A fast reaction - slow diffusion limit for propagating redox fronts in mineral rocks

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Outline of the Talk

Statement of the problem

$$(\mathcal{P}^\varepsilon)\begin{cases} \partial_t u + \operatorname{div}(\mathbf{S_1}\, u) = \varepsilon\,\Delta u + f(u) - \varepsilon^{-1}F(u,v), & \text{in } \Omega\times(0,T] \\ \partial_t v + \operatorname{div}(\mathbf{S_2}\, v) = \varepsilon\,\Delta v + g(v) - \alpha\,\varepsilon^{-1}F(u,v), & \text{in } \Omega\times(0,T] \\ u = \overline{u}, & \text{on } \partial\Omega\times(0,T] \\ v = \overline{v}, & \text{on } \partial\Omega\times(0,T] \\ u(\cdot,0) = u_0, \quad v(\cdot,0) = v_0, & \text{on } \Omega \end{cases}$$

- u, v mass concentrations of reactants
- f, g interspecific competition terms (e.g. $f(u) = u(1-u)$, $g(v) = v(1-v)$)
- F intraspecific production term (e.g. $F(u,v) = u^p v^q$, $p > 1, q > 1$)
- ϵ is the ratio of two characteristic time scales

Aim: Study the asymptotic behavior $\epsilon \to 0$ ...

Some related work:

- L. C. Evans, Houston J. Math.(1980)
- Fasano, Primicerio, Ricci, Rendiconti di Matematica (1990)
- D. Hilhorst/R. van der Hout/L.A. Peletier: J. Math. Anal. Appl.(1996), J. Math. Sci. Uni. Tokyo (1997), Nonlinear Analysis (2000)
- E. N. Dancer, D. Hilhorst, M. Mimura, L. A. Peletier: Eur. J. Appl. Math. (1999)
- E. C. Crooks, E. N. Dancer, D. Hilhorst, M. Mimura, H. Ninomiya: Nonlinear Analyis (2004)
- M. Bazant/Stone: Physica D (2000), T. Seidman/L. Kalachev: J. Math. Anal. Appl. (2003), T. Seidman/Soane/Gobbert: Nonlinear Anal. RWA (2005), S. Meier, A. Muntean, CASA report (TU Eindhoven, 2008), ...

Assumptions

Production by reaction:

- $F \in C^1((0,1] \times (0,1]) \cap C((0,1] \times (0,1])$,
- $F(0,s) = F(\tilde{s},0) = 0$ for $s \in [0,1]$, $\tilde{s} \in [0,1]$,
- $F(u,v) > 0$ for $(u,v) \in (0,1] \times (0,1]$,
- F is nondecreasing in u and v.

Intra-specific source terms:

- f and g are continuously differentiable on $[0,+\infty)$ such that $f(0) = g(0) = 0$;
- $f(s) < 0$, $g(s) < 0$ for all $s > 1$.

Initial and boundary conditions:

- $\overline{u}$ and $\overline{v}$ are functions with values in $[0,1]$,
- $\overline{u}, \overline{v} \in C^{2,1}(\overline{\Omega} \times \mathbb{R}^+)$,
- $u_0 = \overline{u}(\cdot,0)$, $v_0 = \overline{v}(\cdot,0)$.

Existence, uniqueness, estimates for $(\mathcal{P}_\varepsilon)$

Theorem

Problem $(\mathcal{P}^\varepsilon)$ admits a unique classical solution

$$(u_\varepsilon, v_\varepsilon) \in C^{2,1}(\overline{\Omega} \times (0,T]) \cap C(\overline{\Omega} \times [0,T]) \text{ with } 0 \le u_\varepsilon, v_\varepsilon \le 1.$$

Proof idea: For instance, apply arguments from Lunardi (*Analytic semigroups and optimal regularity in parabolic problems, Progress in Nonlinear Diff. Eqs. Birkhaeuser(2005))* + the maximum principle.

Lemma (Interspecific source term: estimates)

There exists a positive constant c_0 which does not depend on ε such that

$$\varepsilon^{-1}\iint_{Q_T} F(u_\varepsilon, v_\varepsilon) \le c_0.$$

Proof of Lemma 2: Integrating the equation for v_ε over Q_T yields

$$\begin{aligned}
&\varepsilon^{-1}\iint_{Q_T} F(u_\varepsilon, v_\varepsilon)\\
&\quad= \alpha^{-1}\left(\iint_{Q_T}\varepsilon\,\Delta v_\varepsilon + \iint_{Q_T}\operatorname{div}(\mathbf{S_2} v_\varepsilon) + g(v_\varepsilon) - \int_\Omega v_\varepsilon(\cdot, T) + \int_\Omega v_0\right)\\
&\quad= \alpha^{-1}\left(\int_0^T\int_{\partial\Omega}\varepsilon\,\partial_n v_\varepsilon + \int_0^T\int_{\partial\Omega} v_\varepsilon\,\mathbf{S_2}\cdot\mathbf{n} + g(v_\varepsilon) - \int_\Omega v_\varepsilon(\cdot, T) + \int_\Omega v_0\right)\\
&\quad\le \alpha^{-1}\left(\operatorname{mes}(\Omega)\left(2 + T\,\|g\|_{L^\infty(0,1)}\right) + \operatorname{mes}(\partial\Omega)\,\|\mathbf{S_2}\|_{\ell^\infty}\,T\right).
\end{aligned}$$

Energy estimates ...

Lemma

There are positive constants c_1 and c_2 which do not depend on ε such that

$$\varepsilon \iint_{Q_T} |\nabla u_\varepsilon|^2 \leq c_1.$$

$$\varepsilon \iint_{Q_T} |\nabla v_\varepsilon|^2 \leq c_2.$$

Compactness ?

Idea: Use Riesz-Frechet-Kolmogorov compactness theorem/Simon's paper

For $r > 0$ sufficiently small, say $r \in (0, \hat{r})$, we define

$$\Omega_r = \{x \in \Omega,\ B(x, 2r) \subset \Omega\}, \qquad \Omega'_r = \bigcup_{x \in \Omega_r} B(x, r) \subset \Omega,$$

For any $\mathcal{F} \in L^\infty(Q_T)$:

$$\begin{array}{lll} \forall \xi \in \overline{B(0, r)}, & \forall (x, t) \in \Omega'_r \times (0, T), & \mathcal{S}_\xi \mathcal{F}(x, t) := \mathcal{F}(x + \xi, t), \\ \forall \tau \in (0, T), & \forall (x, t) \in \Omega \times (0, T), & \mathcal{T}_\tau \mathcal{F}(x, t) := \mathcal{F}(x, t + \tau). \end{array}$$

Lemma

For each $r \in (0, \hat{r})$, the following properties hold:

(*i*) *There exist $G_i \geq 0$ s.t. $G_i(\xi) \to 0$ as $\xi \to 0$ and*

$$\forall \xi \in \overline{B(0,r)}, \qquad \int_0^T \int_{\Omega_r} |\mathcal{S}_\xi u_\varepsilon - u_\varepsilon| \leq G_1(\xi), \quad \int_0^T \int_{\Omega_r} |\mathcal{S}_\xi v_\varepsilon - v_\varepsilon| \leq G_2(\xi).$$

(*ii*) *There exist c_3 and c_4 s. t.*

$$\forall \tau \in (0,T), \qquad \int_0^{T-\tau} \int_{\Omega_r} |\mathcal{T}_\tau u_\varepsilon - u_\varepsilon| \leq c_3\sqrt{\tau}, \quad \int_0^{T-\tau} \int_{\Omega_r} |\mathcal{T}_\tau v_\varepsilon - v_\varepsilon| \leq c_4\sqrt{\tau}.$$

(*iii*) *For any $\eta > 0$, there exists $\omega \Subset Q_T$ which does not depend on ε such that $\|u_\varepsilon\|_{L^1(Q_T\setminus\omega)} < \eta$, $\|v_\varepsilon\|_{L^1(Q_T\setminus\omega)} < \eta$.*

L^1 compactness. Reactants *separation* in space

Lemma (Strong convergence results)

Letting $\varepsilon \to 0$, *there exists* $(u, v) \in (L^\infty(Q_T; [0,1]))^2$ *such that, up to a subsequence of* $\{\varepsilon\}$,

$$\begin{array}{ccll} u_\varepsilon & \to & u & \text{in } L^1(Q_T). \\ v_\varepsilon & \to & v & \text{in } L^1(Q_T). \end{array}$$

Lemma (Segregation principle)

One has:

$$uv = 0, \quad \text{a.e. in } Q_T.$$

New variable:

$$w_\varepsilon = u_\varepsilon - \frac{v_\varepsilon}{\alpha}, \qquad w = u - \frac{v}{\alpha}.$$

There exists $w \in L^\infty(Q_T)$ *s. t.*

$$u_\varepsilon - \frac{v_\varepsilon}{\alpha} \to w, \qquad u = w^+, \qquad v = \alpha w^-.$$

Definition (Strong formulation of the fast reaction problem)

We define Problem $(\mathcal{P}^\star)$ as the following nonlinear transport problem:

$$(\mathcal{P}^\star)\begin{cases} \partial_t w + \operatorname{div}(\mathbf{S}(w)) = \mathcal{F}(w), & \text{in } \Omega \times (0,T], \\ w = \overline{w}, & \text{on } \partial\Omega \times (0,T], \\ w(\cdot,0) = w_0, & \text{on } \Omega. \end{cases}$$

with the flux function $s \mapsto \mathbf{S}(s)$ and source term $s \mapsto \mathcal{F}(s)$:

$$\mathbf{S}(s) := \mathbf{S_1}\, s^+ - \frac{\mathbf{S_2}}{\alpha}\, s^- \quad \mathcal{F}(s) := f(s^+) - \frac{g(-\alpha s^-)}{\alpha}.$$

Show that the limit of the sequence w_ε, denoted w, is the so-called "*unique weak entropy solution*" of

Theorem

The sequence w_ε strongly converges to w in $L^1(Q_T)$. Moreover, the function w is the unique entropy solution *of Problem $(\mathcal{P}^\star)$, i.e. satisfying*

$$\int_{Q_T} \left\{ (w-k)^\pm \, \partial_t \varphi + \mathrm{sgn}_\pm(w-k) \Big(\mathbf{S}(w) - \mathbf{S}(k) \Big) \nabla \varphi - \mathrm{sgn}_\pm(w-k) \, \mathcal{F}(w) \, \varphi \right\}$$
$$+ \int_\Omega (w^0 - k)^\pm \varphi(0,\cdot) + \mathcal{L} \int_{\Sigma_T} (\overline{w} - k)^\pm \varphi \geq 0,$$

for all $\varphi \in \mathcal{D}(]-\infty, T[\times \mathbb{R}^d)$, for all $k \in \mathbb{R}$.

Proof following the lines of Malek/Necas/Rokyta/Ruzicka: *Weak and Measure-valued Solutions to Evolutionary PDEs(1996)*, S. Martin: *J. Diff. Eqs. (2007)*

Theorem

Let w be the unique solution of Problem $(\mathcal{P}^\star)$. Assume there exists a closed hypersurface $\Gamma(t)$ and two subdomains $\Omega_u(t)$, $\Omega_v(t)$ s.t.

$$\overline{\Omega} = \overline{\Omega_u(t)} \cup \overline{\Omega_v(t)}, \quad \Gamma(t) = \overline{\Omega_u(t)} \cap \overline{\Omega_v(t)},$$

$$\begin{aligned} w(\cdot, t) > 0, &\quad \text{on } \Omega_u(t) \\ w(\cdot, t) < 0, &\quad \text{on } \Omega_v(t). \end{aligned}$$

Assume $t \mapsto \Gamma(t)$ smooth enough and $(u, v) := (w^+, \alpha w^-)$ is smooth up to $\Gamma(t)$. Then u and v satisfy

$$(\mathcal{P}^\star) \begin{cases} \partial_t u + \mathbf{S_1} \cdot \nabla u = f(u), & \text{in } Q_u := \bigcup_{t \in \mathbb{R}^+} \{\Omega_u(t) \times \{t\}\}, \\ \partial_t v + \mathbf{S_2} \cdot \nabla v = g(v), & \text{in } Q_v := \bigcup_{t \in \mathbb{R}^+} \{\Omega_v(t) \times \{t\}\}, \\ \left[-u + \frac{v}{\alpha}\right] \mathcal{V} \cdot \mathbf{n} = \left[-u\, \mathbf{S_1} + \frac{v}{\alpha}\, \mathbf{S_2}\right] \cdot \mathbf{n}, & \text{on } \Gamma := \bigcup_{t \in \mathbb{R}^+} \{\Gamma(t) \times \{t\}\}, \\ u = \overline{u}, & \text{on } \partial\Omega \times \mathbb{R}^+, \\ v = \overline{v}, & \text{on } \partial\Omega \times \mathbb{R}^+, \\ u(\cdot, 0) = u_0, \quad v(\cdot, 0) = v_0, & \text{on } \Omega. \end{cases}$$

Concentration effect of the reaction term

Previous estimates ensure that $\varepsilon^{-1}F(u_\varepsilon, v_\varepsilon) \rightharpoonup \mu$ in the sense of measures.

Could we be a little bit more precise about μ?

Theorem (Behaviour of the interspecific source term)

Under convenient regularity assumptions, one has

$$\mu(x,t) = \frac{1}{1+\alpha}\left([u+v]\,\mathcal{V}\cdot\mathbf{n} - [u\,\mathbf{S_1} + v\,\mathbf{S_2}]\cdot\mathbf{n}\right)\delta(x-\xi(t)).$$

where $\xi(t)$ is a parametrization of the free boundary $\Gamma(t)$.

Proof: Defining $\mu^\varepsilon = \varepsilon^{-1} F(u_\varepsilon, v_\varepsilon)$ and using $\psi \in C_0^\infty(Q_T)$, we have:

$$\begin{aligned}\iint_{Q_T} \mu^\varepsilon\,\psi &= \iint_{Q_T} \left(u_\varepsilon\,\partial_t\psi + u_\varepsilon\,\mathbf{S_1}\cdot\nabla\psi + f(u_\varepsilon)\psi\right)\\ &= \frac{1}{\alpha}\iint_{Q_T}\left(v_\varepsilon\,\partial_t\psi + v_\varepsilon\,\mathbf{S_2}\cdot\nabla\psi + g(v_\varepsilon)\psi\right).\end{aligned}$$

Passing to the limit $\varepsilon \to 0$ and integrating the result by parts, we obtain

$$\begin{aligned}\iint_{Q_T}\mu\,\psi &= \int_0^T\int_{\Omega_u(t)}\underbrace{\left(-\partial_t u - \mathbf{S_1}\cdot\nabla u + f(u)\right)}_{=0}\psi + \int_0^T\int_{\Gamma(t)}[-u]\,\psi\,(\mathbf{S_1}-\mathcal{V})\cdot\mathbf{n},\\ \alpha\iint_{Q_T}\mu\,\psi &= \int_0^T\int_{\Omega_v(t)}\underbrace{\left(-\partial_t v - \mathbf{S_2}\cdot\nabla v + g(v)\right)}_{=0}\psi + \int_0^T\int_{\Gamma(t)}[v]\,\psi\,(\mathcal{V}-\mathbf{S_2})\cdot\mathbf{n}\end{aligned}$$

The case of a dissolution front propagating into a mineral

Corollary

Assume that $\alpha = 1$ *and* $\mathbf{S_2} = 0$*. Then*

$$\mu(x,t) \quad = \quad [u]\, \mathcal{V} \cdot \mathbf{n}\, \delta(x - \xi(t))$$

or equivalently

$$\mu(x,t) \quad = \quad \frac{[-u]\,[v]}{[-u+v]}\, \mathbf{S_1} \cdot \mathbf{n}\, \delta(x - \xi(t))$$