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Traveling Waves for Gas–Solid Reactions in a Porous Medium*

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ABSTRACT. The paper deals with traveling waves for gas–solid reactions when the diffusivity is nonlinear and the porosity increases with the consumption of the solid. We obtain existence and uniqueness results as well as criteria for the presence of conversion and penetration fronts.

1. INTRODUCTION

We shall study traveling waves for gas–solid reactions taking into account both the nonlinear diffusivity of a generalized porous medium and the increase in porosity due to solid consumption. The case of constant diffusivity was treated in [5] and [7]. Problems leading to similar equations also occur in geophysical settings (see [2] and [3]), and in populations dynamics (see [4], for instance).

As a gas diffuses through a porous solid and reacts with some species in the solid matrix, this solid species is being consumed with a corresponding increase in porosity. The diffusivity of the gas depends on its concentration and will be taken as a generalized form of the one occurring for the porous medium equation (see [8] and [1], for instance). The reaction itself is assumed to be isothermal, irreversible and distributed throughout the medium with a power-law reaction rate. Let the nondimensional concentration of the gas and the reactive solid species be denoted by C and S, respectively. Mass balances then yield the equations

$$S_t = -S^m C^p, \quad (\epsilon C)_t - \Delta G(C) = -S^m C^p (= S_t) \tag{0.1}$$

where Δ is the Laplacian, m and p are positive constants, and the nondimensional porosity ϵ is given by

$$\epsilon = \epsilon_0 + \epsilon_1 (1 - S), \quad \epsilon_0 > 0, \ \epsilon_1 \geq 0. \tag{0.2}$$

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Rewriting the diffusion term as

$$\Delta G(C) = \operatorname{div}[G'(C)\operatorname{grad} C],$$

we recognize $G'(C)$ as the diffusivity. When $G(C) = C^k$, $k = 1$ corresponds to constant diffusivity, $k > 1$ to slow diffusion (as occurs in the usual porous medium equation), and $k < 1$ to fast diffusion. We choose $G(C)$ to generalize the case $C^k (k > 0)$ by requiring G to satisfy the properties

$$\left.\begin{array}{l} G \text{ maps } [0,\infty) \text{ onto itself} \\ G \in C[0,\infty) \cap C^2(0,\infty) \\ G' > 0 \text{ on } (0,\infty) \\ G(0) = 0\,,\ G(1) = 1\,. \end{array}\right\} \tag{0.3}$$

The inverse of G will be denoted by g which also satisfies (1.3).

Since our interest here is in traveling waves, we shall seek solutions of (1.1) in the form

$$C(x,t) = u(x - at)\,,\ S(x,t) = w(x - at)\,, \tag{0.4}$$

where x is the direction of propagation of the wave and the positive constant a is its velocity. Substitution in (1.1) leads to a pair of ordinary differential equations for u and w:

$$[G(u)]'' + a(\epsilon u)' = u^p w^m\,, \tag{0.5}$$

$$aw' = u^p w^m\,, \tag{0.6}$$

where

$$\epsilon = \epsilon(w) = \epsilon_0 + \epsilon_1(1 - w)\,. \tag{0.7}$$

For simplicity, the original independent variable $x - at$ in these ordinary differential equations will be relabeled x in the sequel.

We look for nonnegative solutions of (1.5)–(1.6) on the real line, obeying the boundary conditions

$$w(-\infty) = 0\,,\ w(+\infty) = 1\,,\ u(+\infty) = 0\,, \tag{0.8}$$

which characterize a wave moving from left to right while consuming the solid reactive species. We see from (1.6) that w is nondecreasing. A solution $(u(x), w(x))$ of (1.5)–(1.8) remains a solution upon translation in either direction. The equivalence class of all translations of a solution represents the same physical wave and will be called a *wave profile*. Uniqueness statements will be made for profiles rather than for individual solutions. When studying the dependence on parameters, however, we need to compare suitably "normalized" solutions; since $w(x)$ is strictly increasing, except possibly where $w = 0$ or $w = 1$, we often find it convenient to normalize solutions through the condition $w(0) = \frac{1}{2}$.

By combining (1.5) and (1.6), we obtain $[G(u)]'' + a(\epsilon u)' - aw' = 0$, so that $[G(u)]' + a\epsilon u - aw = A$, where A is a constant. The boundary conditions show that $[G(u)]'$ tends to the constant $A + a$ as $x \to +\infty$; since $G(0+) = 0$, $G(u) \to 0$ as $x \to +\infty$. These two limits are compatible only if $A + a = 0$, so that

$$[G(u)]' + a\epsilon u + a(1 - w) = 0\,, \tag{0.9}$$

where ϵ depends on w through (1.7). It follows from (1.9) that $G(u(x))$, and hence $u(x)$, is nonincreasing. As $x \to -\infty$, $w \to 0$ so that $[G(u)]'(-\infty) \le -a$, which implies that $G(u(-\infty)) = +\infty$ and therefore $u(-\infty) = +\infty$. To avoid this physically unrealistic property, the solution will only be used, in applications, on a semi-infinite interval of the form $x > \alpha$.

We base our further study on the first-order system consisting of (1.6) and (1.9):

$$[G(u)]' = -a\epsilon u - a(1 - w)\,, \qquad [\epsilon(w) = \epsilon_0 + \epsilon_1(1 - w)] \tag{0.10}$$

$$w' = \frac{1}{a}\, u^p\, w^m \tag{0.11}$$

with the boundary conditions (1.8) to which we add the condition $u(-\infty) = +\infty$ which we just derived. In other words, we are seeking a solution $(u(x), w(x))$ of (1.10)–(1.11) connecting $(+\infty, 0)$ to the only equilibrium pont $(0, 1)$.

By setting

$$v \doteq G(u)\,,\ u = G^{-1}(v) \doteq g(v)\,, \tag{0.12}$$

we can rewrite (1.10)–(1.11) in the standard form

$$v' = -a\epsilon(w)\, g(v) - a(1 - w) \tag{0.13}$$

$$w' = \frac{1}{a}\, g^p(v)\, w^m \tag{0.14}$$

with the boundary conditions

$$w(-\infty) = 0\,,\ v(-\infty) = +\infty\,,\ w(+\infty) = 1\,,\ v(+\infty) = 0\,. \tag{0.15}$$

As already pointed out, g satisfies conditions (1.3). Moreover, v, like u, is a nonincreasing function of x which vanishes if and only if u vanishes. We look for solutions of (1.13)–(1.15) in the half-strip R (see (3.1)) of the $v - w$ plane; information obtained for $v(x)$ is easily converted to information about $u(x)$. The right side of (1.13)–(1.14) is smooth in the interior of R, but may fail to be Lipschitz on the edge $v = 0$ (if $m < 1$) or on the edge of $w = 0$ (if g or g^p has an unbounded derivative there). This non-Lipschitz behavior leads to interesting phenomena as was shown in [5] and [7] in the case $G(u) = u$: for $m < 1$, there exists a *conversion front* with the solid fully converted ($w \equiv 0$) behind the front and $w > 0$ ahead of it; for $p < 1$, there exists a penetration front with $u \equiv 0$ (and hence $w \equiv 1$) ahead of the front and $u > 0$ (and hence $w < 1$) behind it.

The remainder of the paper is organized as follows. In Section 2, we prove necessary and sufficient conditions for the existence of fronts. In Section 3, we prove existence and uniqueness for the system (1.13)–(1.15) by phase–plane methods, and we also obtain estimates relating the velocity of propagation to the profile.

2. EXISTENCE OF FRONTS

A conversion front separates the region (say, $x \leq x_F$) where $w \equiv 0$ from the region $x > x_F$ where $w > 0$. The conversion front is really a feature of the profile rather than of an individual solution: a translation of the solution in either direction merely changes x_F while retaining the front.

Theorem 0.1 *There is a conversion front if and only if $m < 1$.*

Proof. Without a conversion front, $w(x) > 0$ for all x so that (1.11) yields $(m \neq 1)$

$$1 - w^{1-m}(x) = \frac{1-m}{a} \int_x^\infty u^p(y)\, dy\,, \quad \forall x\,. \tag{0.16}$$

If $m < 1$, the left side tends to 1 as $x \to -\infty$ while the right side tends to $+\infty$ (since $u(x) \to +\infty$ as $x \to -\infty$). To avoid this contradiction, a conversion front must exist. For $m \geq 1$, we want to show no such front is possible. The right side of (1.13)–(1.14) is now smooth up to the boundary $v > 0$, $w = 0$. Therefore the unique solution of (1.13)–(1.14) with initial value $w(x_0) = 0$, $v(x_0) = v_0 > 0$ is $(v(x), 0)$ where $v(x)$ is the solution of the scalar problem $v'' = -a(\epsilon_0 + \epsilon_1)\, g(v) - a$ with $v(x_0) = v_0$. Since $(v(x), 0)$ does not satisfy (1.15), we must have $w(x) > 0$ for all x. □

The analysis for penetration fronts is a bit more delicate as there are now two troublesome terms in (1.13)–(1.14), namely those with $g(v)$ and $g^p(v)$. A heuristic argument based on the equation for C in (1.1) may steer us in the right direction. In that equation the reaction term $-C^pS^m$ may be regarded as an absorption whereas $-\Delta G(C)$ represents diffusion. Whether or not there will be a penetration front depends on the balance between diffusion and absorption for small gas concentrations. The slower the diffusion and the stronger the absorption, the more likely such a front will exist. In the model case $G(C) = C^k$, the diffusion becomes slower as k increases; even without any absorption, we know that the porous medium equation $(k > 1)$ exhibits fronts; when $k \leq 1$ fronts will occur only if the absorption is sufficiently strong (that is, p sufficiently small). The following Theorem and Corollary state these ideas precisely.

Theorem 0.2 *Let G satisfy (1.3) and let g be its inverse. Then*

(a) If $\displaystyle\int_0^1 \frac{ds}{g(s)} < \infty$, there exists a penetration front.

(b) If $\int\limits_0^1 \frac{ds}{\sqrt{H(s)}} < \infty$, *where* $H(s) = \int\limits_0^s g^p(y)\,dy$, *then there exists a penetration front.*

(c) If both $\frac{1}{G'(u)}$ *and* $\frac{u^{p-1}}{G'(u)}$ *are bounded in* $(0,\delta)$ *for some* $\delta > 0$, *then there is no penetration front.*

Proof.

(a) Let (v,w) be a solution of (1.13)–(1.15) normalized so that $v(0) = 1$. Assuming $v(x) > 0$ for $x > 0$, (1.13) yields

$$\frac{v'}{g(v)} \le -a\epsilon_0\,,$$

which, when integrated from 0 to x, gives

$$\int_{v(x)}^1 \frac{ds}{g(s)} \ge a\epsilon_0 x\,.$$

Under the hypothesis in (a), this inequality is inconsistent for large x so that we conclude that $v(x)$ must vanish for some finite positive value x_P for which we have the bound

$$x_P \le \frac{1}{a\epsilon_0}\int_0^1 \frac{ds}{g(s)}\,.$$

(b) Consider a solution (v,w) normalized so that $w(0) = \frac{1}{2}$. Using (1.5) and (1.7), we obtain

$$v'' \ge w^m g^p(v)\,,\ x > 0\,.$$

Let A be the positive value of v at $x = 0$; then

$$v'' \ge \left(\frac{1}{2}\right)^m g^p(v)\,,\ x > 0\,;\quad v(0) = A\,,\ v(+\infty) = 0\,,$$

so that v is a subsolution to the problem

$$z'' = \left(\frac{1}{2}\right)^m g(z)^p\,,\ x > 0\,;\quad z(0) = A\,,\ z(+\infty) = 0\,. \tag{0.17}$$

Multiplication by $2z'$ followed by integration gives

$$(z')^2 = \left(\frac{1}{2}\right)^{m-1} H(z) + C\,.$$

At $x = +\infty$, z, $H(z)$ and z' all vanish so that $C = 0$, and, since z is nonincreasing,

$$z' = -\left(\frac{1}{2}\right)^{\frac{m-1}{2}} \sqrt{H(z)}\,,$$

which, when integrated from 0 to x, yields

$$\int_{z(x)}^{A} \frac{ds}{\sqrt{H(s)}} = \left(\frac{1}{2}\right)^{\frac{m-1}{2}} x. \tag{0.18}$$

The hypothesis in (b) implies that $\int_0^A \frac{ds}{\sqrt{H(s)}}$ is finite, leading to a contradiction in (2.3) for large x.

(c) The two conditions in the assumption are equivalent to $g'(v)$ and $(g^p)'(v)$ being bounded in some interval $0 < v < D$. The right side of (1.13) and (1.14) is then Lipschitz in a neighborhood of $(v = 0, w = 1)$ so that the unique solution to (1.13)–(1.14) with the initial values $v = 0$, $w = 1$ is $v \equiv 0$, $w \equiv 1$. Since this solution does not satisfy (1.15), there cannot exist a penetration front. □

Corollary 0.3 *If $G(u) = u^k$, $k > 0$, then the necessary and sufficient condition for the existence of a penetration front is $k > \min(p, 1)$. In particular if $k = 1$, the condition is $p < 1$ as in* [7].

Proof. We have $g(s) = s^{1/k}$ so that hypothesis (a) holds if $k > 1$; now $H(s) = \frac{s^{1+(p/k)}}{1+(p/k)}$ and hypothesis (b) holds if $k > p$. Thus, a front exists if $k > \min(p, 1)$. On the other hand,

$$(1/G'(u)) = (1/k)\, u^{1-k} \quad \text{and} \quad (u^{p-1}/G'(u)) = (1/k)\, u^{p-k}$$

will both be bounded as $u \to 0$ if and only if $k \le \min(p, 1)$. Hence a penetration front exists if and only if $k > \min(p, 1)$. □

Remark 2.4 If $G(u)$ satisfies (1.3) and can be written as $u^k b(u)$ with $b(0) > 0$ and b' bounded near zero, calculations similar to those in Corollary 2.3 show again that the necessary and sufficient condition for a penetration front is $k > \min(p, 1)$.

Remark 2.5 The function $G(u) = u^k e^{-1/u}$ satisfies (1.3) for any $k \ge 0$. Hypothesis (a) holds for all $k \ge 0$ so that a penetration front always exists.

3. EXISTENCE AND UNIQUENESS OF PROFILES

With fixed structural constants $\epsilon_0 > 0$, $\epsilon_1 \ge 0$, $m > 0$, $k > 0$, we want to show that to each velocity $a > 0$ corresponds one and only one profile for (1.13)–(1.15). The phase plane is the (v, w) plane where we seek a trajectory (profile) starting at $(+\infty, 0)$ and ending at (0,1) as x goes from $-\infty$ to $+\infty$. We have already determined that v is nonincreasing and w is nondecreasing in x, so that our trajectory lies in the half-strip

$$R = \{(v, w) : 0 \le v,\ 0 \le w \le 1\}, \tag{0.19}$$

and $w(v)$ is nonincreasing.

It is convenient to make the change of variables $s = -x$ so that (1.13) and (1.14) become

$$\begin{cases} \dfrac{dv}{ds} = a\epsilon(w)\, g(v) + a(1-w)\,, \\ \dfrac{dw}{ds} = -\dfrac{1}{a}\, g^p(v)\, w^m\,. \end{cases} \tag{0.20}$$

Under the transformation the trajectories remain the same, but are traversed in the opposite direction. We are therefore seeking a trajectory in R leading from $(0,1)$ to $(+\infty,0)$ as s goes from $-\infty$ to $+\infty$. The region R is invariant for (3.2), since the associated vector field points inwards on the half–line $\{v > 0,\, w = 1\}$ and on the segment $\{v = 0,\, 0 < w < 1\}$, while the half–line $\{v > 0,\, w = 0\}$ is a trajectory. Thus, any trajectory entering R remains in R.

Theorem 0.4 *Let G satisfy (1.3) with the additional condition that G' be bounded away from zero in a neighborhood of $+\infty$. Then for each velocity $a > 0$ there exists a unique profile (or equivalently, a unique solution normalized by $w(0) = 1/2$, say).*

Remark 3.2 For the model problem $G(u) = u^k$, the additional condition on G' requires $k \geq 1$.

Proof. The orbits in (3.2) satisfy

$$\frac{dw}{dv} = -\frac{g^p(v)w^m}{a^2[1-w+\epsilon(w)g(v)]} \doteq f(v,w)\,, \tag{0.21}$$

where $f \leq 0$ in R. We note the inequality

$$f(v,w) = -\frac{g^p w^m}{a^2(1-w+\epsilon g)} \leq -\frac{g^p w^m}{a^2[1+(\epsilon_0+\epsilon_1)g]} \doteq -w^m h(v)\,. \tag{0.22}$$

Substituting this inequality in (3.3) and dividing by $w^m (w > 0)$, we can integrate between two points (v_0, w_0) and (v, w) interior to R. We then find for $m \neq 1$,

$$\frac{1}{1-m}\,[w(v)^{1-m} - w_0^{1-m}] \leq -\int_{v_0}^{v} h(s)\, ds\,, \tag{0.23}$$

which yields for $m < 1$

$$0 \leq [w(v)]^{1-m} \leq w_0^{1-m} - (1-m)\int_{v_0}^{v} h(s)\, ds\,, \tag{0.24}$$

while for $m > 1$ and $w > 0$,

$$\frac{1}{[w(v)]^{m-1}} \geq \frac{1}{w_0^{m-1}} + (m-1)\int_{v_0}^{v} h(s)\, ds\,. \tag{0.25}$$

We now assume that G' is bounded away from zero in a neighborhood of $+\infty$. In that case

$$\int_{v_0}^{v} h(s)\, ds = \int_{g(v_0)}^{u} \frac{\tau^p G'(\tau)}{a^2[1+(\epsilon_0+\epsilon_1)\tau]}\, d\tau\,,$$

implies that $\int_{v_0}^{\infty} h(s)\, ds = +\infty$ for any $p > 0$. Under the additional condition on G', (3.6) yields a contradiction for large v, so that $w(v)$ must vanish identically for sufficiently large v; this in turn implies that $w(G(u))$ vanishes identically for sufficiently large u when $m < 1$. If $m > 1$ then (3.7) shows that $w(v) \to 0$ as $v \to \infty$ and hence $w(G(u))$ also vanishes identically for u sufficiently large. A similar argument applies when $m = 1$.

To prove uniqueness, we first note from the definition of f in (3.3) that $\dfrac{\partial f}{\partial w} < 0$ for (v, w) in the interior of R. We conclude that if $w(v_1) > \tilde{w}(v_1)$ for some $v_1 > 0$, then $w(v) - \tilde{w}(v)$ is strictly increasing as $v \downarrow 0$. Thus, trajectories cannot intersect on the edge $\{v = 0,\, w > 0\}$; nor can they intersect in the interior of R since the vector field in (3.2) is smooth there. Although two trajectories might have a half-line $\{v \geq v_1,\, w = 0\}$ in common, we have shown the uniqueness of the trajectory of (3.2) connecting $(0, 1)$ to $(+\infty, 0)$.

The proof of existence uses a simple topological argument as in [6] and [5]. Let us first shoot from any point $(0, A)$ with $0 < A < 1$. To any such A corresponds a unique trajectory $w_A(v)$. The set $\{w_A(v)\}_{0<A<1}$ is a family of monotone, nonintersecting, ordered curves. The same is true for the family $\{w_B(v)\}_{B>0}$ of trajectories starting from $(B, 1)$ with $B > 0$. The solution $w^*(v)$ of our problem can then be characterized by

$$w^* = \sup_{0<A<1} w_A = \inf_{B>0} w_B\,,$$

which acts as a separatrix between the trajectories w_A and w_B. □

For many applications, particularly to semi-infinite regions, it is important to know the relation between $u(0)$ and the velocity a. Obviously such a relation can only be derived for a normalized solution. We choose to normalize the solution by setting $w(0) = 1/2$. By multiplying equations (1.10) and (1.11), we find, for $w > 0$,

$$-u^p\,[G(u)]' = a^2 w' w^{-m}\,[u\epsilon(w) + 1 - w]\,,$$

and, after setting $K(u) = \int_0^u G'(s)s^p\, ds$, we have

$$-\frac{d}{dx} K(u(x)) = a^2 \left[\frac{d}{dx} F_m(w) + \epsilon(w)\, u w' w^{-m}\right] \tag{0.26}$$

where the constant of integration in F_m has been chosen so that $F_m(1/2) = 0$:

$$F_m(w) = \frac{w^{1-m} - (1/2)^{1-m}}{1-m} - \frac{w^{2-m} - (1/2)^{2-m}}{2-m}\,, \quad m \neq 1, 2\,.$$

Integration of (3.8) from 0 to $+\infty$ yields

$$K(u(0)) = a^2 \left[F_m(1) + \int_0^\infty u\epsilon(w)\, w^{-m} w'\, dx \right] . \tag{0.27}$$

Since the integrand in (3.9) is positive, we immediately deduce the upper bound for a^2 in (3.11). For a lower bound, we replace $u(x)$ in the integrand by its maximal value $u(0)$. The remaining integral can be performed explicitly using the expression (1.7) for $\epsilon(w)$ so that

$$K(u(0)) \leq a^2[F_m(1) + u(0)\alpha_m] , \tag{0.28}$$

where

$$\alpha_m = \frac{\epsilon_0 + \epsilon_1}{1-m} [1 - (1/2)^{1-m}] - \frac{\epsilon_1}{2-m} [1 - (1/2)^{2-m}] .$$

Combining the lower bound for a^2 from (3.10) with the previous upper bound gives

$$\frac{K(u(0))}{F_m(1) + \alpha_m u(0)} \leq a^2 \leq \frac{K(u(0))}{F_m(1)} , \quad m \neq 1, 2 . \tag{0.29}$$

Similar bounds are easily derived in the cases $m = 1$ and $m = 2$.

When $G(u) = u^k$ with $k \geq 1$, we have $K(u) = [k/(p+k)]\, u^{p+k}$, and (3.11) becomes

$$\frac{[u(0)]^{p+k}}{F_m(1) + \alpha_m u(0)} \leq \frac{p+k}{k} a^2 \leq \frac{[u(0)]^{p+k}}{F_m(1)} , \quad m \neq 1, 2 .$$

Again we can easily modify this result for the cases $m = 1, 2$.

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