Optimal solutions for a free boundary problem for crystal growth

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Abstract. We consider a free boundary problem modeling the growth/dissolution of a crystal in a radially symmetric setting. Existence of an optimal boundary control, minimizing a cost functional of a standard 'integral-quadratic' form, is already known and we here consider the characterization and computation of such an optimal control.

1. Introduction

In [**7**] an existence proof was given for an optimal boundary control minimizing a fairly standard sort of cost functional $\mathcal{J}$ with dynamics given by a free boundary problem corresponding to a model of growth (dissolution) of a radially symmetric crystal grain. Our present concerns are: the development of the corresponding optimality conditions, with some consequent additional regularity, and also the computational aspects of the optimization.

Consider a solution of some substance surrounding a 'crystal grain' of the pure material. Letting $\Omega = \Omega(t)$ be the (bounded) spatial region in $\mathbb{R}^d$ occupied by the solution, we assume that the concentration C will satisfy in $\mathcal{Q} := \{(t,x) : x \in \Omega(t),\ 0 < t < T\}$ a (nonlinear) diffusion-reaction equation of standard form:

$$C_t = \Delta C + F(C). \tag{1.1}$$

We consider the problem only in a context of radial symmetry: $0 \le r := |x| \le 1$ with the crystal grain occupying $0 \le r \le R(t)$ so

$$\Omega(t) = \{x : R(t) < r := |x| < 1\}.$$

Note that by a suitable choice of units, we have taken the diffusion coefficient and the outer radius each to be 1; we will also use units for which the concentration for the crystal, itself, is 1. We then consider the data $\alpha(\cdot)$ for the Dirichlet boundary condition

$$C(t,x) = \alpha(t) \qquad \text{for } |x| = 1,\ 0 < t \le T \tag{1.2}$$

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as our *boundary control.*

The motion of the crystal boundary is given by $\dot{R} = h$ for a suitable function $h(\cdot)$: growth for $h > 0$, dissolution for $h < 0$. If h were given *a priori*, then we could simply adjoin the 'conservation of mass' boundary condition (2.3) at $r = R(t)$ to have a *moving boundary problem*, specified by the pair $[\alpha, h]$ and the initial conditions. Actually, the crystal growth is determined by a *constitutive relation* of the form:[1]

$$h = H(\omega, R) \qquad \text{with } \omega := C|_{r=R+} \tag{1.3}$$

and, coupling with this, we have the free boundary problem of the title. We note that the most commonly used special form of this constitutive relation is

$$H(\omega, R) = K(\omega - C_*(R)) \qquad \text{with } C_*(R) = \gamma_0 e^{\gamma/R}, \tag{1.4}$$

following Gibbs-Nernst and Ostwald-Freundlich, cf. [**2**]. The problem will then be radially symmetric and we can reduce to one space dimension, replacing ΔC by $[C_{rr} + \frac{d-1}{r} C_r]$ in taking C as $C(t, r)$. Indeed, we later introduce the variable $y := \frac{1-|x|}{1-R}$ to work with the *fixed* spatial domain $(0, 1)$.

We note at this point that (under suitable conditions) well-posedness of the free boundary problem is demonstrated in [**3**] for smooth $\alpha(\cdot)$ while an existence and closure result (needed for the existence of optimal boundary controls) is given in [**7**] for less smooth α; more detail later. Our theoretical goal in this paper is to obtain the optimality condition (first order necessary conditions) characterizing minimizers of the cost functional $\mathcal{J}$. Since we do not even have uniqueness of the solution map: $\alpha \mapsto C$, much less differentiability of $\mathcal{J}$ as a function of α, for α with the regularity known for the optimal control, there are some technical problems involved in the justification and computation of these conditions. Our approach will be to note differentiability of $\mathcal{J}$ as a function of the pair $[\alpha, h]$ for the decoupled problem and then to use the Implicit Function Theorem, along with the existence result noted above, for the coupled problem.

We then also present some corresponding numerical computation for the optimal boundary control. For this computation we will take Ω to be 2-dimensional ($d = 2$) and will take $K = 1$, $\gamma_0 = .01$, and $\gamma = 1$ in (1.4) so, written in terms of ω and $\rho = 1/(1 - R)$, we will then be considering the specific relation

$$H = \omega - .01\, e^{1/(1-1/\rho)}. \tag{1.5}$$

2. Statement of the Problem

[1] If it were not for the assumption of radial symmetry, we would have H as a function of the local concentration ω and of the *curvature* κ; see, e.g., [**5**]. Here, that dependence is on $R = 1/\kappa$.

We consider somewhat more precisely the problem under consideration. We begin with the *decoupled problem* which, in its first formulation, consists of (1.1) on $\mathcal{Q} = \mathcal{Q}_T$ given by $\mathcal{Q} := \{(t,x) : R(t) < r := |x| < 1,\ 0 < t < T\}$, with $R(\cdot) > 0$ given by the ordinary differential equation

$$\dot{R} = h(\cdot), \tag{2.1}$$

together with the initial conditions

$$R(0) = R_0, \qquad C(0,\cdot) = C_0(\cdot) \quad \text{on } (R_0, 1), \tag{2.2}$$

the Dirichlet boundary condition (1.2) at $r = 1$, and the flux boundary condition

$$C_r = (1 - C)h \qquad \text{at } r = R(t), \tag{2.3}$$

corresponding to conservation of mass at the moving crystal boundary, with the concentration normalized to 1 for the crystal itself. We assume throughout that:

$$(\mathbf{H}) \qquad \begin{cases} (i) & F \text{ is nonincreasing with } F(0) \geq 0 \geq F(1); \\ (ii) & 0 < R_0 < 1 \text{ and } 0 \leq C_0 \leq 1 \text{ on } (R_0, 1); \\ (iii) & 0 \leq \alpha \leq 1 \text{ on } (0, T); \\ (iv) & h \text{ is bounded and gives } 0 \leq R \leq 1 \text{ on } (0, T) \end{cases}$$

with F smooth and C_0, α, h measurable. Fixing the initial data, we expect a map $[\alpha, h] \longmapsto [C, \omega]$ so we will have $\mathcal{J}$ well-defined as a function of $[\alpha, h]$. The free boundary problem couples this with (1.3), and we assume that

$$H \text{ is smooth with } H(\cdot, 0) \leq 0. \tag{2.4}$$

Note that this is certainly satisfied (for $R > 0$) for H as in (1.4).

As indicated earlier, it is convenient to reformulate the problem in order to work on a fixed, one-dimensional spatial domain. Thus we make a change of variables: $x \mapsto y$, setting

$$u(t,y) = C(t,x) \qquad \text{with } y := \frac{1 - |x|}{1 - R(t)}. \tag{2.5}$$

Note that $y = \rho(1 - r)$ where $\rho(\cdot) := 1/(1 - R(\cdot)) > 1$ so $R = 1 - 1/\rho$ and $|x| = r = 1 - y/\rho$. The problem [(2.1), (1.1), (1.2), (2.3), (2.2)] now just becomes:

$$\begin{cases} \dot{\rho} = \rho^2 h & \text{on } (0,T) \\ u_t = \rho^2 u_{yy} - \psi u_y + F(u) & \text{on } (0,T) \times (0,1) \\ -\rho u_y = (1 - \omega)h & \text{at } y = 1 \\ u = \alpha \ [= \text{control}] & \text{at } y = 0 \\ \rho = \rho_0 \text{ and } u = u_0(\cdot) & \text{at } t = 0 \end{cases} \tag{2.6}$$

where $\psi := \rho\left[\dfrac{(d-1)\rho}{\rho - y} + yh\right]$ and $\omega := u(\cdot, 1)$ with $\rho_0 = 1/(1 - R_0) > 1$. Note that $y = 0, 1$ correspond to $r = 1, 0$. Of course we obtain $\rho_0 > 1$ and $u_0(\cdot)$ on $(0,1)$ from (2.2). The free boundary problem just couples this with (1.3), no longer taking h as given; we assume H is now formulated as $H(\omega, \rho)$.

Theorem 1 [[**7**], [**3**]]. *Assume* **(H)**-(i, ii) *and (2.4). Then there is a (weak) solution* $u \in L^\infty(\to [0,1])$ *of the coupled problem (2.6), (1.3) for each* $\alpha \in L^\infty(\to [0,1])$*; the set of such* $[\alpha, u, h]$ *(with* h *given by (1.3) and necessarily satisfying* **(H)**-(iv)*) is closed (in, say, the weak* L^2 *product topology). If* $\alpha \in H^1(0,T)$*, then the solution* u *is unique.*

Some caution is needed here. Since the existence results of [**7**] and [**3**] only give existence on some interval $(0, T_\alpha)$, it is then an assumption of the control problem that we can consider controls for which $T_\alpha \geq T$. We remark that existence may fail on the full interval $[0,T]$ only by having $R \to 0$ or $R \to 1$. We also note that [**7**] does not assert uniqueness of the solution but, under the stronger regularity assumptions, this is given by the different argument of [**3**]. Each of these proves existence first for a modified problem and then uses a maximum principle argument to show the modification has no effect. Finally, and most important for our subsequent considerations, we note that the existence argument of [**7**], using interior regularity results for parabolic equations, gives (local) $L^2(\to H^1)$ regularity for u away from the outer boundary $y = 0$ — where trace theory tells us that we *cannot* achieve this without requiring $\alpha \in H^{1/2}[0,T]$; we write $\mathcal{H}$ for this space of functions "H^1 away from $y = 0$" so $u \in L^2(\to \mathcal{H})$. On the other hand, the resulting function h will be as regular as the smoothness of F and H will permit.

We will be somewhat specific and consider here an integral cost functional of the fairly standard quadratic type:

$$\mathcal{J} = \frac{1}{2}\int_0^T (\rho - \rho_*)^2 + \frac{\mu}{2}\int_0^T (\alpha - \alpha_*)^2 \tag{2.7}$$

with ρ_*, α_* given. This is not quite the form considered in [**7**] but, as the argument is essentially identical, we take as proven there for *this* functional the following existence result:

Theorem 2 [[**7**]]. *Assume* **(H)**-(i, ii) *and (2.4); assume there is at least one admissible control* $\alpha \in L^\infty(\to [0,1])$ *for which one has existence on* $[0,T]$*, making* $\mathcal{J}$ *finite. Then there is an optimal boundary control* $\hat{\alpha} \in L^\infty(\to [0,1])$*, minimizing the cost functional* $\mathcal{J}$ *of (2.7), subject to (2.6), (1.3) as constraints.*

Our objective is the characterization and computation of this $\hat{\alpha}$. We will obtain the (first order) optimality condition for $\hat{\alpha}$ and will also use this to obtain some improved regularity, showing that the minimizer is actually in $H^1(0,1)$ (with greater regularity on intervals for which the constraints $0 \leq \hat{\alpha} \leq 1$ are not active. (We do this for $\mathcal{J}$ given by (2.7) but note that the arguments would be essentially the same for a variety of cost functionals of roughly similar form.)

3. Differentiability

In this section and the next we present our main theoretical results, regarding the optimality condition characterizing the optimal boundary control whose existence was shown in [**7**]. In order to obtain such conditions one needs some form of differentiability of the cost functional with respect to variation of the control α and, unfortunately, we do not even know uniqueness, much less continuity or differentiability of the dependence of the solution u on α. We approach this by observing that u depends nicely on the pair $[\alpha, h]$ if one were to consider the *uncoupled problem* and that one can then apply the Implicit Function Theorem to obtain the effect of the exogenous constraint (1.3).

THEOREM 3. *Assume* **(H)**. *Then there is a unique (weak) solution u of (2.6) in $L^2(\to \mathcal{H}) \cap L^\infty(\to L^2)$ for each admissible pair $[\alpha, h]$. This solution u (and $\omega := u(\cdot, 1)$) depend Frechet differentiably on $[\alpha, h]$.*

PROOF: The system (2.6) is of a quite standard form for a quasilinear parabolic PDE once one has obtained $\rho(\cdot)$ from h and then shifted u by the (fixed) solution $\tilde{u}$ of the *linear* equation

$$\tilde{u}_t = \rho^2 \tilde{u}_{yy} - \psi \tilde{u}_y; \qquad \tilde{u} = \alpha \;\; [y = 0]; \quad -\rho \tilde{u}_y + h\tilde{u} = h \;\; [y = 1],$$

There is then no difficulty in obtaining (by entirely standard methods, e.g., treating the nonlinearity by a contraction argument) $u - \tilde{u}$ as the unique solution of the resulting nonlinear equation (now with homogeneous BC). [We note that, at this point, there is no need for the hypotheses that $0 \le \alpha \le 1$, $0 \le u_0 \le 1$.]

Now consider the same system, replacing α by $\hat{\alpha} = \hat{\alpha}^\varepsilon := \alpha + \varepsilon\bar{\alpha}$ and h by $\hat{h} = \hat{h}^\varepsilon := h + \varepsilon\bar{h}$ with $\varepsilon \neq 0$; let the solution be $\hat{u} = \hat{u}^\varepsilon$. Note that $\alpha, h, \hat{\alpha}, \hat{h}$ are all arbitrary functions in, say, $L^2(0, T)$ except that **(H)**-(iv) holds for $h, \hat{h}$.

Now consider $\bar{u}^\varepsilon := (\hat{u}^\varepsilon - u)/\varepsilon$. This (together with the corresponding divided differences corresponding to ρ, ω, etc.) then satisfies a system which we will not bother to write out explicitly — other than to note that there is a term: $[F(u + \varepsilon\bar{u}^\varepsilon) - F(u)]/\varepsilon$ to which we may apply the Mean Value Theorem, etc.

It is not difficult to estimate $\bar{u}^\varepsilon$ with a bound (in the same space as for the existence of u) independent of ε, for $0 \neq \varepsilon$ near 0. Thus, as $\varepsilon \to 0$, one always obtains weakly convergent subsequences.

For any such subsequence one then easily sees, again by a standard argument, that the weak limit $\bar{u}$ satisfies the (formally obtained) limit system:

$$(3.1) \qquad \begin{cases} \dot{\bar{\rho}} = (2\rho h)\bar{\rho} + \rho^2 \bar{h} & \text{on } (0, T) \\ \bar{u}_t = \rho^2 \bar{u}_{yy} - \psi \bar{u}_y + F'(u)\bar{u} + a\bar{\rho} + b\bar{h} & \text{on } (0, T) \times (0, 1) \\ -\rho \bar{u}_y = -h\bar{\omega} - [h(1 - \omega)/\rho]\bar{\rho} + (1 - \omega)\bar{h} & \text{at } y = 1 \\ \bar{u} = \bar{\alpha} & \text{at } y = 0 \\ \bar{\rho} = 0 \text{ and } \bar{u} = 0 & \text{at } t = 0, \end{cases}$$

where $a := 2\rho u_{yy} - \psi_\rho u_y$, $b := -y\rho u_y$ and $\bar{\omega} := \bar{u}(\cdot, 1)$. Since (3.1) is easily seen to have a unique solution, this shows that $\bar{u}$ is, indeed, the derivative of the (nonlinear) solution map $\mathbf{U} : [\alpha, h] \mapsto u$ of (2.6) at $[\alpha, h]$ in the direction of $[\bar{\alpha}, \bar{h}]$, i.e., this solution map is differentiable with a Gateaux derivative $\mathbf{U}'(\alpha, h) : [\bar{\alpha}, \bar{h}] \mapsto \bar{u}$ defined by (3.1); our interest really will be in the induced map: $[\bar{\alpha}, \bar{h}] \mapsto \bar{\omega}$. Some caution is needed as to the space in which to consider $\bar{u}$ in view of our concerns as to the regularity of u, and so of u_{yy} appearing in a, etc. The important consideration for us is that this concern applies only near $y = 0$ and we have no difficulties at all, in this respect, in treating the trace $\bar{\omega}$ on $y = 1$, where the regularity is essentially independent of the regularity of $\hat{\alpha}$, $\bar{\alpha}$. The observation that this is actually a Frechet derivative follows on verification of the continuous dependence of the operator on $[\alpha, h]$ in L^2.

The system (3.1) is the *variational system* for the decoupled problem given by (2.6). We now consider the relation of this to the free boundary problem, obtained by coupling (2.6) with (1.3). We begin with the obvious differential corollary to the constraint (1.3):

$$\bar{h} = H_\omega \bar{\omega} + H_\rho \bar{\rho}$$

and use this to eliminate $\bar{h}$ in (3.1), obtaining

$$\text{(3.2)} \qquad \begin{cases} \dot{\bar{\rho}} = \rho c_1 \bar{\rho} + \rho d_1 \bar{\omega} & \text{on } (0, T) \\ \bar{u}_t = \rho^2 \bar{u}_{yy} - \psi \bar{u}_y + F'(u)\bar{u} + c_2 \bar{\rho} + d_2 \bar{\omega} & \text{on } (0, T) \times (0, 1) \\ -\rho \bar{u}_y = c_3 \bar{\rho} - d_3 \bar{\omega} & \text{at } y = 1 \\ \bar{u} = \bar{\alpha} & \text{at } y = 0 \end{cases}$$

with homogeneous initial condition at $t = 0$ as before and setting:

$$\begin{aligned} c_1 &:= 2h + \rho H_\rho & d_1 &:= \rho H_\omega \\ c_2 &:= 2\rho u_{yy} - \psi_\rho u_y - \rho y H_\rho & d_2 &:= -y u_y H_\omega \\ c_3 &:= (1 - \omega)[H_\rho - h/\rho] & d_3 &:= h - (1 - \omega) H_\omega \end{aligned}$$

THEOREM 4. *Assume* **(H)**-(i, ii) *and let* $\hat{\alpha}, \hat{h}, \hat{u}$, *etc., satisfy the coupled problem [(2.6), (1.3)] with, necessarily,* $\hat{\rho} > 1$ *continuous. Then (locally, for* α *in an* L^2 *neighborhood of this* $\hat{\alpha}$*) there is a (uniquely) well-defined and differentiable map:* $\alpha \mapsto [h, \omega]$ *(giving* h, u *close to* $\hat{h}, \hat{u}$*). The derivative of this is the linear map:* $\bar{\alpha} \mapsto [\bar{h}, \bar{\omega}]$*, given by (3.2). This also gives a bounded linear operator*

$$\text{(3.3)} \qquad \mathbf{L} = \mathbf{L}(\hat{\alpha}, \hat{u}) : \bar{\alpha} \mapsto \bar{\rho} : L^2(0, T) \to L^2(0, T).$$

PROOF: This will follow from the Implicit Function Theorem, applied to the map $\mathbf{D} : [\alpha, h] \mapsto [h - H(\omega, \rho)]$, as given by (2.6). It is clear that $\mathbf{D}$ is (continuously) Frechet differentiable and we must verify that $\mathbf{D}_h$ (at $[\hat{\alpha}, \hat{h}]$) is a boundedly invertible linear operator on, say, $L^2(0, T)$.

Note that $\mathbf{D}_h : \bar{h} \mapsto [\bar{h} - H_\omega \bar{\omega} + H_\rho \bar{\rho}]$, with $\bar{\omega}, \bar{\rho}$ obtained from (3.1) with $\hat{\alpha} = 0$. Since it is clear that $\bar{\omega}, \bar{\rho}$ depend compactly on $\bar{h}$, we have $\mathbf{D}_h = [\mathbf{I} + (compact)]$ and spectral theory tells us that the bounded invertibility follows if 0 is not an eigenvalue, i.e., from the observation (e.g., by a Gronwall estimate) that the system (3.2), has only the unique trivial solution when $\bar{\alpha} = 0$. The Implicit Function Theorem then asserts the local existence of a C^1 map: $\alpha \mapsto h$ giving (1.3), as desired, with derivative $[\mathbf{D}_h]^{-1}\mathbf{D}_\alpha$ — just corresponding to (3.2).

Note that this ensures that the optimal boundary control, whose existence is guaranted by Theorem 2, cannot be isolated (among admissible controls for which the free boundary problem has a solution) and that one will have (directional) differentiability of $\mathcal{J}$ with respect to the relevant 'directions' $\bar{\alpha}$ of admissible variation — where we call $\bar{\alpha}$ *admissible* provided $\alpha = \hat{\alpha} + s\bar{\alpha}$ satisfies **(H)**-(iii) for sufficiently small $s \geq 0$.

COROLLARY. *The solution map: $\alpha \mapsto u$ for the free boundary problem — as in Theorem 1 — is well-defined and continuous from $L^2((0,T) \to [0,1])$.*

PROOF: We have *local* continuity and, by [**3**], uniqueness from $H^1((0,T) \to [0,1])$ — whose density then gives global uniqueness.

4. Optimality conditions

From Theorem 4 we may differentiate $\mathcal{J}$ at $\hat{\alpha}$ (using $\hat{u}$, etc., for evaluation) to obtain

$$\langle \mathcal{J}', \bar{\alpha} \rangle = \langle \hat{\alpha} - \alpha_*, \bar{\alpha} \rangle + \mu \langle \hat{\rho} - \rho_*, \bar{\rho} \rangle \tag{4.1}$$

for every admissible variation $\bar{\alpha}$. Note that we can rewrite this as $\langle \mathcal{J}', \bar{\alpha} \rangle = \langle \hat{\alpha} - \hat{\beta}, \bar{\alpha} \rangle$ with

$$\hat{\beta} := \alpha_* + \mu \mathbf{L}^*(\hat{\rho} - \rho_*) \tag{4.2}$$

where $\mathbf{L}$ is given, as in (3.3), by (3.2).

To use this we must be able to calculate the adjoint $\mathbf{L}^*$ and we now proceed to do this. We are considering $\bar{\rho}$ related to $\bar{\alpha}$ by (3.2) and wish to find a mapping: $\zeta \mapsto \Upsilon$ such that $\int_0^T \zeta \bar{\rho} = \int_0^T \Upsilon \bar{\alpha}$.

Consider φ, v satisfying

$$\begin{cases} -\dot{\varphi} = c_1 \varphi + f_1 & \text{on } (0,T) \\ -v_t = \rho^2 v_{yy} - \psi v_y + F'(u)v & \text{on } (0,T) \times (0,1) \\ \rho v_y = f_2 & \text{at } y = 1 \\ \quad v = 0 & \text{at } y = 0 \end{cases} \tag{4.3}$$

where

$$f_1 := [\zeta + (\int_0^T c_2 v) - \rho c_3 v|_{y=1}]$$

$$f_2 := [d_1\varphi + (\int_0^T d_2 v) + [d_3 - \psi/\rho]v|_{y=1}]$$

and $\Upsilon := \rho^2 v_y|_{y=0}$ with homogeneous 'initial condition' at $t = T$ and using c_1, etc., as in (3.2). Note that the integrals appearing in the definitions of f_1 and f_2 are with respect to y, over $(0,1)$. (In particular, we have (from c_2) such an integral of $2\rho u_{yy} v$ and we use an integration by parts to rewrite this term as $-2[(1-\omega)hv|_{y=1} + \rho\int_0^T u_y v_y]$; there is some question about the regularity of u_y near $y = 0$ but we have enough regularity for v there to compensate, giving f_1 in $L^1(0,T)$.)

LEMMA 4.2. *Let* $\mathbf{L}$ *be given as in (3.3). Then the adjoint is given, through (4.3), by* $\mathbf{L}^* : \zeta \mapsto \Upsilon := \rho^2 v_y|_{y=0}$.

PROOF: From the initial conditions we have $\int_0^T [\dot{\bar\rho}\varphi + \bar\rho\dot\varphi] = 0$ and $\int_0^T\int_\Omega [\bar u_t v + \bar u v_t] = 0$. Now use the PDEs to substitute for $\bar u_t, v_t$; then integrate by parts and use the boundary conditions to obtain:

$$\int_0^T \zeta\bar\rho = \int_0^T \Upsilon\bar\alpha + \int_0^T f_1\bar\rho + \int_0^T \rho[(f_2 - d_1\varphi) - \rho v_y|_{y=1}]\bar\omega.$$

Using the identity $\int_0^T f_1\bar\rho = \int_0^T \rho d_1\varphi\bar\omega$, obtained from the ODEs, then gives $\mathbf{L}^*\zeta = \Upsilon$.

THEOREM 5. *Assume* **(H)**-(i, ii) *and (2.4) and let* $\hat\alpha, \hat u$ *be such that the cost functional* $\mathcal{J}$ *of (2.7) is minimized, subject to (2.6), (1.3), over* $\alpha \in L^\infty(\to [0,1])$. *Then the optimal boundary control* $\hat\alpha$ *is given by*

$$\hat\alpha = \begin{cases} 1 & \text{when } \alpha_* + \Upsilon \geq 1 \\ 0 & \text{when } \alpha_* + \Upsilon \leq 0 \\ \alpha_* + \Upsilon & \text{when } 0 \leq \alpha_* + \Upsilon \leq 1 \end{cases} \tag{4.4}$$

where $\Upsilon = \rho^2 v_y|_{y=0}$ *from (4.3) with* $\zeta := \mu(\hat\rho - \rho_*)$ *— and this is to be further coupled with [(2.6), (1.3)].*

PROOF: At the minimizer $\hat\alpha$ we have $\langle \mathcal{J}', \bar\alpha\rangle \geq 0$ for any admissible $\bar\alpha$. Let $\Upsilon := \rho^2 v_y|_{y=0}$ be given by (4.3) with $\zeta := \mu(\hat\rho - \rho_*)$ so (4.2) gives $\hat\beta := \alpha_* + \Upsilon$. Now, for $\varepsilon > 0$, consider $\mathcal{S} = \{t : \hat\alpha \leq (1-\varepsilon), (\hat\beta - \varepsilon)\}$ and let $\bar\alpha =$ (characteristic function of $\mathcal{S}$); one easily sees that $\bar\alpha$ is admissible. However, $(\hat\alpha - \hat\beta) \leq -\varepsilon$ on $\mathcal{S}$ so $\langle \hat\alpha - \hat\beta, \bar\alpha\rangle \leq -\varepsilon|\mathcal{S}|$ — which would contradict the non-negativity of $\langle \mathcal{J}', \bar\alpha\rangle$ unless the measure $|\mathcal{S}|$ were 0. As $\varepsilon > 0$ was arbitrary, this gives $\hat\alpha \geq \min\{1, \hat\beta\}$ ae. We get $\hat\alpha \geq \max\{0, \hat\beta\}$ ae similarly and together these give (4.4).

COROLLARY. *The optimal boundary control $\hat{\alpha}$ obtained by Theorem 2 is actually in $H^1(0,T)$ if α_* is.*

PROOF: By (4.4), it is sufficient to show that $\Upsilon \in H^1$ For which we need only see that (4.3) gives sufficient regularity for v near $y=0$. We can *almost* just cite [**6**] to get $v \in H^{1,2}$ as we have $F'(u) \in L^2$, etc. We must observe that regularity for parabolic equations localizes so we can ignore the question near $y=1$ and then note that the only relevant boundary data is that at $y=0$ — obviously smooth; the leading coefficient $\hat{\rho}^2$ is smooth enough not to interfere with this.

Our arguments do not permit us to treat the case $\mu = 0$ in (2.7) directly but it is interesting to consider this as a limit. If α_μ denotes a minimizer corresponding to $\mu > 0$, then the constraint ensures existence of a subsequence $\alpha_\mu \rightharpoonup \alpha_0$ weakly convergent in $L^2(0,T)$ for which the arguments of [**7**] give suitable convergence to a minimizer of the limit functional. It is then only necessary to pass to the limit in Theorem 5 to obtain the optimality condition for α_0; the relevant change is that we now have $\zeta = 0$ in f_1 as used in (4.3). Clearly, this argument does not preserve, for α_0, the regularity obtained in the Corollary above.

5. Numerical results

We will consider numerically the problem

$$\min_{\alpha \in U} \left\{ \mathcal{J}(\alpha) \equiv \frac{1}{2} \int_0^1 (\rho(t) - \rho_*(t))^2 \, dt \right\} \tag{5.1}$$

subject to the 'constraint' that (ρ, u) satisfies the nonlinear parabolic system (2.6) with H specifically as in (1.4) — i.e.,

$$\begin{cases} \dot{\rho}(t) = \rho(t)^2 \big(u(t,1) - \gamma_0 e^{\delta\rho(t)/(\rho(t)-1)}\big), \; t \in (0,1) \\ \dot{u}(t,y) = \rho(t)^2 u_{yy}(t,y) - \rho(t) \left[\dfrac{\rho(t)}{\rho(t)-y} + y\big(u(t,1) - \gamma_0 e^{1/(1-1/\rho(t))}\big) \right] u_y, \\ \qquad\qquad\qquad\qquad y \in (0,1), \; t \in (0,1) \end{cases} \tag{5.2}$$

with the boundary conditions

$$\begin{cases} u(t,0) = \alpha(t) \\ u_y(t,1) = -\dfrac{1}{\rho(t)} (1 - u(t,1)) \big(u(t,1) - \gamma_0 e^{1/(1-1/\rho(t))}\big), \; t \in (0,1) \end{cases} \tag{5.3}$$

and the initial conditions

$$\begin{cases} \rho(0) = \rho_0 \\ u(0,y) = u_0(y), \qquad y \in (0,1). \end{cases} \tag{5.4}$$

Note that (5.1) corresponds to (2.7) with $\mu = 0$. The set of admissible controls is $U = \{\alpha \mid \alpha_{\min} \le \alpha \le \alpha_{\max}\}$.

One can derive discrete analogues to (5.1)–(5.4) in standard ways: we have employed the trapezoidal rule for computing $J(\alpha)$, the finite element method with linear elements for the spatial discretization of (5.2)–(5.3), and the implicit Euler method for time discretization. The resulting nonlinear state system can then be solved, for example, by a combination of Newton and overrelaxation methods. In order to apply efficient nonlinear programming algorithms for minimizing the discretized cost functional $\mathcal{J}$, one must be able to compute the (discretized) gradient $\nabla_\alpha \mathcal{J}$. This can be done in a well known manner by applying the adjoint state technique for the discretized state system (see [**4**]).

Example 5.1. In (5.1)–(5.4) let $\rho_*(t) = 2 + 2t$ (i.e., $R_*(t) = 1 - 1/(2+2t)$), $\gamma_0 = 0.01$, $\rho_0 = 2$ and $u_0(y) = -y(y-2)$ (i.e.

$$C(0,r) = C_0(r) = \begin{cases} 1, & 0 \le r \le 1/2 \\ -4r(r-1), & 1/2 < r \le 1 \text{).} \end{cases}$$

In the numerical results presented here we have taken $\Delta y = 1/20$ for the space discretization and $\Delta t = 1/20$ for the time discretization. As a result one has 21 unknowns in the minimization of $\mathcal{J}$. The conjugate gradient algorithm with box constraints $\alpha_{\min} = 0.05$ and $\alpha_{\max} = 0.85$ was then used for this minimization.

As an initial guess for α we have chosen a constant control, $\alpha(t) \equiv 0.15$ (Figure 5.1). Figure 5.2 shows $R(t)$ (— line) and $R_*(t)$ (--- line). In Figure 5.3 we see the corresponding concentration $C(t,r)$.

In Figure 5.4 we then see the numerical approximation to the optimal control α after 3 iterations of the conjugate gradient algorithm. Figure 5.5 shows corresponding value of $R(t)$ (— line) and $R_*(t)$ (--- line) and Figure 5.6 shows the corresponding values of the evolving concentration.

Figure 5.1

Figure 5.2

Figure 5.3

Figure 5.4

Figure 5.5

Figure 5.6

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A forthcoming paper of the authors' will provide further details on the numerical realization of algorithms for finding optimal controls in such crystal growth/dissolution problems.

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