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DEPOSITION REACTOR**

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OPTIMAL CONTROL OF CHEMICAL VAPOR DEPOSITION REACTOR

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Abstract. We study a simple model of chemical vapor deposition on a silicon wafer. The control is a flux of chemical species, and the objective is to grow the semiconductor film so that its surface attains, as nearly as possible, a prescribed profile. The surface is spatially fast oscillating due to the small feature scale, and therefore the problem is formulated in terms of its homogenized approximation. We prove that the optimal control is bang-bang, and we use this information to develop a numerical scheme for computing the optimal control.

1. The Problem. Chemical vapor deposition is one of the steps in semiconductor processing. Figure 1 shows schematically a chemical vapor deposition reactor with silicon wafer placed on a table. A flux g of chemical species (plasma) is injected from the top, and it diffuses onto the wafer. The feature size on the semiconductor surface is submicron, approximately 10^{-6} the linear size of the reactor. Because of the small feature size, the evolving surface of the semiconductor film affects the actual deposition of the plasma on the film, and must therefore be taken into account in the model.

A problem of interest is: How to choose the control variable g so that the surface of the film will approximate a prescribed desired profile.

We shall consider a simple model where the reactor is a 2-d rectangle:

$$\Omega_0 = \{(x_1, x_2); \quad -a < x_1 < a, \quad 0 < x_2 < b\}$$

and the wafer occupies the entire base

$$\Gamma = \{(x_1, 0); \quad -a < x_1 < a\}.$$

The surface of the film over the wafer is then a moving boundary

$$\Gamma_\varepsilon(t) : \quad x_2 = \varepsilon f_\varepsilon(x_1, t), \quad -a < x_1 < a$$

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Figure 1.

where ε is a small positive parameter, of the same order of magnitude as the feature size. We expect f_ε to be nonnegative, and set

$$\Omega_\varepsilon(t) = \{(x_1, x_2) \in \Omega_0; \varepsilon f_\varepsilon(x_1, t) < x_2 < b\}.$$

We assume that the plasma consists of just one active species with concentration u , and that u satisfies the diffusion equation

$$(1.1) \quad u_t - \Delta u = 0 \quad \text{for } x = (x_1, x_2) \in \Omega_\varepsilon(t),$$

and the boundary conditions

$$(1.2) \quad \frac{\partial u}{\partial n} = g \quad \text{on } \Gamma_b = \{(x_1, b); -a < x_1 < a\},$$

$$(1.3) \quad \frac{\partial u}{\partial x_1} = 0 \quad \text{on } x_1 = \pm a,$$

$$(1.4) \quad \frac{\partial u}{\partial n} + p(x_1, \frac{x_1}{\varepsilon})u = 0 \quad \text{on } \Gamma_\varepsilon(t)$$

where n is the outward normal.

Setting

$V_N =$ velocity of points on $\Gamma_\varepsilon(t)$ in the direction n ,

the equation of the continuity is

$$V_N = \varepsilon \frac{\partial u}{\partial n},$$

or, by (1.4),

$$(1.5) \quad V_N = -\varepsilon p u \quad \text{on } \Gamma_\varepsilon(t).$$

Finally, we prescribe initial conditions

$$(1.6) \quad u(x, 0) = 0, \quad f_\varepsilon(x_1, 0) = f_0(x_1, \frac{x_1}{\varepsilon}).$$

Our basic assumptions on p and f_0 are:

$$(1.7) \quad \begin{aligned} (a) \quad & p(x_1, \xi_1) \text{ and } f_0(x_1, \xi_1) \text{ are smooth functions in} \\ & (x_1, \xi_1) \in [-a, a] \times \mathbb{R}, \text{ 1-periodic in } \xi_1, \\ (b) \quad & p_{x_1}(\pm a, \xi_1) = p_{\xi_1}(\pm a, \xi_1) \equiv 0, \quad (f_0)_{x_1}(\pm a, \xi_1) = (f_0)_{\xi_1}(\pm a, \xi_1) \equiv 0, \\ (c) \quad & p(x_1, \xi_1) \geq p_0 > 0, \quad f_0(x_1, \xi_1) \geq 0. \end{aligned}$$

Note that (1.5) can be written in the form

$$(1.8) \quad \frac{\partial f_\varepsilon}{\partial t} = p u \left\{ 1 + \left(\frac{\partial(\varepsilon f_\varepsilon)}{\partial x_1} \right)^2 \right\}^{1/2} \quad \text{on } \Gamma_\varepsilon(t).$$

The function $g = g(x_1, t)$ is a control variable defined in the rectangle

$$Q = \{(x_1, t); \quad -a \leq x_1 \leq a, \quad 0 \leq t \leq T\}.$$

We shall consider two classes of control sets:

$$\begin{aligned} \mathfrak{A} &= \{g \in L^\infty(Q); \quad 0 \leq g \leq K\}, \\ \mathfrak{A}_M &= \{g \in L^\infty(Q); \quad 0 \leq g \leq K, \quad \int_Q g dx_1 dt \leq M\} \end{aligned}$$

where $KT > M$.

Friedman and Hu [6] proved that for any $g \in \mathfrak{A}$ there exists a unique classical solution $(u_\varepsilon, f_\varepsilon)$ of (1.1)–(1.7) for $0 \leq t \leq T_0$, where T_0 depends only on K , and

$$(1.9) \quad \max_{0 \leq t \leq T_0} \|u_\varepsilon - u_0\|_{L^2(\Omega_\varepsilon(t))} \leq C\varepsilon,$$

$$(1.10) \quad \max_{0 \leq t \leq T_0} \left\| f_\varepsilon(x_1, t) - f\left(x_1, \frac{x_1}{\varepsilon}, t\right) \right\|_{L^2(\Omega_\varepsilon(t))} \leq C\varepsilon;$$

here (u_0, f) form the unique solution of the homogenized problem

$$(1.11) \quad \frac{\partial u_0}{\partial t} - \Delta u_0 = 0 \quad \text{for } x \in \Omega_0,$$

$$(1.12) \quad \frac{\partial u_0}{\partial n} = g(x_1, t) \quad \text{on } \Gamma_b = \{x_2 = b\},$$

$$(1.13) \quad \frac{\partial u_0}{\partial x_1} = 0 \quad \text{on } \{x_1 = \pm a\},$$

$$(1.14) \quad \frac{\partial u_0}{\partial n} + Pu_0 = 0 \quad \text{on } \Gamma = \{x_2 = 0\},$$

$$(1.15) \quad u_0(x, 0) = 0 \quad \text{on } \Omega_0$$

where

$$(1.16) \quad P(x_1, t) = \int_0^1 p(x_1, \xi_1) \left[1 + (f_{\xi_1}(x_1, \xi_1, t))^2 \right]^{1/2} d\xi_1,$$

and

$$(1.17) \quad \begin{aligned} f_t(x_1, \xi_1, t) &= p(x_1, \xi_1) u_0(x_1, 0, t) \left[1 + (f_{\xi_1}(x_1, \xi_1, t))^2 \right]^{1/2}, \\ f(x_1, \xi_1, 0) &= f_0(x_1, \xi_1). \end{aligned}$$

Let $G(x_1, \xi_1, s)$ be the solution of the hyperbolic equation

$$(1.18) \quad \frac{\partial G}{\partial s} = p(x_1, \xi_1) \left[1 + G_{\xi_1}^2 \right]^{1/2}, \quad 0 \leq s \leq S,$$

with initial condition

$$(1.19) \quad G(x_1, \xi_1, 0) = f_0(x_1, \xi_1).$$

Then we can represent f in the form

$$(1.20) \quad f(x_1, \xi_1, t) = G\left(x_1, \xi_1, \int_0^t u_0(x_1, 0, \tau) d\tau\right).$$

Note that S can be taken to be any positive number such that the characteristics of (1.18), (1.19) do not intersect each other for all times $0 \leq s \leq S$.

One can check that the function

$$\|g\|_{L^\infty} \cdot \left(x_2 + \frac{1}{p_0} \right)$$

satisfies (1.11)–(1.15) with “ $\geq$ ” in (1.12), (1.14), (1.15), and consequently it is $\geq u_0$.

Hence

$$(1.21) \quad 0 \leq u_0 \leq K \left(b + \frac{1}{p_0} \right).$$

As in the proof of Theorem 5.1 in [6] one can then show that T_0 can be taken to be any number satisfying

$$T_0 \leq T, \quad T_0 K \left(b + \frac{1}{p_0} \right) \leq S$$

provided ε is small enough, say $\varepsilon \leq \varepsilon_0$. We shall henceforce choose T such that

$$T \leq \frac{S}{K(1 + 1/p_0)}$$

and take $0 < \varepsilon < \varepsilon_0$; then for any $g \in \mathfrak{A}$ there exists a unique classical solution of (1.1)–(1.7) for $0 \leq t \leq T$.

Let $c_\varepsilon(x_1, t)$ be a positive continuous function for $(x_1, t) \in Q$, and let $\psi(t)$ be a continuous positive function for $0 \leq t \leq T$. We introduce the functional

$$\tilde{J}[g] = \int_0^T \int_{-a}^a \psi(t) \left(f_\varepsilon(x_1, t) - c_\varepsilon(x_1, t) \right)^2 dx_1 dt.$$

We wish to find g which minimizes this functional.

In view of the estimate (1.10), if we replace $f_\varepsilon(x_1, t)$ by $f(x_1, x_1/\varepsilon, t)$ we incur a small error, $O(\varepsilon)$. We shall henceforce make this replacement, and also take c_ε to have the form:

$$(1.22) \quad c_\varepsilon = c(x_1, x_1/\varepsilon, t) \text{ where } c(x_1, \xi_1, t) \text{ is a continuous positive function for } -a \leq x_1 \leq a, \xi_1 \in \mathbb{R}, 0 \leq t \leq T, \text{ 1-periodic in } \xi_1.$$

The functional we shall consider is

$$(1.23) \quad J[g] = \int_0^T \int_{-a}^a \int_0^1 \psi(t) \left(f(x_1, \xi_1, t) - c(x_1, \xi_1, t) \right)^2 d\xi_1 dx_1 dt.$$

Problem (P).

$$(1.24) \quad \text{minimize } \{J[g]; \quad g \in \mathfrak{A}\}$$

where (f, u_0) is the solution of (1.11)–(1.17).

Problem (P_M).

$$(1.25) \quad \text{minimize } \{J[g]; \quad g \in \mathfrak{A}_M\}$$

where (f, u_0) is the solution of (1.11)–(1.17).

Optimal control problems for chemical vapor deposition reactor were recently considered in [12] [13]; the models in these articles are based on ODE and do not incorporate the moving surface of the film.

The model of stationary film surface

$$x_2 = \varepsilon f(x_1, \frac{x_1}{\varepsilon})$$

with p as in (1.7) was considered by Belyaev [1] [2] (see also [14]), assuming that u satisfies the Poisson equation; matched asymptotic expansion was employed in [8] [9] [10] to study the same problem. Articles [5; Chap 10] [8] [9] and [11] describe the physical aspects of the model. A more general stationary boundary

$$x_2 = f_0(x_1) + \varepsilon f_1(x_1, \frac{x_1}{\varepsilon}) + \varepsilon^2 f_2(x_1, \frac{x_1}{\varepsilon}, \frac{x_1}{\varepsilon^2})$$

was considered in [7].

In §2 we shall derive an optimality condition, using a method similar to [3] [4]. We shall apply this condition, in §3, to obtain some information on the structure of any optimal control g_0 . Section 4 deals with final-time objective function. Finally, in §5 we provide a numerical scheme based on the results of §3.

2. An optimality condition. The existence of an optimal control g_0 to problems (P) or (P_M) can be established by a standard compactness argument.

Let (u_0, f) be the solution of (1.11)–(1.17) corresponding to g_0 , with $P = P_0$, that is,

$$(2.1) \quad P_0(x_1, t) = \int_0^1 p(x_1, \xi_1) \left\{ 1 + G_{\xi_1}^2 \left(x_1, \xi_1, \int_0^t u_0(x_1, 0, \tau) d\tau \right) \right\}^{1/2} d\xi_1.$$

Take any function $l(x_1, t)$ such that

$$g_0 + \delta l \in \mathfrak{A} \quad (\text{or } \in \mathfrak{A}_M) \quad \text{for any small } \delta > 0,$$

and denote the corresponding solution of (1.11)–(1.17) by (u_l, f_l) , Then

$$(2.2) \quad \begin{aligned} \frac{\partial u_l}{\partial t} - \Delta u_l &= 0 \quad \text{for } x \in \Omega_0, \\ \frac{\partial u_l}{\partial n} &= g_0 + \delta l \quad \text{on } \Gamma_b, \\ \frac{\partial u_l}{\partial x_1} &= 0 \quad \text{on } \{x_1 = \pm a\}, \\ \frac{\partial u_l}{\partial n} + P_l u_l &= 0 \quad \text{on } \Gamma \end{aligned}$$

where

$$(2.3) \quad P_l(x_1, t) = \int_0^1 p(x_1, \xi_1) \left\{ 1 + G_{\xi_1}^2 \left(x_1, \xi_1, \int_0^t u_l(x_1, 0, \tau) d\tau \right) \right\}^{1/2} d\xi_1.$$

It follows that

$$(2.4) \quad \begin{aligned} P_l - P_0 = & \int_0^1 \left\{ p(x_1, \xi_1) \frac{\partial}{\partial s} \left[1 + G_{\xi_1}^2(x_1, \xi_1, s) \right]^{1/2} \right\} \Big|_{s=\int_0^t u_0(x_1, 0, \tau) d\tau} \\ & \times \int_0^t (u_l - u_0)(x_1, 0, \tau) d\tau \Big\} d\xi_1 + O\left(\left| \int_0^t (u_l - u_0)(x_1, 0, \tau) d\tau \right|^2 \right). \end{aligned}$$

By comparison we can estimate $u_l - u_0$, in terms of $\sup |P_l - P_0|$ (cf. the derivation of (1.21)), and this (together with (2.4)) yields an integral inequality for

$$\|u_l - u_0\|_{L^\infty(\Omega_0 \times \{t\})}.$$

By Gronwall's inequality it then follows that

$$(2.5) \quad \|u_l - u_0\|_{L^\infty} \leq C\delta.$$

Using parabolic estimates as well as integration along characteristics, as in [7], we can deduce from (2.5) estimates for higher order derivatives of $u_l - u_0$; in particular,

$$\|u_l - u_0\|_{C^1([0, T]; C^\alpha(\bar{\Omega}_0))} \leq C\delta \quad \text{for any } 0 < \alpha < 1.$$

It follows that, for any $0 < \beta < \alpha$,

$$(2.6) \quad \frac{u_l - u_0}{\delta} \rightarrow z_l \quad \text{in } C^\beta(\bar{\Omega}_0 \times [0, T])$$

for a sequence $\delta \rightarrow 0$.

Since

$$\frac{\partial(u_l - u_0)}{\partial n} + P_0(u_l - u_0) = -u_l(P_l - P_0) \quad \text{on } \Gamma = \{x_2 = 0\},$$

by using (2.4) we get

$$\begin{aligned} \frac{\partial z_l}{\partial n} + P_0 z_l = & - \frac{\partial}{\partial s} \int_0^1 \left\{ p(x_1, \xi_1) \left[1 + G_{\xi_1}^2(x_1, \xi_1, s) \right]^{1/2} \right\} \Big|_{s=\int_0^t u_0(x_1, 0, \tau) d\tau} \\ & \times \int_0^t z_l(x_1, 0, \tau) d\tau \Big\} d\xi_1 \cdot u_0(x_1, 0, t) \\ = & - \frac{\partial}{\partial t} P_0 \cdot \int_0^t z_l(x_1, 0, \tau) d\tau, \end{aligned}$$

or

$$(2.7) \quad \frac{\partial z_l}{\partial n} + \frac{\partial}{\partial t} \left\{ P_0 \int_0^t z_l(x_1, 0, \tau) d\tau \right\} = 0 \quad \text{on } \Gamma.$$

It will be convenient to introduce the function

$$(2.8) \quad \zeta(x_1, t) = \int_0^t z_l(x_1, 0, \tau) d\tau.$$

It satisfies:

$$(2.9) \quad \frac{\partial \zeta}{\partial t} - \Delta \zeta = 0 \quad \text{for } x \in \Omega_0,$$

$$(2.10) \quad \frac{\partial \zeta}{\partial n} = \int_0^t l(x_1, \tau) d\tau \quad \text{on } \Gamma_b,$$

$$(2.11) \quad \frac{\partial \zeta}{\partial x_1} = 0 \quad \text{on } \{x_1 = \pm a\},$$

$$(2.12) \quad \frac{\partial \zeta}{\partial n} + P_0(x_1, t)\zeta = 0 \quad \text{on } \Gamma$$

and

$$(2.13) \quad \zeta = 0 \quad \text{for } t = 0.$$

Observe that since ζ (or z_l) is uniquely determined, the convergence in (2.6) holds for *any* sequence $\delta \rightarrow 0$.

By optimality

$$J[g_0 + \delta l] \geq J[g_0]$$

i.e.,

$$\begin{aligned} & \int_0^T \int_{-a}^a \int_0^1 \psi(t) \left\{ \left[G(x_1, \xi_1, \int_0^t u_l(x_1, 0, \tau) d\tau) - c(x_1, \xi_1, t) \right]^2 \right. \\ & \left. - \left[G(x_1, \xi_1, \int_0^t u_0(x_1, 0, \tau) d\tau) - c(x_1, \xi_1, t) \right]^2 \right\} d\xi_1 \geq 0. \end{aligned}$$

Dividing by δ and letting $\delta \rightarrow 0$, we easily obtain

$$(2.14) \quad \int_0^T \int_{-a}^a \sigma(x_1, t) \zeta(x_1, 0, t) dx_1 dt \geq 0$$

where

$$(2.15) \quad \begin{aligned} \sigma(x_1, t) = & \psi(t) \int_0^1 \left[G(x_1, \xi_1, \int_0^t u_0(x_1, 0, \tau) d\tau) - c(x_1, \xi_1, t) \right] \\ & \cdot \left[G_s(x_1, \xi_1, \int_0^t u_0(x_1, 0, \tau) d\tau) \right] d\xi_1. \end{aligned}$$

We next wish to recast (2.14) in a more useful form. To do that we introduce the “adjoint” problem to (2.9)–(2.13):

$$(2.16) \quad \frac{\partial w}{\partial t} + \Delta w = 0 \quad \text{for } x \in \Omega_0,$$

$$(2.17) \quad \frac{\partial w}{\partial n} = 0 \quad \text{on } \Gamma_b,$$

$$(2.18) \quad \frac{\partial w}{\partial x_1} = 0 \quad \text{on } \{x_1 = \pm a\},$$

$$(2.19) \quad \frac{\partial w}{\partial n} + P_0(x_1, t)w = \sigma(x_1, t) \quad \text{on } \Gamma$$

with terminal condition

$$(2.20) \quad w = 0 \quad \text{for } t = T.$$

Then

$$\begin{aligned} 0 &= \int_0^T \int_{\Omega_0} (\zeta w)_t dx dt = \int_0^T \int_{\Omega_0} (w \Delta \zeta - \zeta \Delta w) dx dt \\ &= \int_0^T \int_{\Gamma_b} \left(\frac{\partial \zeta}{\partial n} w - \frac{\partial w}{\partial n} \zeta \right) + \int_0^T \int_{\Gamma} \left[\left(\frac{\partial \zeta}{\partial n} + P_0 \zeta \right) w - \left(\frac{\partial w}{\partial n} + P_0 w \right) \zeta \right], \end{aligned}$$

or

$$\int_0^T \int_{-a}^a \left(\int_0^t l(x_1, \tau) d\tau \right) w(x_1, b, t) dx_1 dt = \int_0^T \int_{-a}^a \sigma(x_1, t) \zeta(x_1, 0, t) dx_1 dt \geq 0$$

by (2.14). Setting

$$(2.21) \quad W(x, t) = \int_t^T w(x, \tau) d\tau,$$

we summarize:

THEOREM 2.1. *If (g_0, u_0) is an optimal solution of problem (P) (or (P_M)), then for any l such that $g_0 + \delta l \in \mathfrak{A}$ (or $\in \mathfrak{A}_M$) for all small $\delta > 0$, there holds:*

$$(2.22) \quad \int_0^T \int_{-a}^a W(x_1, b, t) l(x_1, t) dx_1 dt \geq 0,$$

where W is defined by (2.21) and w is the solution to (2.16)–(2.20).

3. Properties of the minimizers. In this section we use Theorem 2.1 to derive properties of g_0 .

THEOREM 3.1. *Let (g_0, u_0) be a solution of problem (P) or (P_M) , and assume that*

$$(3.1) \quad \int_{-a}^a \sigma^2(x_1, t) dx_1 \neq 0 \quad \text{for a.e. } t \in (0, T).$$

Then

$$(3.2) \quad g_0 = K\chi_A$$

where A is a subset of Q .

This means that the optimal control is bang-bang.

Proof. Consider first the case where (g_0, u_0) is a solution to problem (P). If the assertion (3.2) is not true then there is a sufficiently large integer n and a subset B of Q with positive measure, such that

$$\frac{1}{n} \leq g_0 \leq K - \frac{1}{n} \quad \text{on } B.$$

By Fubini's theorem, there is a set $\Sigma \subset [0, T]$ of positive measure such that, for any $t \in \Sigma$, the set

$$\Sigma_t = \{(x_1, t) \in B\}$$

has positive measure.

For any l bounded and supported on B , $g_0 + \delta l$ is in $\mathfrak{A}$ if δ is a small positive number. Hence, by Theorem 2.1,

$$\int_0^T \int_{-a}^a \left(\int_t^T w(x_1, b, \tau) d\tau \right) l(x_1, t) dx_1 dt \geq 0.$$

Since the same is true for $-l$,

$$(3.3) \quad \int_t^T w(x_1, b, \tau) d\tau = 0 \quad \text{on } B,$$

and, by differentiation,

$$(3.4) \quad w(x_1, b, t) = 0 \quad \text{a.e. in } B.$$

We may assume that every point in B is a point of Lebesgue density 1. Since $w(x, t)$ is C^∞ in $(\Omega_0 \cup \Gamma_b) \times (0, T)$, it follows that the successive derivatives

$$\partial_{x_1}^m \partial_t^n w(x_1, b, t) \quad (m + n = 1, 2, \dots)$$

also vanish on B . Recall, by (2.17), that

$$\frac{\partial}{\partial x_2} w(x_1, b, t) \equiv 0 \quad \text{in } B.$$

Using (2.16) we deduce that

$$\frac{\partial^2}{\partial x_2^2} w(x_1, b, t) = 0 \quad \text{in } B$$

and, as before,

$$\frac{\partial^2}{\partial x_2^2} \partial_{x_1}^m \partial_t^n w(x_1, b, t) = 0 \quad \text{in } B.$$

We next differentiate (2.16) in x_2 and deduce that

$$\frac{\partial^3}{\partial x_2^3} w(x_1, b, t) \equiv 0 \quad \text{in } B;$$

by another differentiation,

$$\frac{\partial^4}{\partial x_2^4} w(x_1, b, t) \equiv 0 \quad \text{in } B, \text{ etc.}$$

Thus all the derivatives of w vanish on the set $\{(x_1, b, t); (x_1, t) \in B\}$. Since $w(x, t)$ is analytic in x in $\Omega_0 \cup \Gamma_b$, it follows that

$$w(x, t) \equiv 0 \quad \text{for } x \in \Omega_0,$$

for a.e. $t \in \Sigma$. Recalling (2.19) we conclude, in particular, that $\sigma(x_1, t) = 0$ if $-a < x_1 < a$, for a.e. $t \in \Sigma$, which is a contradiction to the assumption (3.1).

In the case of (P_M) , we need to impose on l the restriction $\int_B l \leq 0$, and we therefore obtain (by imposing just the condition $\int_B l = 0$), instead of (3.3), the relation

$$\int_t^T w(x_1, b, \tau) d\tau = \text{constant} \quad \text{on } B.$$

Differentiating in t we get (3.4), and we can then proceed as before. $\square$

Remark 3.1 A by-product of the above proof is the assertion that each set $\{W = \mu\}$ has measure zero.

We next wish to get some information on the set A .

THEOREM 3.2. *Under the assumptions of Theorem 3.1 there exists a $\lambda \leq 0$ such that*

$$(3.5) \quad \begin{aligned} g_0 &= K \quad \text{a.e. on } \{(x_1, t) \in Q, W(x_1, b, t) < \lambda\}, \\ g_0 &= 0 \quad \text{a.e. on } \{(x_1, t) \in Q, W(x_1, b, t) > \lambda\}; \end{aligned}$$

furthermore, $\lambda = 0$ for a minimizer of problem (P) , or for a minimizer of problem (P_M) if $\int_Q g_0 < M$.

Proof. We first prove that (3.5) for some constant λ . Suppose this is not the case. Then there exist subsets B_1, B_2 of Q of positive measure, and a large positive integer n , such that

$$g_0 = K \quad \text{in } B_1, \quad g_0 = 0 \quad \text{in } B_2$$

and

$$(3.6) \quad W(x_1, b, t) > W(\bar{x}_1, b, \bar{t}) + \frac{1}{n}$$

for any $(x_1, t) \in B_1$, $(\bar{x}_1, \bar{t}) \in B_2$. We may assume that B_1 and B_2 have the same measure.

Take $l = -1$ on B_1 , $l = 1$ on B_2 , $l = 0$ elsewhere. Then $g_0 + \delta l$ is admissible control for both problems (P) and (P_M) if δ is positive and small. Hence, by Theorem 2.1,

$$\int_{B_1} W(x_1, b, t) \leq \int_{B_2} W(x_1, b, t),$$

which is a contradiction to (3.6).

If (g_0, u_0) is a solution (to either problem (P) or problem (P_M)), then $g_0 = 0$ on the set $\{W(x_1, b, t) > 0\}$; for otherwise there is a subset B of positive measure on which $g_0 = K$ on B . We can take $l = -1$ on B and zero elsewhere and get a contradiction to (2.22). This proves that $\lambda \leq 0$.

Similarly, for problem (P) (or for problem (P_M) when $\int_Q g_0 < M$), g_0 must equal to K on the set $\{W(x_1, b, t) < 0\}$, so that (3.5) holds with $\lambda = 0$. $\square$

Remark 3.2 If g_0 is a control satisfying the necessary conditions of Theorem 3.2, then $J[g]$ cannot take maximum at g_0 in the sense that

$$(3.7) \quad J[g_0 + \delta l] \leq J[g_0]$$

for some $l \neq 0$ a.e., and a sequence $\delta = \delta_n \rightarrow 0+$. Indeed, otherwise, we get the reverse inequality to (2.22), namely

$$(3.8) \quad \int_0^T \int_{-a}^a W(x_1, b, t) l(x_1, t) dx_1 dt \leq 0.$$

However, since $g_0 + \delta l$ is admissible,

$$\begin{aligned} l &\leq 0 \quad \text{on } \{g_0 = K\}, \\ l &\geq 0 \quad \text{on } \{g_0 = 0\}, \end{aligned}$$

so that $\text{sgn } l = \text{sgn}(W - \lambda)$. Since further $l \neq 0$ and $W - \lambda \neq 0$ a.e. in Q , it follows that $\int_Q (W - \lambda)l > 0$, a contradiction to (3.8) if $\lambda = 0$. If $\lambda < 0$, then we are in the constrained case (P_M) with $\int_Q g_0 = M$, and consequently $\int_Q l \leq 0$. Hence

$$\int_Q Wl \geq \int_Q (W - \lambda)l > 0,$$

a contradiction to (3.8). In the above analysis we could have taken $-l$ instead of l ; hence the restriction $\delta > 0$ can be removed, and we have actually proved the following results:

If g_0 satisfies the optimality condition of Theorem 3.2, then $J[g]$ takes strict local minimum at g_0 in any direction l ($l \neq 0$ a.e.):

$$J[g_0 + \delta l] > J[g_0] \quad \text{if } \delta \text{ is small enough, and } g_0 + \delta l \in \mathfrak{A} \text{ (or } \in \mathfrak{A}_M).$$

Thus the necessary optimality condition is (roughly) also sufficient, provided (3.1) is satisfied.

Remark 3.3 The function $c(x_1, \xi_1, t)$ is the goal we wish to achieve for $f(x_1, \xi_1, t)$. It is natural to assume that

$$f(x_1, \xi_1, 0) < c(x_1, \xi_1, 0),$$

i.e., initially (before the deposition) the surface of the film has the lower profile than the desire surface. If this situation prevails for all $t \leq T$, i.e., if

$$f(x_1, \xi_1, t) < c(x_1, \xi_1, t),$$

for all $(x_1, \xi_1, t) \in [-a, a] \times [0, 1] \times [0, T]$ then, by (1.20),

$$G\left(x_1, \xi_1, \int_0^t u_0(x_1, 0, \tau) d\tau\right) - c(x_1, \xi_1, t) < 0,$$

and, since $G_s > 0$,

$$(3.9) \quad \sigma(x_1, t) < 0.$$

THEOREM 3.3. *Let (g_0, u_0) be a solution to problem (P) or (P_M) and assume that*

$$(3.10) \quad \sigma(x_1, t) \leq 0, \quad \int_{-a}^a \sigma^2(x_1, t) dx_1 \neq 0 \quad \text{a. e.}$$

Then the set $\{g_0 = K\}$ is a subgraph, i.e., there exists a function $\varphi(x_1)$ ($-a \leq x_1 \leq a$) such the symmetric difference

$$(3.11) \quad \{g_0 = K\} \triangle \{(x_1, t) \in Q; 0 \leq t \leq \varphi(x_1)\}$$

has zero measure; if further $\sigma(x_1, T) \not\equiv 0$, then $\varphi(x_1)$ is C^∞ in a neighborhood of any point $\bar{x}_1$ such that $-a \leq \bar{x}_1 \leq a$ and $0 < \varphi(\bar{x}_1) < b$.

Proof. Since $\sigma \leq 0$, (2.19) implies that

$$\frac{\partial w}{\partial n} + P_0 w \leq 0$$

and, by maximum principle, $w \leq 0$. Consequently

$$\frac{\partial W}{\partial t} = -w \geq 0,$$

i.e., $W(x, t)$ is monotone increasing in t , and (3.11) follows from Theorem 3.2.

Under the additional assumption that $\sigma(x_1, T) \not\equiv 0$, w is strictly negative on Q (by strong maximum principle), and then

$$(3.12) \quad \frac{\partial W(x_1, b, t)}{\partial t} \neq 0 \quad \text{on } Q.$$

The function $t = \varphi(x_1)$ is determined by solving

$$W(x_1, b, t) = \lambda$$

for $t = t(x_1)$. Since (3.12) holds, and since W is in C^∞ away from Γ , the implicit function theorem asserts that φ is uniquely defined and it belongs to C^∞ in a neighborhood of any point $\bar{x}_1$ such that $-a < \bar{x}_1 < a$ and $0 < \varphi(\bar{x}_1) < b$. The solution u_0 can be extended by reflection across $x_1 = \pm a$ (see [6]) and, consequently, the above is valid also if $\bar{x}_1 = \pm a$. $\square$

Note that since $W(x, t) \leq 0$ for $t < T$ (when (3.10) holds), Theorem 3.2 implies that, for the problem (P), $\varphi(x_1) \equiv T$ i.e., $g_0 \equiv K$ a.e.

4. Final-time control. In this section we study the optimal control for the problem where we are interested only in the profile at the final time $t = T$. The functional of (1.23) is replaced by:

$$(4.1) \quad J^T[g] = \int_{-a}^a \int_0^1 \left(f_\varepsilon(x_1, \xi_1, T) - c(x_1, \xi_1) \right)^2 d\xi_1 dx_1.$$

Problem (P^T).

$$(4.2) \quad \text{minimize } \{J^T[g]; \quad g \in \mathfrak{A}\}$$

where (f, u_0) is the solution of (1.11)–(1.17).

Problem (P_M^T).

$$(4.3) \quad \text{minimize } \{J^T[g]; \quad g \in \mathfrak{A}_M\}$$

where (f, u_0) is the solution of (1.11)–(1.17).

The existence of an optimal control g_0 to problems (P^T) or (P_M^T) can be established by a standard compactness argument.

For the optimality condition, we can argue as in Section 2. Using the functional in (4.1), we deduce, instead of (2.14), the inequality

$$(4.4) \quad \int_{-a}^a \sigma(x_1) \zeta(x_1, 0, T) dx_1 \geq 0$$

where

$$(4.5) \quad \begin{aligned} \sigma(x_1) = & \int_0^1 \left[G(x_1, \xi_1, \int_0^T u_0(x_1, 0, \tau) d\tau) - c(x_1, \xi_1) \right] \\ & \cdot \left[G_s(x_1, \xi_1, \int_0^T u_0(x_1, 0, \tau) d\tau) \right] d\xi_1. \end{aligned}$$

We now proceed to define the adjoint problem: For any small $\eta > 0$, let $w = w_\eta$ be the solution of the problem:

$$(4.6) \quad \frac{\partial w}{\partial t} + \Delta w = 0 \quad \text{for } x \in \Omega_0,$$

$$(4.7) \quad \frac{\partial w}{\partial n} = 0 \quad \text{on } \Gamma_b,$$

$$(4.8) \quad \frac{\partial w}{\partial n} = 0 \quad \text{on } \{x_1 = \pm a\},$$

$$(4.9) \quad \frac{\partial w}{\partial n} + P_0(x_1, t)w = \frac{\chi_{[T-\eta, T]}}{\eta} \sigma(x_1) \quad \text{on } \Gamma$$

with terminal condition

$$(4.10) \quad w = 0 \quad \text{for } t = T.$$

As in Section 2 we obtain, for $W(x, t) = \int_t^T w(x_1, x_2, \tau) d\tau$,

$$(4.11) \quad \int_0^T \int_{-a}^a W(x_1, b, t) l(x_1, t) dx_1 dt = \frac{1}{\eta} \int_{T-\eta}^T \int_{-a}^a \sigma(x_1) \zeta(x_1, 0, t) dx_1 dt.$$

It is clear that $W = W_\eta$ satisfies:

$$(4.12) \quad \frac{\partial W}{\partial t} + \Delta W = 0 \quad \text{for } x \in \Omega_0,$$

$$(4.13) \quad \frac{\partial W}{\partial n} = 0 \quad \text{on } \Gamma_b,$$

$$(4.14) \quad \frac{\partial W}{\partial n} = 0 \quad \text{on } \{x_1 = \pm a\},$$

$$(4.15) \quad \begin{aligned} \frac{\partial W}{\partial n} + P_0(x_1, t)W = & \int_t^T \frac{\chi_{[T-\eta, T]}(\tau)}{\eta} \sigma(x_1) d\tau \\ & + \int_t^T (P_0)_t(x_1, \tau) W(x_1, b, \tau) d\tau \quad \text{on } \Gamma \end{aligned}$$

with the terminal condition

$$(4.16) \quad W = 0 \quad \text{for } t = T.$$

If we let $\eta \rightarrow 0$ and use also (4.4) and (4.11), we obtain the following optimality condition:

THEOREM 4.1. *If (g_0, u_0) is an optimal solution of problem (P^T) (or (P_M^T)), then, for any l such that $g_0 + \delta l \in \mathfrak{A}$ (or $\in \mathfrak{A}_M$) for all small $\delta > 0$, there holds:*

$$(4.17) \quad \int_0^T \int_{-a}^a W(x_1, b, t) l(x_1, t) dx_1 dt \geq 0,$$

where W is the solution of the following system:

$$(4.18) \quad \frac{\partial W}{\partial t} + \Delta W = 0 \quad \text{for } x \in \Omega_0,$$

$$(4.19) \quad \frac{\partial W}{\partial n} = 0 \quad \text{on } \Gamma_b,$$

$$(4.20) \quad \frac{\partial W}{\partial n} = 0 \quad \text{on } \{x_1 = \pm a\},$$

$$(4.21) \quad \frac{\partial W}{\partial n} + P_0(x_1, t)W = \sigma(x_1) + \int_t^T (P_0)_\tau(x_1, \tau)W(x_1, b, \tau) d\tau \quad \text{on } \Gamma$$

with terminal condition

$$(4.22) \quad W = 0 \quad \text{for } t = T.$$

We can also prove, under appropriate assumptions, that optimal control is bang-bang.

THEOREM 4.2. *Let (g_0, u_0) be a solution of problem (P^T) (or (P_M^T)), and assume that*

$$(4.23) \quad \int_{-a}^a \left\{ \sigma(x_1) + \int_t^T (P_0)_\tau(x_1, \tau)W(x_1, b, \tau) d\tau - P_0(x_1, t)W(x_1, b, t) \right\}^2 dx_1 \neq 0$$

for a.e. $t \in [0, T]$,

Then

$$(4.24) \quad g_0 = K\chi_A \quad \text{a.e. in } Q.$$

where A is a subset of Q .

The proof is the same as in Section 3 and will not be repeated here.

Remark 4.1 If

$$\int_{-a}^a \sigma^2(x_1) dx_1 \neq 0,$$

then (4.23) holds if $T - \gamma < t < T$ for some small $\gamma > 0$, and (4.24) is thus valid in $Q \cap \{T - \gamma < t < T\}$.

Remark 4.2 If the diffusion coefficient is very large, then we may also consider the elliptic system with the time t as a parameter. For this system (with a free boundary), the homogenized system was derived in [6]. The optimality conditions of Sections 3–5 extend also to such a system.

5. Numerical results. In this section we give some numerical results for the problems (P) and (P_M) .

The restriction (3.1) under which we proved the bang-bang principle seems quite weak, and is undoubtedly satisfied “generically”. The numerical scheme described below assumes that (3.1) holds, so that any optimal control possesses the property established in Theorem 3.2.

I. Direct Iteration:

We base our method on the following successive iteration scheme:

For $g_j \in \mathfrak{A}$ (or $\mathfrak{A}_M$), we solve the system (1.11)–(1.20) using a finite difference scheme. Then we solve the parabolic system (2.16)–(2.20) for w_j using again the finite difference scheme. Next we integrate w_j to get W_j and define the new g_{j+1} by (3.5), and iterate.

In defining g_{j+1} we choose $\lambda = 0$ in (3.5) for problem (P), and for problem (P_M) if $\int_Q g_{j+1}$ turns out to be $< M$. For Problem (P_M) , if the choice $\lambda = 0$ does not give a g_{j+1} which satisfies the constraint, then we shall solve $\lambda = \lambda_{j+1}$ and g_{j+1} at the same time, using the constraint equation $\int_Q g_{j+1} = M$.

It is clear that W_j depends continuously on the L^1 norm of g_j . The new g_{j+1} is basically determined by solving the equation $W_j = \lambda_{j+1}$. Thus the continuity of g_{j+1} in the L^1 norm as a function of W_j depends on the non-vanishing of $(W_{j,t}, W_{j,x_1})$ on the set $W_j = \lambda_{j+1}$. We stop the iteration process if the error $\int_Q |g_{j+1} - g_j|$ first becomes smaller than $tol \cdot (2Ka)$ where the tolerance factor tol is around 10^{-2} .

At $t = T$, $w_j = 0$. Thus W_j decreases quadratically to zero if $T - t \rightarrow 0$, and consequently g_{j+1} is not as sharply determined near $t = T$. To overcome this difficulty we use a smaller mesh size in t near $t = T$.

Our experiments show that this scheme converges in just a few iterations if (3.9) holds for each iteration steps. Figure 2 is a computational result for the problem (P_M)

with the following choice of data:

$$\begin{aligned}
& \text{the domain } 0 < x_1 < 1, \quad 0 < x_2 < 1, \quad 0 < t < 1, \\
& p(x_1, \xi_1) = 2 + \sin(\pi x_1) + \frac{1}{\pi} \sin(2\pi \xi_1), \\
& c(x_1, \xi_1, t) \equiv c(x_1, \xi_1) = 2 + \sin\left(\frac{\pi}{2} x_1\right) + \cos(2\pi \xi_1), \\
& f_0(x_1, \xi_1) = 1 + \cos\left(\frac{\pi}{2} x_1\right) + \frac{1}{\pi} \sin(2\pi \xi_1), \\
& \text{initial data } q(x) \equiv 0.2, \\
& K = 1 \quad \text{and} \quad M = \frac{1}{2}.
\end{aligned}$$

Note that in the theory developed in the preceding sections we have taken initial data $q(x) \equiv 0$. However all the results extend to general smooth initial data $q(x)$ which are ≥ 0 and which satisfy the consistency condition at $t = 0$ with respect to the boundary conditions of both u_ε and u_0 at $\partial\Omega_\varepsilon$ and $\partial\Omega_0$, respectively (Actually, consistency at $x_2 = b$ is not needed). Notice that the choice $q(x) \equiv 0.2$ does not satisfy the consistency condition, but it will not cause any problem for numerical computations, since the time step is very small. The reason for choosing q positive is in order to obtain significant advancement of the free boundary quickly in time.

Accelerated Scheme.

Our experiments show that when (3.9) is not satisfied the Direct Iteration Scheme is either slowly convergent, or not convergent at all. To improve convergence we introduce Accelerated Scheme which includes a penalty term in each iteration so that the step length $g_{j+1} - g_j$ will not be “too large”. Suppose that g_j is already known; then we consider, instead of (1.23), the functional

$$(5.1) \quad J_j[g] = J[g] + \frac{\mu_j}{2} \int_0^T \int_{-a}^a \left(g(x_1, t) - g_j(x_1, t) \right)^2 dx_1 dt;$$

where μ_j is a positive constant which converges to 0 as $j \rightarrow \infty$. We denote a minimizer of (5.1) by g_{j+1} . Note that if g_j is a minimizer of J , then J_j has the unique minimizer g_j . For this reason we expect a minimizer of J_j to be a good approximation to the actual minimizer, if g_j is near this minimizer. We can proceed as in Section 2 to derive the following inequality:

$$(5.2) \quad \int_0^T \int_{-a}^a \left[W_j(x_1, b, t) + \mu_j (g_{j+1}(x_1, t) - g_j(x_1, t)) \right] l(x_1, t) dx_1 dt \geq 0,$$

where W_j is defined by (2.21) with $w = w_j$. From this optimality condition, one can obtain, as in Section 3, for problem (P),

$$(5.3) \quad \begin{aligned} g_{j+1} &= K && \text{a.e. on } \{(x_1, t) \in Q, W_j(x_1, b, t) < -\mu_j(K - g_j(x_1, t))\} \\ g_{j+1} &= 0 && \text{a.e. on } \{(x_1, t) \in Q, W_j(x_1, b, t) > \mu_j g_j(x_1, t)\}. \end{aligned}$$

Note that we have not specified the value of g_{j+1} in the set

$$S = \left\{ -\mu_j K \leq W_j(x_1, b, t) - \mu_j g_j(x_1, t) \leq 0 \right\}.$$

Since this set is small (as $\mu_j \rightarrow 0$ if $j \rightarrow \infty$) we arbitrarily set $g_{j+1} = 0$ in $S \cap \left\{ -\frac{1}{2}\mu_j K \leq W_j(x_1, b, t) - \mu_j g_j(x_1, t) \right\}$ and $g_{j+1} = K$ in the complementary subset of S . Thus

$$(5.4) \quad \begin{aligned} g_{j+1} &= K && \text{a.e. on } \{(x_1, t) \in Q, W_j(x_1, b, t) < -\mu_j\left(\frac{K}{2} - g_j(x_1, t)\right)\} \\ g_{j+1} &= 0 && \text{a.e. on } \{(x_1, t) \in Q, W_j(x_1, b, t) > -\mu_j\left(\frac{K}{2} - g_j(x_1, t)\right)\}. \end{aligned}$$

Although μ_j converges to zero, for the penalty term to be effective μ_j should not converge too fast to zero. A good choice seems to be

$$\mu_j = \max \left\{ tol, \frac{1}{2Ka} \|g_j - g_{j-1}\|_{L^1((-a,a) \times [0,T])} \right\} \cdot \|W_j(\cdot, b, \cdot)\|_{L^\infty((-a,a) \times [0,T])}$$

where tol is a predetermined small number, and we stop the process if

$$\|g_j - g_{j-1}\|_{L^1((-a,a) \times [0,T])} + \|g_{j+1} - g_j\|_{L^1((-a,a) \times [0,T])} \leq 2 \cdot tol \cdot (2Ka).$$

This Scheme converges much faster than the previous one. We experimented with a variety of data and found that it converges in most cases, although sometimes the convergence is slow (twenty iterations). Figure 3 uses the Accelerated Scheme for the problem (P_M) with the following data:

$$\begin{aligned} &\text{the domain } 0 < x_1 < 1, \quad 0 < x_2 < 1, \quad 0 < t < 1, \\ &p(x_1, \xi_1) = 3 + \sin(4\pi x_1) + \sin(2\pi \xi_1), \\ &c(x_1, \xi_1, t) \equiv c(x_1, \xi_1) = 3 + 4(x_1 - 0.5)^2 + \cos(2\pi \xi_1), \\ &f_0(x_1, \xi_1) = 2 + (1 - x_1) + \frac{1}{\pi} \sin(2\pi \xi_1), \\ &\text{initial data } q(x) \equiv 0.5, \\ &\text{and } K = 1, \end{aligned}$$

and we choose tol to be around 10^{-2} .

In both cases the control is bang-bang, i.e., $g_0 = K\chi_A$. In Figure 2 the set A is a subgraph whereas in Figure 3 it is not.

Figure 2.

Figure 3.

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