Proceedings of the 9th International Symposium on
Dynamics and Control of Process Systems (DYCOPS 2010),
Leuven, Belgium, July 5-7, 2010
Mayuresh Kothare, Moses Tade, Alain Vande Wouwer, Ilse Smets (Eds.)

Optimal control of transport-reaction system with time varying spatial domain

James Ng, Stevan Dubljevic

Department of Chemical and Materials Engineering, University of Alberta, Alberta, T6G 2V4, Canada, (e-mail: jcng,Stevan.Dubljevic@ualberta.ca).

Abstract: This paper considers the multiscale optimal control of crystal growth. The optimal control is realized for the crystal pulling arm modeled by the standard rigid body dynamics, while the underlying dynamics of the diffusion of heat in the crystal growth region is given by parabolic partial differential equations (PDEs) with time varying spatial domain. The underlying transport-reaction system is developed from the first principles and the associated dynamics is analyzed in appropriate functional state space setting. The complete description of the evolutionary parabolic domain time varying PDE is provided and explored within the coupled master-slave control setting. Numerical simulations demonstrate an optimal pulling evolution rate and its effects on the temperature profile in the crystal with the time varying domain.

Keywords: Multiscale dynamics, Rigid Body Dynamics, Transport-reaction system, Parabolic PDEs, Time varying spatial domain, Optimal control.

1. INTRODUCTION

The application of optimal control to industrial processes is highly desirable where the benefits are realized in the quality of process outputs in addition to the economic gains that arise from the reduction in associated production costs. In order to maximize the benefits of control application, the appropriate model of the process must be determined. Often in processing, the material undergoes some property transition over an interval of time that is reflected as a change of state or shape of the material. This implies that the dynamical features of the system will be transformed and therefore the process model must incorporate the time-dependent evolution of the material domain to remain valid over the given interval of time. The development of physical models of the governing dynamics of systems with time varying spatial domains and the application of control to these systems therefore represents an important area of research. In some cases, it is possible to apply control to the domain in order to obtain the desired operating characteristics. The dynamics of transport-reaction processes are typically modelled by parabolic PDEs and in simple model dynamics representation are usually restricted to regions with fixed domains. However, there is a significant number of industrially important processes in which the material and/or process controlled volume evolve in time, by changing the shape or just undergo change due to underlying velocity field, see Brown et al. (1991). In particular, a prime example of time-varying domain transport-reaction process is a Czochralski crystal growth, see Derby and Brown (1987, 1986a,b); Brown (1988), see Fig.1, in which the solidified crystal of high purity is pulled out from the melt, so

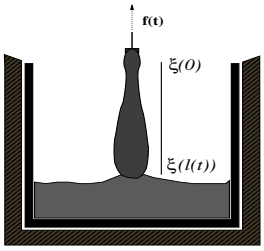

Fig. 1. An example of a process with time varying domain is given by the Czochralski crystal growth process.

that the crystal controlled volume changes in a shape and size as the solidification process takes place at the crystal-melt interface. In particular, the shape and crystal size evolves and contributes to the time varying nature of the process parameters which are of the prime interest to be controlled. There are several works which consider control of Czochralski crystal growth, see Armaou and Christofides (2001), and control of time-varying domain parabolic PDEs, see Armaou and Christofides (1999), in which time dependent domain evolution was usually prespecified. Existing works have also considered the application of proportional control to crystal growth, see Derby et al. (1987), however the need to optimally control the process arises from the high importance of maintaining the temperature distribution through the crystal and crystal-melt interface for production of high-purity crystals. Along the same line of work, the optimal control realization of the process with time varying boundary described by the parabolic PDEs has been considered, where the multiscale model of rigid body dynamics is incorporated in the optimal control regulation of the crystal temperature, see Wang (1990, 1995).

Therefore, motivated by these works our primary objective in this paper is to provide a detailed formulation of

⋆ Financial support from Office of the Dean of Engineering and Chemical & Materials Engineering Department at the University of Alberta is gratefully acknowledged.

the parabolic PDE model of a transport-reaction process with time varying domain in the framework of Czochralski crystal growth and to demonstrate the application of optimal control through the actuation of the pulling arm which affects the movement of the underlying parabolic PDE boundary. We provide a multiscale model description which consists of a model of rigid body dynamics entangled with the parabolic PDE model of temperature distribution in the growing crystal slab. The underlying time varying nature of the temperature distribution is defined in well posed functional state space setting, and in this work we do not consider any temperature based actuation within domain, whereas the finite dimensional optimal control is applied to the pulling of the crystal out of melt. We provide a novel insight into this multiscale optimal control problem and the immediate realization of the optimal control strategy for Czochralski crystal growth process.

2. PRELIMINARIES

The process model is formulated starting from the first principles dynamical equations for continuum mechanics for the purpose of incorporating the time-dependent evolution of the spatial domain in the model description. In particular, we will utilize the Reynolds Transport Theorem in ensuing model development, see Leal (1992). We define the physical space region as the open set, $\Omega \subset \mathcal{R}^3$ with material points, $\hat{\xi} = (\hat{\xi}_1, \hat{\xi}_2, \hat{\xi}_3)$, and consider an arbitrary time dependent, moving subregion of Ω which is the open set $\mathcal{U}(t_0, t_1) \subset \Omega$ with volume element dv and spatial points $\xi = (\xi_1, \xi_2, \xi_3)$. The surface of $\mathcal{U}(t_0, t_1)$ is the piecewise C^1 boundary $\partial\mathcal{U}(t_0, t_1)$ and consists of the element ds. The *regular motion* of the boundary is described by the flow of $\partial\mathcal{U}(t_0, t_1)$ along the spatial velocity field $w(\xi, t)$, where w is the continuous and invertible mapping $w : \Psi(\Omega) \to \mathcal{R}^3$, such that $\mathcal{U}(t_0, t_1) = \Psi(\mathcal{U}_0)$ is the region at time t in the interval $[t_0, t_1]$ relative to its initial configuration at t_0. The regularity of the motion presumes the boundary $\partial\mathcal{U}(t_0, t_1)$ remains intact such that $\mathcal{U}(t_0, t_1)$ is not, for example, divided or penetrated. We note the relationship between the spatial points $\xi \in \mathcal{U}(t_0, t_1)$ from $\hat{\xi} \in \Omega$ as the mapping $\xi = \Psi(\hat{\xi})$ and define x as a *scalar physical quantity* (for example, temperature or concentration) at $t \in [t_0, t_1]$ at position ξ. Due to the proper definition of the mappings between ξ and $\hat{\xi}$ space, we invoke the *Transport theorem* on $\mathcal{U}(t_0, t_1)$ as follows, see Marsden and Hughes (1983); Leal (1992).

Let $x = x(\xi, t)$ be a bounded C^1 function on the open set $\mathcal{U}(t_0, t_1) \subset \Omega$ that is continuous on the moving boundary $\partial\mathcal{U}(t_0, t_1)$. By the *Transport theorem*, see Marsden and Hughes (1983), the time rate of change of x in $\mathcal{U}(t_0, t_1)$ is expressed as:

$$c\rho \frac{d}{dt} \int\limits_{\mathcal{U}(t_0,t_1)} x dv = c\rho \int\limits_{\mathcal{U}(t_0,t_1)} \left(\frac{\partial x}{\partial t} + \nabla \cdot (xw) \right) dv \quad (1)$$

where c is the *specific heat capacity* and ρ is the *mass density*. It is assumed that the physical properties, c and ρ, remain invariant for the interval of time $[t_0, t_1]$ and throughout the region $\mathcal{U}(t_0, t_1)$. The interchange of the differentiation and integration over $\mathcal{U}(t_0, t_1) = \Psi(\mathcal{U}_0)$ is validated by the initial assumption of the continuity of the mapping Ψ that preserves the structure of the domain for $\xi \in \mathcal{U}(t_0, t_1)$ in the interval $[t_0, t_1]$. The heat flux, $f(\xi, t)$, across ds and internal reactionary heat sources and sinks, $h(\xi, t)$, are given as:

$$f = -\kappa \nabla x \quad (2)$$

$$h = \rho g - \gamma x \quad (3)$$

where κ, γ and g denote *thermal conductivity*, *heat loss* and *heat generation*, respectively. The negative assignment for the term in f reflects the direction of heat transfer relative to the normal component of the boundary while the sign assignments for the terms in h correspond to the possible exothermic or endothermic reactions occurring in the region. The *Conservation Law* provides that the total heat flow balance in a region $\mathcal{U}(t_0, t_1)$ is:

$$c\rho \frac{d}{dt} \int\limits_{\mathcal{U}(t_0,t_1)} x dv = \int\limits_{\mathcal{U}(t_0,t_1)} h dv \quad - \int\limits_{\partial\mathcal{U}(t_0,t_1)} f \cdot n \, ds \quad (4)$$

with n denoting the unit outward normal component of surface element ds. Eq.4 represents the *integral form* of the *Conservation Law*. The *material form* of the *Conservation Law*, see Marsden and Hughes (1983), can be determined from its integral form by substituting Eq.2 into Eq.4, arrangement of terms and invoking the *divergence theorem* for the integrand over $\partial\mathcal{U}(t_0, t_1)$, to obtain:

$$\int\limits_{\mathcal{U}(t_0,t_1)} \left[c\rho \frac{dx}{dt} - \nabla \cdot (\kappa \nabla x) - h \right] dv = 0 \quad (5)$$

The material form of the *Conservation Law* arises from the assumption of continuity throughout the region over the interval $[t_0, t_1]$ which implies the vanishing of the integrand over $\mathcal{U}(t_0, t_1)$, in Eq.5. The substitution of Eq.1 into Eq.5 and arrangement of terms yields the following general expression of the heat equation for the region $\mathcal{U}(t_0, t_1)$ where the boundary, $\partial\mathcal{U}(t_0, t_1)$, is moving with the velocity field w:

$$c\rho \frac{\partial x}{\partial t} = \nabla \cdot (\kappa \nabla x) - c\rho \nabla \cdot (xw) + h \quad (6)$$

One can notice that Eq.6 differs from the standard well known material derivative expression for transport of a scalar property for the term $c\rho\nabla \cdot (xw)$, see Leal (1992), demonstrating that the inclusion of the time dependent spatial domain provides a more detailed description of the system dynamics. Further, we note that the dilatation or contraction of the moving region, $\mathcal{U}(t_0, t_1)$, is due to the motion of the boundary, $\partial\mathcal{U}(t_0, t_1)$, along the spatial velocity field, w, that determines the configurations of $\mathcal{U}(t_0, t_1)$ in the interval $[t_0, t_1]$. The expansion of the expression $\nabla \cdot (xw)$ gives:

$$\nabla \cdot (xw) = x\nabla \cdot w + w \cdot \nabla x \quad (7)$$

Therefore, due to the assumption of density invariance which implies incompressibility of $\mathcal{U}(t_0, t_1)$, the divergence of the velocity field vanishes such that $\nabla \cdot w = 0$. In consideration of the mapping of points, $\hat{\xi}$, in Ω to ξ in $\mathcal{U}(t_0, t_1)$, the relation among the spatial and material coordinates is given by velocity field, $w(\xi, t) = \partial\Psi(\hat{\xi}, t)/\partial t = d\xi/dt$, so that contribution of the moving boundary to the scalar quantity, x, is obtained as:

$$w \cdot \nabla x = \frac{d\xi_j}{dt} \frac{\partial x}{\partial \xi_j} \quad (8)$$

for $j = \{1, 2, 3\}$. In other words, this term can be viewed as the type of convective transport due to the motion of the subregion $\mathcal{U}(t_0, t_1)$. From the Eqs.6-7-8, we obtain the expression for the heat equation for the region $\mathcal{U}(t_0, t_1)$ with moving boundary, $\partial\mathcal{U}(t_0, t_1)$, as follows:

$$c\rho\frac{\partial x}{\partial t} = \nabla \cdot (\kappa \nabla x) - c\rho(w \cdot \nabla x) + h \tag{9}$$

In the case when the domain becomes constant Eq.9 leads to the well known expression of the reaction diffusion parabolic PDE. The general form of the boundary conditions imposed upon Eq.9 for prescribed functions a, b, r over $\partial\mathcal{U}(t_0, t_1)$, where $\partial x/\partial n$ is the outward normal component to the boundary of the domain, is expressed as:

$$a\, x + b\frac{\partial x}{\partial n}\bigg|_{\partial\mathcal{U}(t_0,t)} = r \tag{10}$$

The boundary conditions of Eq.10 relate the temperature, x, on the boundary of the region and the flux of x through $\partial\mathcal{U}(t_0, t_1)$. In the ensuing work, the definitions of *Dirichlet*, *Neumann* and *Robin* boundary conditions can be applied without loss of generality in a three or lower dimensional space setting.

3. MODEL DYNAMICS OF CZOCHRALSKI CRYSTAL GROWTH

The process model in Eq.9-10 provides the complete physical description of transport of heat or diffusion in a moving region with a time dependent spatial domain. In this work, we consider the one-dimensional case of Czochralski crystal formation governed by the dynamics described by Eq.9-10 such that the domain is the Hilbert space $\mathbb{L}_2(0, l)$ where $l = l(t)$ is the length of the domain at each time $t \in [t_0, t_1]$. The evolution of the boundary with respect to time is determined by the realization of the pulling arm motion, see Wang (1990); Brown (1988), with dynamics governed by the second order rigid body dynamics equation for mechanical systems:

$$M\ddot{l}(t) - \nu\dot{l}(t) + \eta l(t) = f_c(t) \tag{11}$$

where M is the *mass* of the system and ν, η, $f_c(t)$ are the respective *dampening coefficient*, *elastic coefficient* and *control force* of the system. We make a reasonable assumption that the velocity of the boundary, $w = \dot{l}(t)$, is bounded for all t, implying that $f_c(t)$ is finite in magnitude as $t \to \infty$. The governance of the domain motion by the rigid body equation results in a coupled system consisting of Eq.9-11. To facilitate the discussion of dynamic behaviour of this system, we consider Eq.9-10 in the absence of heat sources and sinks. Further, we assume that the *thermal conductivity*, κ, is constant throughout the region and define the *diffusivity constant* as $k = \kappa/c\rho$ so that Eq.9 is reduced to the following equation:

$$\frac{\partial x}{\partial t} = k\frac{\partial^2 x}{\partial \xi^2} - w\frac{\partial x}{\partial \xi} \tag{12}$$

For the general case of boundary conditions imposed on Eq.12 one can take process parameters $a = 1$, $b = 1$ and $r = 0$ in Eq.10, so that the boundary conditions associated in Eq.12 become:

$$x(0, t) - \frac{\partial x}{\partial \xi}(0, t) = 0 \tag{13}$$

$$x(l, t) + \frac{\partial x}{\partial \xi}(l, t) = 0 \tag{14}$$

The negative sign in Eq.13 is assigned because $\partial x/\partial n = -1$ at the point $\xi = 0$. The initial temperature distribution is given as:

$$x(\xi, 0) = x_0 \tag{15}$$

Equations 12-13-14-15 provide a well posed PDE problem that is coupled with the standard rigid body equation, Eq.11, for mechanical systems determining the evolution of the domain. In order to ascertain the dynamics of the system we determine the structure of the time varying spatial operator. We note that Eq.12 can be written as:

$$\frac{\partial x}{\partial t} - \mathcal{L}x = 0 \tag{16}$$

with the associated boundary conditions of Eq.13-14 where $\mathcal{L}$ is the second order ordinary differential equation that gives the time-varying spatial operator as:

$$\mathcal{L}(\,\cdot\,) = k\frac{d^2(\,\cdot\,)}{d\xi^2} - w\frac{d(\,\cdot\,)}{d\xi} \tag{17}$$

In consideration of Eq.17 we seek solutions of the following eigenvalue problem:

$$\mathcal{L}\phi = -\lambda\phi \tag{18}$$

for the eigenvalue λ. In lieu of the boundary conditions, Eqs.13-14, the eigenvalue problem for the time varying spatial domain operator becomes:

$$k\frac{d^2\phi}{d\xi^2} - w\frac{d\phi}{d\xi} = -\lambda\phi \tag{19}$$

$$\phi(0) - \phi'(0) = 0 \tag{20}$$

$$\phi(l) + \phi'(l) = 0 \tag{21}$$

In order to obtain solutions to Eq.19, we let $z_1 = \phi(\xi)$ and $z_2 = \phi'(\xi)$ to transform the second order differential equation to a system of first order ordinary differential equations represented as $\dot{z}(\xi) = \tilde{\Gamma} z(\xi)$. A non-trivial, unique solution may be found for the boundary conditions given in Eq.20-21 so that problem is well-posed and a solution is found in the form of:

$$z(\xi) = \Gamma z(\xi_0) \tag{22}$$

where $z(\xi_0)$ is the vector of the boundary conditions at $\xi = 0$. In the case of Czochralski crystal growth, we assume that the boundary conditions are *natural (Neumann) boundary conditions*. The physical interpretation of these boundary conditions is that the pulling arm is well insulated from the crystal so that $z_2(0) = 0 = \partial x(0)/\partial\xi$, while the temperature of the crystal at this boundary is $z_1(0)$. There is also zero flux across the interface between the crystal and the melt so that $z_2(l) = 0$ and the temperature of the crystal and the melt, $z_1(l)$, is the same

at the interface. From the Eq.22 we obtain the expression corresponding to the prescribed boundary conditions as:

$$2\lambda\mu^{-\frac{1}{2}}e^{\frac{w}{2k}l(t)}\sinh\left(\frac{l(t)}{2k}\mu\right)z_1(0)=0 \tag{23}$$

where $\mu = w^2 - 4k\lambda$. The trivial solution to Eq.23 occurs when $\lambda = 0$, such that $\phi(\xi) = 0$ for all $l(t)$ and singular solutions occur when $\lambda = w^2/(4k)$. The two remaining cases for $\mu > 0$ and $\mu < 0$ reveal the possible eigenvalues and associated eigenfunctions that satisfy Eq.23. For $\mu > 0$, we have that $\lambda < w^2/(4k)$ and the resulting eigenfunctions correspond to exponential growth in time and therefore they are not physically realistic descriptions of the diffusion problem that is naturally dissipative in the absence of internal and external sources of heat. For the case where $\mu < 0$, we have that $\lambda > w^2/(4k)$ and there exists a countable infinite set of eigenvalues $\{\lambda_n, n \in \mathbb{N}\}$ that satisfy Eq.23 where:

$$\lambda_n(t) = -\left[k\left(\frac{n\pi}{l(t)}\right)^2 + k\left(\frac{w}{2k}\right)^2\right] \tag{24}$$

In consideration of Eq.18 we obtain a set of corresponding eigenfunctions:

$$\phi_n(\xi,t) = B_n e^{\frac{w}{2k}\xi}\left[\cos\left(\frac{n\pi}{l(t)}\xi\right) - \frac{w}{2k\frac{n\pi}{l(t)}}\sin\left(\frac{n\pi}{l(t)}\xi\right)\right] \tag{25}$$

with coefficients B_n to be determined. It can be verified that Eq.25 satisfies Eq.19 for the eigenvalues defined in Eq.24. In order to determine the coefficients B_n, we defined the adjoint eigenfunctions as $\phi_n^*(\xi,t) = e^{-\frac{w}{k}\xi}\phi_n(\xi,t)$ with orthogonality relation:

$$\int_{\mathbb{L}_2(0,l)} \Phi(\xi,t)\phi_n(\xi,t)\phi_m(\xi,t)d\xi = 0\,, \qquad n \neq m \tag{26}$$

where $\Phi(\xi,t)$ is a weighting function. Due to the orthogonality of eigenfunctions, that is $\langle\phi_n, \phi_m^*\rangle_\Phi = 0$, by taking $n = m$ in Eq.26, the set of coefficients B_n can be determined as:

$$B_n(\xi,t) = \sqrt{\frac{2}{l(t)}}\left[1 + \left(\frac{w}{2k\frac{n\pi}{l(t)}}\right)^2\right]^{-\frac{1}{2}} \tag{27}$$

One can notice that the operator $\mathcal{L}$ given in Eq.17 with associated boundary conditions Eqs.20-21 has a similar features as Sturm-Liouville system, see Ray (1981), which describes an axial dispersion model of homogeneous chemical reactor in which a zero-order exothermic reaction takes place. Moreover, the eigenvalue and eigenfunction expressions of Eqs.24-25 are in agreement with the operator arising from the heat/diffusion parabolic PDE natural boundary conditions problem fixed domain expressions, that is, in the limit $t \to \infty$, $w \to 0$ and $l(t) = const$. Another important characteristic of a model with the moving domain is that usual notion of the "energy" of the system which is in the case of the parabolic system described by the spectrum of the operator $\mathcal{L}$ in its expression posses the term which has a feature of the "kinetic energy" associated with the moving boundary, $E_k = \frac{1}{2k}\frac{w^2}{2}$. Fig.2 shows time evolution of the first two eigenfunctions defined in Eqs.25-27 and for two times $t = 2$ and $t = 100$ where evolution of

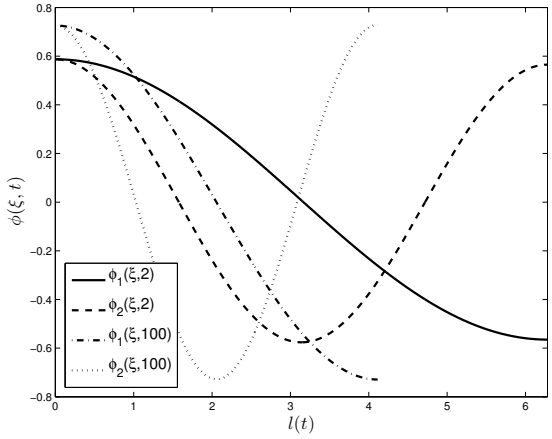

Fig. 2. Time evolution of first two eigenfunctions $\phi_1(\xi,t)$ and $\phi_2(\xi,t)$.

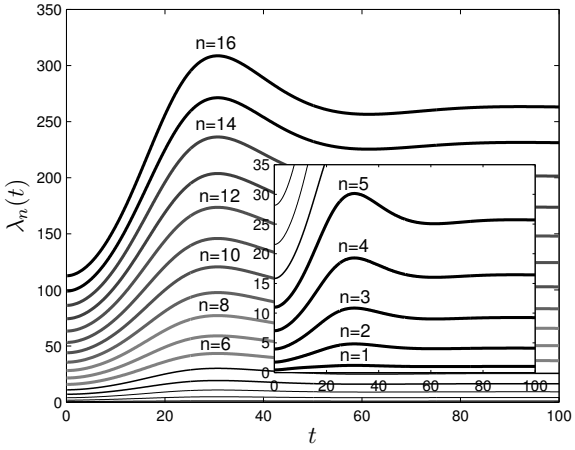

Fig. 3. Eigenvalues evolution given by the Eq.24 and under the implementation of the control law Eq.34.

$l(t)$ is generated as a solution of optimal control problem given as Eqs.32. Fig.2 illustrates the different behavior of the first two eigenfunctions for two time instances. Complementary to the evolution of eigenfunctions one obtains the evolution of eigenvalues defined in Eq.24, see Fig.3. One can notice that the eigenvalue problem for the operator $\mathcal{L}$ given by Eqs.19-20-21 for the each fixed time yields a point spectrum which does not have accumulation point, in other words, this continuous spectrum at each time instance can be viewed as a point spectrum of the operator $\mathcal{L}$. In this paper, we do not prove properties of time varying operator $\mathcal{L}$, and we will assume that at each time instance the operator $\mathcal{L}$ is a spectral operator, see Curtain and Zwart (1995), which has underlying eigenfunctions utilized in the construction of the time varying Hilbert space, see Wang (1990).

4. CONTROLLER FORMULATION

In this section, we provide an optimal control law synthesis which is associated with the pulling arm dynamics and affects the properties of the underlying parabolic PDEs through the boundary evolution. We define the appro-

priate time varying separable Hilbert spaces, $\mathcal{V}(t)$ and $\mathcal{H}(t)$ consisting of functions defined on $\mathcal{U}(t_0,t)$ such that $\mathcal{V}(t) \subset \mathcal{H}(t) \subset \mathcal{V}'(t)$, the dual of $\mathcal{V}(t)$, with $\mathcal{V}(t)$ dense in $\mathcal{H}(t)$, $\mathcal{H}(t)$ dense in $\mathcal{V}'(t)$ and with continuous corresponding injections. We introduce the notion of the bilinear forms on $\mathcal{V}(t) : \phi, \psi \rightarrow a(t;\phi,\psi)$ with the following two properties, 1.) $\forall \phi,\ \psi$, the function $a(t;\phi,\psi)$ is measurable such that following holds, $\|a(t;\phi,\psi)\| \leq c\|\phi\|_{\mathcal{V}'(t)}\|\psi\|_{\mathcal{V}'(t)}$, 2.) $a(t;\phi,\phi) + \lambda\|\phi\|^2_{\mathcal{H}_u(t)} \geq \alpha_0\|\phi\|^2_{\mathcal{V}_u(t)},\ \forall\ \phi \in \mathcal{V}'(t)$, for appropriately chosen constants which do not depend on time. Let $\mathcal{A}(t)$ be an operator from $\mathcal{G}(\mathcal{V}(t),\mathcal{V}'(t))$ defined by $a(t;\phi,\psi) = \langle \mathcal{A}(t)\phi,\psi\rangle$, so that for dependence of $\langle\varphi,\psi\rangle$ on the time dependent spatial domain $\mathcal{U}(t_0,t_1)$, we obtain $\langle\varphi,\psi\rangle = \int_{\mathcal{U}(t_0,t_1)} \varphi\psi dv$. Since, the $\mathcal{V}(t)$ has a time dependent countable basis $\{\phi_1(t),\phi_2(t),\cdots\}$, we seek Galerkin approximation of the solutions Eqs.12-13-14 in the form,

$$x(\xi,t) = \sum_{n=1}^{N} a_n(t)\phi_n(\xi) \tag{28}$$

where N is the order of the approximation. We utilize the orthonormal eigenfunctions as a basis on to which we project our system of equations to get the state representation as:

$$\dot{a}(t) = A_d(t)a(t) \tag{29}$$

In this work, we only consider the application of optimal control to the moving arm dynamics governing the motion of the boundary Eq.11, coupled with the dynamics of the Czochralski crystal growth process, Eq.12-13-14-15. Although, the natural dissipation of heat in the absence of generation terms implies inherent stability of the system, and since we do not consider heat input injection in this model, our objective is to demonstrate and investigate the effect of control on the temperature distribution of the system, through the optimal motion of the boundary. One can see from Eq.24-25-27 that both the length and change of the domain will impact dynamics of the system. The system representation of Eq.11 is obtained by letting $y_1 = l(t)$ and $y_2 = \dot{l}(t)$, with $\tilde{\nu} = \nu/M$, $\tilde{\eta} = \eta/M$ and $\tilde{f}(t) = f_c(t)/M$ to get:

$$\begin{bmatrix}\dot{y}_1\\ \dot{y}_2\end{bmatrix} = \begin{bmatrix}0 & 1\\ -\tilde{\nu} & -\tilde{\eta}\end{bmatrix}\begin{bmatrix}y_1\\ y_2\end{bmatrix} + \begin{bmatrix}0\\ 1\end{bmatrix}\tilde{f}(t) \tag{30}$$

The general form of Eq.30 can be expressed compactly as $\dot{y}(t) = A_m y(t) + B_m\tilde{f}(t)$. The dependence of the process the evolution of the boundary requires the augmentation of the state matrix of Eq.29. The state matrix, A_d, is partitioned to include only the terms $(n\pi/l(t))^2$, and it is combined with Eq.30 to obtain the augmented state system for the diffusion problem coupled with the rigid body equation:

$$\begin{bmatrix}\dot{y}\\ \dot{a}\end{bmatrix} = \begin{bmatrix}A_m & 0\\ 0 & A_d\end{bmatrix}\begin{bmatrix}y\\ a\end{bmatrix} - \frac{y_2^2}{4k}\begin{bmatrix}0 & 0\\ 0 & I\end{bmatrix}\begin{bmatrix}y\\ a\end{bmatrix} + \begin{bmatrix}B_m\\ 0\end{bmatrix}\tilde{f}(t) \tag{31}$$

Equivalently, we denote the system given by Eq.31 as

$$\dot{q}(t) = A(t)q(t) - P(t)q(t) + B\tilde{f}(t) \tag{32}$$

where $q = [y\ \ a]^T$ is a state vector. The state matrix, $A(t)$, contains only decoupled diagonal elements so that the design of optimal state feedback for the system given in Eq.30, reduces to the solution of the finite dimensional solution of the Riccati equation:

$$0 = A_m'P + PA_m + Q - PB_mR^{-1}B_m'P \tag{33}$$

with appropriately chosen weights on Q and R. The resulting LQR control law is

$$\tilde{f}(t) = -\frac{1}{2}R^{-1}B_m'Py(t) = -\mathcal{K}y(t) \tag{34}$$

where P is a positive definite solution to the LQR-ARE Eq.33.

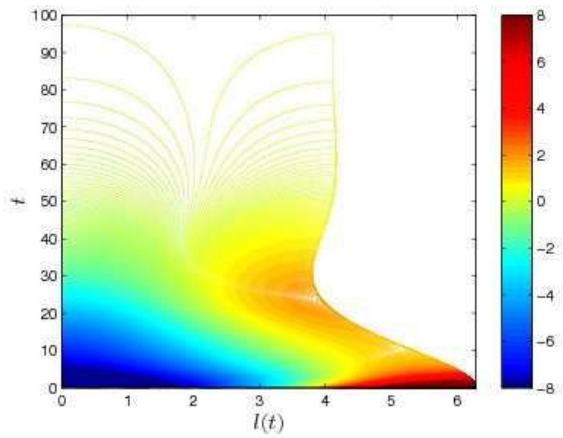

Fig. 4. Closed loop temperature distribution under optimal control given by Eq.34.

5. SIMULATION AND NUMERICAL RESULTS

Simulations of the system given in Eq.32 were carried out over a maximum domain length of 2π and a time interval of $t \in [0, 100]$ seconds. The parameters of the pulling arm for Eq.30 were prescribed by setting the dampening constant of $\nu = -0.002$, elastic coefficient, $\eta = 7$ and the mass of system was $M = 10$. For the process state equation, the diffusivity constant was set at $k = 1.5$. Under these process conditions, the gain matrix, for $Q = 0.5$ and $R = 0.01$, was determined to be $\mathcal{K} = [2.95\ \ 10.4]$ resulting in the closed loop eigenvalues of $[-0.522 + 0.850i, -0.522 - 0.850i]$. The $N = 16$ order approximation is used to simulate the temperature distribution. The closed loop temperature distribution over the time interval and domain is shown in Fig.4. The temperature of the crystal reaches the final state in approximately 90 seconds as the domain motion approaches its nominal position of 3.8 from an initial perturbed position of 2π and initial velocity of zero. Fig. 5 shows the evolution of the boundary over the time interval with the oscillations due to the contribution of the elastic coefficient of the control arm. The temperature of the system reaches the desired state only when the length of the domain reaches the nominal value. This clearly demonstrates that the dynamics of the system are dependent on the evolution of the domain and must be considered to obtain an accurate model of the process.

6. CONCLUSION

In this work, we developed model dynamics of time-dependent domain of transport-reaction process which describes the industrially important problem of Czochralski

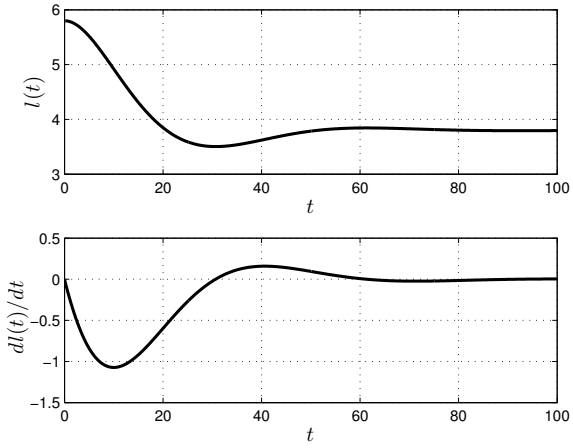

Fig. 5. Controller driven domain motion.

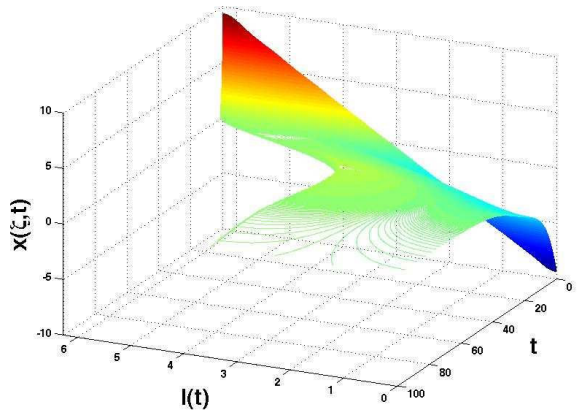

Fig. 6. Three-dimensional representation of closed loop temperature distribution under optimal control given by Eq.34.

crystal growth. The complete description of the time dependent parabolic PDE within the operator description in appropriate functional space setting is considered. The optimal control realization is associated with the mechanical based part of the multiscale process model. In particular, we provide the optimal control associated with the pulling force which controls the boundary time evolution and therefore affects the underlying parabolic PDE properties. The process model for the temperature distribution in the crystal was considered in the 1-dimensional case with *natural* boundary conditions. Future works will consider the process model in higher dimensional cases, different coordinate systems and the associated boundary conditions to obtain the complete representation of the physical system. At this stage, we did not consider the spatially distributed heating source which in realistic process realization of Czochralski crystal growth, is crucial for the tight temperature control in the crystal slab. In the future work, we will consider optimal control realizations which include spatially distributed heating, and require satisfaction of input and state constraints.

REFERENCES

Armaou, A. and Christofides, P.D. (1999). Robust control of parabolic PDE systems with time-dependent spatial domains. *Automatica*.

Armaou, A. and Christofides, P.D. (2001). Crystal temperature control in the czochralski crystal growth process. *AIChE J.*, **47**, 79–106.

Brown, H.S., Kevrekidis, I.G., and Jolly, M.S. (1991). A minimal model for spatio-temporal patterns in thin film flow. In *Pattern and Dynamics in Reactive Media*, 11–31. R. Aris, D. G. Aronson, and H. L. Swinney, ed., Springer-Verlag.

Brown, R. (1988). Theory of transport processes in single crystal growth from the melt. *AIChE J*, 34, 881–911.

Curtain, R.F. and Zwart, H. (1995). *An introduction to Infinite-Dimensional Linear Systems Theory*. Springer-Verlag, New York.

Derby, J., Atherton, L., Thomas, P., and Brown, R. (1987). Finite-element methods for analysis of the dynamics and control of czochralski crystal growth. *J. Cryst. Growth*, 2, 297–343.

Derby, J. and Brown, R. (1986a). Thermal-capillary analysis of czochralski and liquid encapsulated czochralski crystal growth. I. simulation. *J. Cryst. Growth*, 74, 605–624.

Derby, J. and Brown, R. (1986b). Thermal-capillary analysis of czochralski and liquid encapsulated czochralski crystal growth. II. processing strategies. *J. Cryst. Growth*, 75, 227–240.

Derby, J. and Brown, R. (1987). On the dynamics of czochralski crystal growth. *J. Cryst. Growth*, 83, 137–151.

Leal, G. (1992). *Laminar Flow and Convective Transport Processes*. Butterworth-Heinemann, Boston, U.S.A.

Marsden, J. and Hughes, T. (1983). *Mathematical Foundations of Elasticity*. Dover Publications, New York, U.S.A.

Ray, W. (1981). *Advanced Process Control*. McGraw-Hill, New York, New York.

Wang, P.K.C. (1990). Stabilization and control of distributed systems with time-dependent spatial domains. *J. Optim. Theor. & Appl.*, 65, 331–362.

Wang, P.K.C. (1995). Feedback control of a heat diffusion system with time-dependent spatial domains. *Optim. Contr. Appl. & Meth.*, 16, 305–320.