Optimal control and well-posedness for a free boundary problem[1]

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ABSTRACT: We consider a free boundary problem modeling growth and dissolution of a crystal in radial geometry with time-dependent data γ at the outer boundary. Well-posedness is shown first for γ in H^1 but then, motivated by an opimal control problem, for γ in L^2.

KEY WORDS: *free boundary problem, diffusion, crystal, well-posed, control.*

1. INTRODUCTION

We consider, in radial geometry, a 'crystal grain' of some substance (radius $0 < R = R(t) < L$; concentration normalized to 1) surrounded by a dilute solution with concentration $u = u(t,r)$ in the 'annulus' $R < |x| = r < L$. We consider a fixed time interval $(0,T)$ and set $\mathcal{Q} := \{(t,x) : 0 < t < T; R(t) < |x| = r < L\}$. The underlying model involves diffusion[2] in the solution with the concentration satisfying the conservation equation

$$\dot{u} = \Delta u = r^{1-d}(r^{d-1}u_r)_r \quad \text{in } \mathcal{Q} \tag{1.1}$$

with the boundary condition

$$u_r = \dot{R}[1-u] \quad \text{at the crystal boundary } r = R(t) \tag{1.2}$$

corresponding to conservation in mass transport 'across' the moving interface. It is convenient to set

$$\dot{R} = h(t) \quad \text{with } R(0) = R_0 \tag{1.3}$$

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[2]One could also add a nonlinear reaction term $\varphi(u)$ in the equation. For simplicity we will take $\varphi \equiv 0$, although there are no essential differences to the arguments provided φ is differentiable (Lipschitzian) with $\varphi(0) \geq 0 \geq \varphi(1)$.

and this may be viewed as an ordinary differential equation from which to obtain the moving boundary $R(\cdot)$ on $[0,T]$. Of course we also have initial conditions for u

$$u(0,r) = u_0(r) \quad \text{for } R_0 < r < L \tag{1.4}$$

and require, of course, that $0 \le u_0 < 1$ so this represents an admissible concentration. We impose Dirichlet conditions

$$u = \gamma = \gamma(t) \quad \text{at the outer boundary } r = L \tag{1.5}$$

and will treat the specification of the function $\gamma(\cdot)$ as a *control*; again, we require that $0 \le \gamma \le 1$.

This problem: [the equations (1.1), (1.3) with (1.4), (1.5), and the coupling (1.2)], we will call $(\mathbf{P_0})$. For the analysis, it is convenient to rescale the time-varying r-interval $[R,L]$ by setting $y := [L-r]/[L-R]$ with a concommittant alteration of the equation to

$$u_t = \rho^2 u_{yy} - \psi u_y \qquad \begin{cases} \rho := \frac{1}{L-R}, \\ \psi := \rho\left[\frac{(d-1)\rho}{\rho-1} + yh\right] \end{cases} \tag{1.6}$$

so the problem now 'lives' on the fixed domain $\hat{\mathcal{Q}} := (0,T) \times (0,1)$. We refer to this equivalent rescaled version as $(\hat{\mathbf{P}}_\mathbf{0})$.

Note that, in addition to the initial data R_0, u_0, the data for $(\mathbf{P_0})$ or $(\hat{\mathbf{P}}_\mathbf{0})$ consists of the pair of functions $[\gamma, h]$ and we will later, artificially, consider the control problem using this pair. As it stands, $(\mathbf{P_0})$ is a moving boundary problem but not a *free* boundary problem. We make it a free boundary problem by using the *constitutive relation*

$$h = H(\kappa,\, u|_{r=R}) \quad \text{with } \kappa := 1/R \tag{1.7}$$

to couple the differential equations. We will work with the problem: [$(\mathbf{P_0})$ with (1.7)], which we refer to as $(\mathbf{P}_*)$ with a similar equivalent rescaled form $(\hat{\mathbf{P}}_*)$. Observe that the pair (1.3), (1.7) combine to give

$$\dot{R} = H(1/R, \omega) \quad \text{with } R(0) = R_0 \tag{1.8}$$

where

$$\omega := u|_{r=R} \quad (\text{or } \omega := u|_{y=1} \text{ for } (\hat{\mathbf{P}}_*)). \tag{1.9}$$

and we view (1.8) as an ordinary differential equation for R, defining a map

$$\mathbf{R} : \omega(\cdot) \mapsto R(\cdot) : L^2((0,T) \to [0,1]) \to H^1(0,T) \tag{1.10}$$

under suitable conditions on H, etc. We assume that H is defined[3] and smooth where relevant and that $H(\cdot,0) \le 0$. It is not difficult to provide

[3] In real applications the function H typically takes the form: $H(\kappa,\omega) := K[\omega - G(\kappa)]$. We note that the most widely used model is the Ostwald–Freundlich law: $G(\kappa) := C_* e^{\delta\kappa}$, although this cannot be expected to remain valid for very small R ($\kappa \to \infty$). In any case, our results do not depend on any specific form for H.

auxiliary structural conditions on the behavior of H for $R \approx 0, L$ which ensure that any solution of the ordinary differential equation (1.8) (for arbitrary $\omega(\cdot)$, taking values in $[0,1]$) remains bounded away from $0, L$ on bounded t-intervals. As a simplification, we assume *some* such auxiliary condition and refer to it as **(C)**. This ensures that (1.8) does, indeed, define a map $\mathbf{R}$ as in (1.10) for which R always stays away from $0, L$.

Francis Conrad discussed some aspects of the *steady-state problem* for this at the last of these conferences, at Irsee. Beginning, actually, *during* that conference, Danielle Hilhorst and I then joined him in looking at the time-dependent problem in the setting described above. Let me note here the principal result of that collaboration:

THEOREM 1: *Assume H is as described above, satisfying* **(C)** *and with $H(\cdot, 0) \leq 0$. We seek a solution pair $[R, u]$ of*
$(\mathbf{P}_*)$ *[(1.1), (1.3), (1.4), (1.5), (1.2), (1.7)]*
for $0 < t \leq T$ but shift to the rescaled version $(\hat{\mathbf{P}}_*)$ for convenience. We consider R in, e.g., $H^1(0,T)$ and, consider u in the usual parabolic space

$$\mathcal{U} := C([0,T] \to L^2(0,1)) \cap L^2((0,T) \to H^1(0,1)).$$

Let $0 < R_0 < 1$ and let $u_0 \in L^2(R-0, L)$ with $0 \leq u_0 \leq 1$ ae; let γ be in $H^1(0,T)$ with $0 \leq \gamma \leq 1$. Then there is a unique solution $[R, u] \in H^1(0,T) \times \mathcal{U}$ and the map: $[R_0, u_0, \gamma] \mapsto [R, u]$ is continuous from $\mathbb{R} \times L^2 \times H^1$ (with the restrictions $0 < R_0 < L$ and $0 \leq u_0, \gamma \leq 1$) to $H^1(0,T) \times \mathcal{U}$ (with the restrictions $0 < R < L$ and $0 \leq u \leq 1$).

PROOF: See [1], [2] but we indicate here the structure of the argument. One begins by considering an artificial problem using truncated functions, modifying H, to obtain certain compactness. Later, a Maximum Principle argument shows that the solution obtained is already a solution of the original problem. This compactness then implies existence of a suitable weighted norm on $L^2((0,T) \to [0,1])$ for which one has strict contractivity of the map $\mathbf{F} = \mathbf{F}_\gamma$ defined by

$$(1.1\mathbf{F}): \omega \xmapsto{\quad \mathbf{R} \quad} R \mapsto \dot{R} =: h \xmapsto{\quad (\hat{\mathbf{P}})_{\mathbf{0}} \quad} u \xmapsto{\quad \text{trace} \quad} u|_{y=1}$$

where, of course, we are keeping u_0, γ fixed in considering $(\hat{\mathbf{P}}_{\mathbf{0}})$. This gives unique existence and the estimates obtained also give the continuity of the solution map. ■

2. OPTIMAL CONTROL

A few weeks after the Irsee conference there was a conference on DPS, control of Distributed Parameter Systems, at Santiago de Compostela and

I discussed some control-theoretic aspect of the crystal problem, viewing $(\mathbf{P}_*)$ as a *boundary control problem* in two senses: we control to make the free boundary $R(\cdot)$ match some desired evolution and we will be using the boundary data γ as the control. Consider a cost functional of the rather standard form

$$\mathcal{J} := \mathcal{J}_0(R) + \frac{1}{2}\int_0^T |\gamma - \gamma_*|^2\,dt \tag{2.1}$$

where $\gamma_*(\cdot)$ is a convenient 'center' for control and $\mathcal{J}_0$ measures the (cost of) deviation from the desired 'profile'. We will assume only that $\mathcal{J}_0$ is lsc from, e.g., $H^1(0,T)$ and may, for example, take

$$\mathcal{J}_0 := \frac{\alpha}{2}\int_0^T |\rho - \rho_*|^2\,dt \tag{2.2}$$

with $\rho := 1/(L-R)$ as in (1.6).

The principal difficulty is that $\mathcal{J}$ is not coercive with respect to the $H^1(0,T)$ topology for γ for which we have our only existence result, Theorem 1, so we seek to extend that.

THEOREM 2: *Assume the same hypotheses on H, R_0, u_0 as for Theorem 1. Then, for every $\gamma \in \mathcal{G} := L^2((0,T) \to [0,1])$, there is at least one solution $[R,u]$ of $(\mathbf{P}_*)$ or, equivalently, of $(\hat{\mathbf{P}}_*)$ where R is in $H^1([0,T] \to (0,L))$ as in Theorem 1 and u is in a compact subspace of the Banach space*

$$\mathcal{V}_* := C([0,T] \to L^2(0,1)) \cap L^2((0,T) \to H^s(\varepsilon,1)) \qquad (s<1;\ \varepsilon>0).$$

Further, the set of such $[\gamma,R,u]$ is closed in $\mathcal{G} \times H^1(0,T) \times \mathcal{U}_*$, using the weak topology for $\mathcal{G}$.

PROOF: We cite [4] for details but, as for Theorem 1, indicate the nature of the argument. Here one considers the same map $\mathbf{F}_\gamma$, given as there by (1.11) with a modified H. Now one need only argue continuity and compactness of $\mathbf{F}$ to obtain existence through application of the Schauder Theorem since we do not assert uniqueness. For the compactness, the trick is to consider (1.6) and write the solution as $u = v + z$ with

$$z_t = \rho^2 z_{yy}; \qquad z|_{t=0} = u_0, \quad z|_{y=0} = \gamma, \quad \rho^2 z_y|_{y=1} = 0.$$

Note that z depends only on γ and the further change of time variable to τ with $d\tau/dt = \rho^2$ enables us easily to verify the regularity of z and show suitable compactness as γ ranges over $\mathcal{G}$, taking advantage of 'interior regularity' results. The resulting equation for v now no longer involves γ explicitly and v can now be estimated by standard 'energy' methods to obtain applicability of the Aubin Compactness Theorem. ∎

COROLLARY 2.1: *Let $\mathcal{J}$ be as in (2.1) with $\mathcal{J}_0$ lsc from $H^1(0,T)$ and let H and the data $[R_0, u_0]$ be as in the Theorem. Then $\mathcal{J}$ attains its minimum, i.e., there exists an optimal triple $[\tilde{\gamma}, \tilde{R}, \tilde{u}]$, minimizing $\mathcal{J}$ subject to satisfying $(\mathbf{P}_*)$ in the sense of Theorem 2.*

PROOF: Consider any minimizing sequence for $\mathcal{J}$: $\{[\gamma_k, R_k, u_k]\}$ satisfying $(\mathbf{P}_*)$. Theorem 2 ensures existence of a convergent subsequence and that the limit $[\tilde{\gamma}, \tilde{R}, \tilde{u}]$ satisfies $(\mathbf{P}_*)$. ■

3. REGULARITY

The results of the last section are somewhat less than satisfactory from the point of view either of partial differential equations or control theory since we do not yet have well-posedness for $\gamma \in \mathcal{G}$. This means that one does not know that $\tilde{\gamma}$ actually *conrols*, in the sense of determining the particular optimal solution pair $[\tilde{R}, \tilde{u}]$, and this makes it rather difficult to attempt a characterization of $\tilde{\gamma}$ through (first order) necessary conditions for optimality: we cannot obtain optimality conditions by differentiating $\mathcal{J}$ with respect to its variable if $\mathcal{J}$ is not actually a function of γ. The trick is to 'decouple' the problem, returning to $(\mathbf{P_0})$.

THEOREM 3: *Assume the same hypotheses on H, R_0, u_0 as for Theorems 1,2. Then the map*

$$(3.1)\quad \mathbf{T} : \gamma \times \mathcal{H} \to C([0,T] \to (0,1)) \times \mathcal{G} : [\gamma, h] \xrightarrow{(\hat{\mathbf{P}})_{\mathbf{0}}} [R, \omega]$$

is well-defined and (continuously) Frechet differentiable for a suitable neighborhood $\mathcal{H} \in L^2(0,T)$. The derivative, at each point, is a compact operator.

PROOF: This is a fairly straightforward computation, leading to a linear system (which we omit here) coupling a partial differential equation on $\hat{\mathcal{Q}}$ with an ordinary differential equation along $y = 1$. See [3]. ■

The desired well-posedness from L^2 is now a simple corollary to this and Theorems 1 and 2.

COROLLARY 3.1: *The problem $(\mathbf{P}_*)$ is well-posed in the context of Theorem 2.*

PROOF: From Theorem 2 we have existence and note a compact set of $h = H(1/R, \omega)$ arising; we take H to be a neighborhood of this set so $\mathbf{R}$ is well-defined. From Theorem 3 we see that the related map $\mathbf{D} : [\gamma, h] \mapsto [h - H(1/R, \omega)]$ is also continuously differentiable and $\mathbf{D}_h$ has the form $\mathbf{I}+[\textit{compact}]$. One easily verifies from the system giving the derivative that $\mathbf{D}_h$ is injective so, by standard spectral theory, it is boundedly invertible. Application of the Implicit Function Theorem then gives local existence of a C^1 map: $\gamma \mapsto h$ for which $\mathbf{D}(\gamma, h) \equiv 0$ — just corresponding to the use of (1.7) as a constraint, converting $(\mathbf{P_0})$ to $(\mathbf{P}_*)$. We thus have a *local* well-posedness for $(\mathbf{P}_*)$. On the other hand, since H^1 is dense in $\mathcal{G}$, we may use Theorem 1 to assert well-posedness globally. ■

For the control problem we note another corollary.

COROLLARY 3.2: *Assume, for (2.1), that γ_* is in $H^1(0,T)$ and that $\mathcal{J}_0$ is 'smooth', say given by (2.2). Then the optimal $\tilde{\gamma}$ of Corollary 2.1 is actually in $H^1(0,T)$.*

PROOF: See [3]. From Theorem 3 and Corollary 3.1 we note that $\mathcal{J}$ is a differentiable function of γ and optimality gives $\langle \mathcal{J}'(\tilde{\gamma}), \delta >\leq 0$ for all admissible variations δ, i.e., such that $\tilde{\gamma} + s\delta$ continues to take values in $[0,1]$. It follows that $\tilde{\gamma}$ is the $[0,1]$-truncation of $\gamma_* + \Upsilon$ where Υ is obtained through the use of the adjoint of $\mathbf{F}'$, from which we can show that Υ is in H^1. ■

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