qualitative influence of the isotherm, on the other hand, can be seen in the far-field behaviour, in particular in the existence of a sharp infiltration front (for the case $C_0 = 0$ and Freundlich-type isotherms) and in the growth of the concentration profile near the front. The results turn out to be the same as for travelling wave solutions, which are asymptotic profiles for large time for a stationary water flow in one direction. This confirms that the qualitative front behaviour is solely due to the nature of the isotherm and not influenced by the underlying flow regime. Of course, the flow speed strongly influences the front speed. To be able to estimate the front position is of paramount importance for the application in groundwater hydrology, as one is then able to decide whether and when pollution may be hazardous for a drinking water supply. This also gives importance to the explicit shock solution for the hyperbolic limit case $D = 0$. The explicit front position obtained here serves as a lower bound for the general case.

Acknowledgements

The authors wish to acknowledge L. A. Peletier (Leiden University) for a number of fruitful discussions and P. A. C. Raats (Institute for Soil Fertility, Haren (Gr.), Netherlands) for bringing this problem to our attention. This work was completed while both authors enjoyed the support and hospitality of the Institute for Mathematics and its Applications.

REFERENCES

- ATKINSON, F. V., & PELETIER, L. A. 1971 Similarity profiles of flows through porous media. *Arch. Rational Mech. Anal.* **42**, 369–79.
- ATKINSON, F. V., & PELETIER, L. A. 1974 Similarity solutions of the nonlinear diffusion equation. *Arch. Rational Mech. Anal.* **54**, 373–92.
- BEAR, J. 1972 *Dynamics of Fluids in Porous Media*. New York: Elsevier (also Dover, 1988).

- FREEZE, R. A., & CHERRY, J. A. 1979 *Groundwater*. Englewood Cliffs, NJ: Prentice-Hall.
- VAN DUJN, C. J., & KNABNER, P. 1991 Solute transport in porous media with equilibrium and non-equilibrium multiple-site adsorption: Travelling waves. *J. Reine Angew. Math.* **415**, 1–49.
- VAN DUJN, C. J., & KNABNER, P. 1992 Travelling waves in the transport of reactive solutes through porous media: Adsorption and binary ion exchange—Part II. *Transport in Porous Media* **8**, 199–226.
- VAN DUJN, C. J., & PELETIER, M. A. 1994 Asymptotic behavior of solutions of a nonlinear transport equation. Preprint, Delft University of Technology.
- WHITHAM, G. B. 1974 *Linear and Nonlinear Waves*. New York: Wiley.