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# THE UNIQUENESS OF INITIAL CONTROL FOR AN ADSORBATE-INDUCED PHASE TRANSITION MODEL

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ABSTRACT. In this paper we are concerned with the uniqueness of initial control for an adsorbate-induced phase transition model. That is, by showing the convexity of the cost functional, we prove that there exists a unique initial control.

## 1. INTRODUCTION

We consider the following initial control problem

$$\text{(P)} \qquad \text{minimize } J(u,v)$$

with the cost functional $J(u,v)$ of the form

$$J(u,v) = \int_0^T \|y(u,v)-y_d\|^2_{H^3(\Omega)}dt + \int_0^T \|\rho(u,v)-\rho_d\|^2_{H^2(\Omega)}dt$$
$$+\gamma\{\|u\|^2_{H^3(\Omega)} + \|v\|^2_{H^2(\Omega)}\}, \qquad (u,v) \in H^3(\Omega)\times H^2(\Omega),$$

where $y = y(u,v)$ and $\rho(u,v)$ is governed by the adsorbate-induced phase transition model:

$$(1.1) \qquad \begin{aligned} &\frac{\partial y}{\partial t} = a\Delta y - dy(y+\rho-1)(1-y) && \text{in } \Omega\times(0,T],\\ &\frac{\partial \rho}{\partial t} = b\Delta\rho + c\nabla\cdot\{\rho(1-\rho)\nabla\chi(y)\} - fe^{\alpha\chi(v)}\rho \\ &\qquad\qquad -g\rho + h(1-\rho) && \text{in } \Omega\times(0,T],\\ &\frac{\partial y}{\partial n} = \frac{\partial \rho}{\partial n} = 0 && \text{on } \partial\Omega\times(0,T],\\ &y(x,0)=u(x), \quad \rho(x,0)=v(x) && \text{in } \Omega. \end{aligned}$$

Here, $\Omega$ is a bounded region in $\mathbb{R}^2$ of $C^3$ class. $n = n(x)$ is the outer normal vector at a boundary point $x \in \partial\Omega$ and $\frac{\partial}{\partial n}$ denotes the differentiation along the vector $n$. $y(x,t)$ denotes the order parameter which represents the structural state of the surface at a position $x \in \Omega$ and a time $t \in [0,\infty)$, and $\rho(x,t)$ the adsorbate coverage of the surface $\Omega$ by a specific kind of molecules. $\chi(y)$ is assumed to be given smooth function for $y$, prototype of $\chi(y)$ is

$$\chi(y) = -y^2(3-2y).$$

$a$ and $b$ are positive diffusion constants. $c, d, f, g, h, \alpha$ and $\gamma$ are assumed to be positive constants. We refer to [5] and [7] for the physical background of (1.1).

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In many situations, the initial condition of the state is unknown or only known partially. This kind of problem is formulated as an nonlinear optimal control problem with the initial value serving as the control variable. Many papers have been published to study the nonlinear control problem ([1], [2], [3], [6]). Recently, Ryu and Jung [9] studied the initial control for an adsorbate-induced phase transition model. In that paper they showed the existence of the initial control and obtained the optimality conditions. In this paper, by showing the convexity of the cost functional, we prove that there exists a unique initial control.

The paper is organized as follows. In Section 2, we recall some known results. Section 3 is devoted to obtaining the uniqueness of the initial control.

**Notations.** $\mathbf{R}$ denotes the sets of real numbers. Let $I$ be an interval in $\mathbf{R}$. $L^p(I;\mathcal{H})$, $1 \le p \le \infty$, denotes the $L^p$ space of measurable functions in $I$ with values in a Hilbert space $\mathcal{H}$. $\mathcal{C}(I;\mathcal{H})$ denotes the space of continuous functions in $I$ with values in $\mathcal{H}$. For simplicity, we shall use a universal constant $C$ to denote various constants which are determined in each occurrence in a specific way by $\delta, M$, and so forth.

## 2. Formulation of problem

Let $A_1 = -a\Delta + a$ and $A_2 = -d\Delta + g$ with the same domain $\mathcal{D}(A_i) = H^2_n(\Omega) = \{z \in H^2(\Omega); \frac{\partial z}{\partial n} = 0 \text{ on } \partial\Omega\}$ $(i = 1, 2)$. Then, $A_i$ are two positive definite self-adjoint operators in $L^2(\Omega)$. $\mathcal{D}(A_i^\theta) = H^{2\theta}(\Omega)$ for $0 \le \theta < \frac{3}{4}$, and $\mathcal{D}(A_i^\theta) = H^{2\theta}_n(\Omega)$ for $\frac{3}{4} < \theta \le \frac{3}{2}$ (see [11]). We set two product Hilbert spaces $\mathcal{V} \subset \mathcal{H}$ as

$$\mathcal{V} = H^3_n(\Omega) \times H^2_n(\Omega), \quad \mathcal{H} = H^2_n(\Omega) \times H^1(\Omega).$$

By identifying $\mathcal{H}$ with its dual space, we consider $\mathcal{V} \subset \mathcal{H} = \mathcal{H}' \subset \mathcal{V}'$. It is then seen that

$$\mathcal{V}' = H^1(\Omega) \times L^2(\Omega),$$

with the duality product

$$\langle \Phi, Y \rangle_{\mathcal{V}' \times \mathcal{V}} = \langle A_1^{1/2}\zeta, A_1^{3/2} y \rangle_{L^2} + (\varphi, A_2\rho)_{L^2}, \quad \Phi = \begin{pmatrix} \zeta \\ \varphi \end{pmatrix}, \; Y = \begin{pmatrix} y \\ \rho \end{pmatrix}.$$

We denote the norms of $\mathcal{V}$, $\mathcal{H}$, and $\mathcal{V}'$ by $\|\cdot\|$, $|\cdot|$, and $\|\cdot\|_*$, respectively. $(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle$ denote the scalar product of $\mathcal{H}$ and the pairing between $\mathcal{V}$ and $\mathcal{V}'$. We denote the scalar products in $\mathcal{V}$ and $\mathcal{V}'$ by $\langle\cdot,\cdot\rangle_{\mathcal{V}}$ and $\langle\cdot,\cdot\rangle_{\mathcal{V}'}$, respectively.

We set also a symmetric bilinear form on $\mathcal{V} \times \mathcal{V}$:

$$a(Y, \tilde{Y}) = (A_1 y, A_1 \tilde{y})_{L^2} + (A_2^{1/2}\rho, A_2^{1/2}\tilde{\rho})_{L^2}, \qquad Y = \begin{pmatrix} y \\ \rho \end{pmatrix}, \tilde{Y} = \begin{pmatrix} \tilde{y} \\ \tilde{\rho} \end{pmatrix} \in \mathcal{V}.$$

Obviously, the form satisfies

$$|a(Y,\tilde{Y})| \le M\|Y\|\|\tilde{Y}\|, \quad Y, \tilde{Y} \in \mathcal{V}, \tag{2.1}$$

$$a(Y,Y) \ge \delta\|Y\|^2, \quad Y \in \mathcal{V} \tag{2.2}$$

with some $\delta$ and $M > 0$. This form then defines a linear isomorphism $A = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$ from $\mathcal{V}$ to $\mathcal{V}'$, and the part of $A$ in $\mathcal{H}$ is a positive definite self-adjoint operator in $\mathcal{H}$ with the domain $\mathcal{D}(A) = H^4_n(\Omega) \times H^3_n(\Omega)$.

(1.1) is, then, formulated as an abstract equation

$$\text{(2.3)} \qquad \begin{cases} \dfrac{dY}{dt} + AY = F(Y), \quad 0 < t \le T, \\ Y(0) = U \end{cases}$$

in the space $\mathcal{V}'$. Here, $F(\cdot) : \mathcal{V} \to \mathcal{V}'$ is the mapping

$$F(Y) = \begin{pmatrix} ay + dy(y+\rho-1)(1-y) \\ c\nabla \cdot \{\rho(1-\rho)\nabla\chi(y)\} - fe^{\alpha\chi(y)}\rho + h(1-\rho) \end{pmatrix}, \qquad Y = \begin{pmatrix} y \\ \rho \end{pmatrix}.$$

Here, $U$ is defined by $U = \binom{u}{v}$.

As verified in [10, Sec. 3], $F(\cdot)$ satisfies the following conditions:

(f.i) For each $\eta > 0$, there exists an increasing continuous function $\phi_\eta : [0,\infty) \to [0,\infty)$ such that

$$\|F(Y)\|_* \le \eta\|Y\| + \phi_\eta(|Y|), \quad Y \in \mathcal{V},$$
$$|F(Y)| \le \eta\|Y\|_{\mathcal{D}(A)} + \phi_\eta(\|Y\|), \quad Y \in \mathcal{D}(A).$$

(f.ii) For each $\eta > 0$, there exists an increasing continuous function $\psi_\eta : [0,\infty) \to [0,\infty)$ such that

$$\|F(\tilde{Y}) - F(Y)\|_* \le \eta\|\tilde{Y} - Y\| + (\|\tilde{Y}\| + \|Y\| + 1)\psi_\eta(|\tilde{Y}| + |Y|)|\tilde{Y} - Y|, \quad \tilde{Y}, Y \in \mathcal{V},$$
$$|F(\tilde{Y}) - F(Y)| \le \eta\|\tilde{Y} - Y\|_{\mathcal{D}(A)} + (\|\tilde{Y}\|_{\mathcal{D}(A)} + \|Y\|_{\mathcal{D}(A)} + 1)\psi_\eta(\|\tilde{Y}\| + \|Y\|)\|\tilde{Y} - Y\|, \quad \tilde{Y}, Y \in \mathcal{D}(A).$$

Furthermore, $F(\cdot)$ is first-order Fréchet differentiable with the derivative

$$F'(Y)Z = \begin{pmatrix} az + dz(y+\rho-1)(1-2y) + dy(z+w)(1-y) \\ c\nabla\{w(1-2\rho)\nabla\chi(y)\} + c\nabla\{\rho(1-\rho)\nabla(\chi'(y)z)\} - f\alpha\chi'(y)ze^{\alpha\chi(y)}\rho \\ -fe^{\alpha\chi(y)}w - hw \end{pmatrix},$$
$$Y = \begin{pmatrix} y \\ \rho \end{pmatrix}, \; Z = \begin{pmatrix} z \\ w \end{pmatrix}.$$

$F'(\cdot)$ satisfies the following estimates (cf. [10, Sec. 3]):

(f.iii) For each $\eta > 0$, there exists an increasing continuous function $\mu_\eta : [0,\infty) \to [0,\infty)$ such that

$$|\langle F'(Y)Z, P\rangle| \le \begin{cases} \eta\|Z\|\|P\| + (\|Y\| + 1)\mu_\eta(|Y|)|Z|\|P\|, & Y, Z, P \in \mathcal{V}, \\ \eta\|Z\|\|P\| + (\|Y\| + 1)\mu_\eta(|Y|)\|Z\||P|, & Y, Z, P \in \mathcal{V}. \end{cases}$$

(f.iv) There exists an increasing continuous function $\nu : [0,\infty) \to [0,\infty)$ such that

$$\|F'(\tilde{Y})Z - F'(Y)Z\|_* \le C\|Z\|(1 + \|\tilde{Y}\| + \|Y\|)\nu(|\tilde{Y}| + |Y|)|\tilde{Y} - Y|, \quad \tilde{Y}, Y, Z \in \mathcal{V}.$$

We then obtain the following result (For the proof, see Ryu and Yagi [8]).

**Theorem 2.1.** *Let* (2.1), (2.2), (f.i), *and* (f.ii) *be satisfied. Then, for any* $U \in \mathcal{V}$, *there exists a unique weak solution*

$$Y \in H^1(0,T(U);\mathcal{H}) \cap \mathcal{C}([0,T(U)];\mathcal{V}) \cap L^2(0,T(U);\mathcal{D}(A))$$

*to* (2.3), *the number* $T(U) > 0$ *is determined by the norm* $\|U\|$.

Now, let $\mathcal{U}_{ad}$ be a closed, bounded, and convex subset in $\mathcal{V}$ and let $S > 0$ be such that for each $U \in \mathcal{U}_{ad}$, (2.3) has a unique weak solution $Y(U) \in H^1(0,S;\mathcal{H}) \cap \mathcal{C}([0,S];\mathcal{V}) \cap L^2(0,S;\mathcal{D}(A))$. Thus the problem (**P**) is obviously formulated as follows:

$$(\overline{\mathbf{P}}) \qquad \text{minimize } J(U),$$

where

$$J(U) = \int_0^S \|Y(U) - Y_d\|^2 dt + \gamma\|U\|^2, \quad U \in \mathcal{U}_{ad}.$$

Here, $Y_d = \binom{y_d}{\rho_d}$ is a fixed element of $L^2(0,S;\mathcal{V})$. $\gamma$ is a positive constant.

By using the compactness of the embedding $\mathcal{V} \hookrightarrow \mathcal{H}$, we obtain the existence of an optimal control $\overline{U} \in \mathcal{U}_{ad}$ for $(\overline{\mathbf{P}})$ (cf. [9, Theorem 2.1]). Moreover, the differentiability of $Y(U)$ with respect to $U$ is obtained.

**Proposition 2.2.** The mapping $Y : \mathcal{U}_{ad} \to H^1(0,S;\mathcal{V}') \cap \mathcal{C}([0,S];\mathcal{H}) \cap L^2(0,S;\mathcal{V})$ is Gâteaux differentiable with respect to $U$. For $V \in \mathcal{U}_{ad}$, $Y'(U)V = Z$ is the unique solution in $H^1(0,S;\mathcal{V}') \cap \mathcal{C}([0,S];\mathcal{H}) \cap L^2(0,S;\mathcal{V})$ of the problem

$$(2.4) \qquad \begin{aligned} &\frac{dZ}{dt} + AZ - F'(Y)Z = 0, \quad 0 < t \le S, \\ &Z(0) = V. \end{aligned}$$

which satisfies

$$(2.5) \qquad |Z|^2 + \int_0^S \|Z(t)\|^2 dt \le C\|V\|^2.$$

Proof. The Gâteaux differentiability of $Y(U)$ was proved in [9, Proposition 3.2]. Therefore, the only thing to be prove here is the estimate (2.5) which will be useful in the next section.

Taking the scalar product of the equation of (2.4) with $Z$ and using (f.iii), we obtain that for $0 < t < S$,

$$(2.6) \qquad \frac{d}{dt}|Z(t)|^2 + \delta\|Z(t)\|^2 \le (\|Y\|^2 + 1)\tilde{\mu}(|Y|^2)|Z(t)|^2,$$

where $\tilde{\mu} : [0,\infty) \to [0,\infty)$ is some increasing continuous function. Using Gronwall's inequality and $|\cdot| \le C\|\cdot\|$, we obtain

$$|Z(t)|^2 \le |V|^2 e^{\int_0^S (\|Y\|^2+1)\tilde{\mu}(|Y|^2)ds} \le C\|V\|^2.$$

Using this result in (2.6) and integrating from 0 and $t$, we have

$$\int_0^S \|Z(t)\|^2 dt \le C\|V\|^2. \quad \Box$$

With aid of Proposition 2.2, the optimality conditions for $(\overline{\mathbf{P}})$ are verified (For the proof, see [9, Theorem 3.3]).

**Theorem 2.3.** Let $\overline{U}$ be an optimal control of $(\overline{\mathbf{P}})$ and let $\overline{Y} \in H^1(0,S;\mathcal{H}) \cap \mathcal{C}([0,S];\mathcal{V}) \cap L^2(0,S;\mathcal{D}(A))$ be the optimal state, that is $\overline{Y}$ is the solution to (2.3) with the control $\overline{U}$. Then, there exists a unique solution $P \in H^1(0,S;\mathcal{V}') \cap C([0,S];\mathcal{H}) \cap L^2(0,S;\mathcal{V})$ to the linear problem

$$-\frac{dP}{dt} + AP - F'(\overline{Y})^* P = \Lambda(\overline{Y} - Y_d), \quad 0 \le t < S,$$
$$P(S) = 0$$

in $\mathcal{V}'$, where $\Lambda : \mathcal{V} \to \mathcal{V}'$ is a canonical isomorphism; moreover, $\overline{U}$ satisfy

$$\langle \frac{1}{\gamma} P(0) + \Lambda\overline{U}, V - \overline{U} \rangle \ge 0 \qquad \text{for all } V \in \mathcal{U}_{ad}.$$

## 3. Uniqueness of the initial control

In this section we obtain the uniqueness of the initial control for the problem $(\overline{\mathbf{P}})$. By a direct calculation, the mapping $F(\cdot) : \mathcal{V} \to \mathcal{V}'$ is second-order Fréchet differentiable and have the following derivatives

$$F''(Y)(Z,Z) = \begin{pmatrix} d\Big(z(z+w)(2-3y) - 2z^2(y+\rho-1) - y(z+w)z\Big) \\ c\Big(-2\nabla\{w^2\nabla\chi(y)\} + 2\nabla\{w(1-2\rho)\nabla(\chi'(y)z)\} + \nabla\{\rho(1-\rho)\nabla(\chi''(y)(z,z))\}\Big) \\ -f\Big((\alpha\chi'(y)z)^2 + \alpha\chi''(y)(z,z)\Big)e^{\alpha\chi(y)}\rho - 2f\alpha\chi'(y)ze^{\alpha\chi(y)}w \end{pmatrix},$$
$$Y = \begin{pmatrix} y \\ \rho \end{pmatrix}, \ Z = \begin{pmatrix} z \\ w \end{pmatrix}.$$

and we have the following estimate.

**Lemma 3.1.** (f.v) There exists an increasing continuous function $\kappa : [0,\infty) \to [0,\infty)$ such that

$$\|F''(Y)(Z,Z)\|_* \le (\|Y\| + 1)\kappa(|Y|)\|Z\||Z|, \qquad Y, Z \in \mathcal{V}.$$

Proof. The proof is similar to that of [10, Sec. 3]. □

Now we prove second-order Gâteaux differentiability of $Y(U)$ which will be useful in the next.

**Proposition 3.2.** The mapping $Y : \mathcal{U}_{ad} \to H^1(0,S;\mathcal{V}') \cap C([0,S];\mathcal{H}) \cap L^2(0,S;\mathcal{V})$ is second-order Gâteaux differentiable with respect to $U$. For $V \in \mathcal{U}_{ad}$, $Y''(U)(V,V) = \Phi$ is the unique solution in $H^1(0,S;\mathcal{V}') \cap C([0,S];\mathcal{H}) \cap L^2(0,S;\mathcal{V})$ of the problem

$$\frac{d\Phi}{dt} + A\Phi - F''(Y)(Z,Z) - F'(Y)\Phi = 0, \quad 0 < t \le S, \qquad (3.1)$$
$$\Phi(0) = 0,$$

where $Z = Y'(U)V$ and $\Phi$ satisfies

$$|\Phi(t)| + \int_0^S \|\Phi(t)\|^2 dt \le C\|V\|^4. \qquad (3.2)$$

Proof. Similar arguments as [9, Proposition 3.2] can be applied to second-order Gateaux derivative. On the other hand, we consider the linear problem (3.1). From (2.1), (2.2), (f.i), (f.ii), (f.iii), and (f.v), we can easily verify that (3.1) possesses a unique weak solution $\Phi \in H^1(0,S;\mathcal{V}') \cap C([0,S];\mathcal{H}) \cap L^2(0,S;\mathcal{V})$ on $[0,S]$ (cf. [4, Chap. XVIII, Theorem 2]). Therefore, we only prove the estimate (3.2).

Taking the scalar product of the equation of (3.1) with $\Phi$ and using (f.iii) and (f.v), we obtain that for $0 < t < S$,

$$(3.3)\quad \frac{1}{2}\frac{d}{dt}|\Phi(t)|^2 + \delta\|\Phi(t)\|^2 \\ \leq \frac{\delta}{2}\|\Phi\|^2 + (\|Y\|^2+1)\tilde{\kappa}(|Y|^2)\|Z\|^2|Z|^2 + (\|Y\|^2+1)\tilde{\mu}(|Y|^2)|\Phi|^2,$$

where $\tilde{\kappa}, \tilde{\mu} : [0,\infty) \to [0,\infty)$ are some increasing continuous functions. Therefore, by Gronwall's inequality and $Y \in \mathcal{C}(0,S;\mathcal{V})$, we obtain

$$\begin{aligned} |\Phi(t)|^2 &\leq e^{\int_0^S (\|Y\|^2+1)\tilde{\mu}(|Y(s)|^2)ds} \int_0^S (\|Y\|^2+1)\tilde{\kappa}(|Y|^2)\|Z(s)\|^2|Z(s)|^2 ds \\ &\leq C\|Z\|^2_{L^2(0,S;\mathcal{V})}\|Z\|^2_{L^\infty(0,S;\mathcal{H})} \end{aligned}$$

and thus, by (2.5),

$$|\Phi(t)|^2 \leq C\|V\|^4.$$

Using this result in (3.3) and integrating from 0 and $t$, we have

$$\int_0^S \|\Phi(t)\|^2 dt \leq C\|V\|^4. \quad \square$$

**Theorem 3.3.** If the time interval $[0,S]$ is short enough, then there is a unique initial control for $(\overline{\mathbf{P}})$.

PROOF. We show uniqueness by showing strict convexity of the following map:

$$U \in \mathcal{U}_{ad} \to J(U).$$

This convexity follows from showing for all $U, V \in \mathcal{U}_{ad}$, $0 < h < 1$,

$$g''(h) > 0,$$

where $g(h) = J(U + h(V-U))$ (cf. [12, Sec. 25.5.]).

We denote $Y^h = Y(U + h(V-U))$. By a direct calculation, we have

$$g''(h) = \int_0^S \langle \Phi, D^*\Lambda(DY^h - Y_d)\rangle dt + \int_0^S \|DZ\|^2 dt + \gamma\|V-U\|^2,$$

where $Z$ is the solution of

$$\begin{aligned} &\frac{dZ}{dt} + AZ - F'(Y^h)Z = 0, \quad 0 < t \leq S, \\ &Z(0) = V - U \end{aligned}$$

and $\Phi$ is the solution of

$$\begin{aligned} &\frac{d\Phi}{dt} + A\Phi - F''(Y^h)(Z,Z) - F'(Y^h)\Phi = 0, \quad 0 < t \leq S, \\ &\Phi(0) = 0. \end{aligned}$$

Therefore, by (2.5) and (3.2), we infer that

$$(3.4)\quad \int_0^S \|\Phi\|^2 dt \leq C\|V-U\|^4.$$

By using (3.4), we have

$$\begin{aligned} g''(h) &\geq -\Big(\int_0^S \|\Phi\|^2 dt\Big)^{1/2}\Big(\int_0^S \|D^*\|^2_{\mathcal{L}}\|DY^h - Y_d\|^2 dt\Big)^{1/2} + \gamma\|V-U\|^2 \\ &\geq (\gamma - C\|D^*\|_{\mathcal{L}}\|DY^h - Y_d\|_{L^2(0,S;\mathcal{V})})\|V-U\|^2, \end{aligned}$$

where $\|\cdot\|_{\mathcal{L}}$ denotes the operator norm. Thus, for fixed $\gamma > 0$, we may choose $S > 0$ small enough so that $\gamma - C\|D^*\|_{\mathcal{L}}\|Y^h - Y_d\|_{L^2(0,S;\mathcal{V})} \geq \alpha > 0$. Hence, we obtain the desired result. □

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# 피흡착질에 의하여 유도된 상전이 모델에 대한 초기치 제어의 유일성 문제

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## 요 약

본 논문에서는 피흡착질에 의하여 유도된 상전이 모델에 대한 초기치 제어의 유일성 문제를 다루고 있다. 구체적으로 비용함수의 제어에 대한 볼록성(convexity)을 보임으로서 초기치 제어의 유일성을 증명하였다.