OPTIMAL CONTROL OF A CLASS OF PARABOLIC TIME-VARYING PDES

James Ng[a], Ilyasse Aksikas[a,b], Stevan Dubljevic[a]

[a]Department of Chemical & Materials Engineering,
University of Alberta, Canada

[b]Department of Mathematics, King Abdelaziz University, Jeddah, KSA

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Catalytic tubular reactor

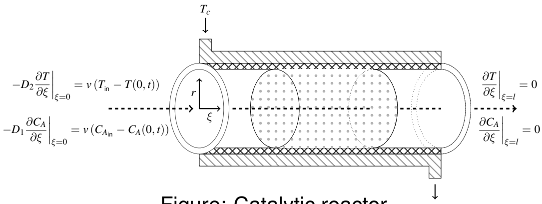


Figure: Catalytic reactor

- Many industrial processes, e.g methanol, ammonia and other petrochemicals
- Diffusion-Convection-Reaction Process
- Tubular reactor systems with catalyst deactivation,
- Loss of catalyst activity $\rightarrow$ Time-varying rates of reaction

$\Longrightarrow$ Parabolic time-varying PDEs

Crystal Growth Process

- Important industrial process utilized for the production of semi-conductor material in the electronics and microprocessor industry.
- Materials produced: Silicon (Si), Germanium (Ge).
- Temperature dynamics: Parabolic PDE with time-varying coefficients
- Convective transport term is time-varying due to the motion of the domain boundary.

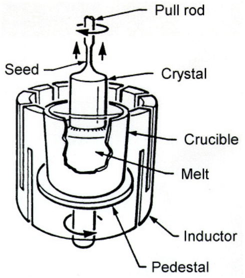


Figure: Crystal Process diagram

INTRODUCTION

§ MOTIVATING EXAMPLES

- Parabolic partial differential equations (PDEs) with time-varying features represent an important class of models for reaction-diffusion-convection processes. e.g.
  - Tubular and packed bed reactor systems with catalyst deactivation,
  - Crystal growth and annealing type processes with time-varying spatial domains
- These time-dependent features play an important role in the system dynamics, and therefore must be incorporated into the model based controller design.

* Approach:

- Evolution systems representation
- Operator differential Riccati equation

INTRODUCTION

§ RELATED WORKS

Nonautonomous PDEs

- *I. Aksikas, J.F. Forbes, and Y. Belhamadia, "Optimal control design for time-varying catalytic reactors: a Riccati equation based approach", Int. J. Control., 2009*
- *I. Aksikas and J.F. Forbes, "Linear quadratic regulator for time-varying hyperbolic distributed parameter systems", IMA. J. Mathematical Control and Information, 2010.*
- *P. Acquistapace, F. Flandoli, and B. Terreni, "Initial boundary value problems and optimal control for nonautonomous parabolic systems," SIAM J. Cont. & Optim., 1991.*
- *A. Smyshlyaev and M. Krstic, "On control design for PDEs with space-dependent diffusivity and time-dependent reactivity, Automatica, 2005.*

PDEs with time-varying spatial domains

- *A. Armaou and P. D. Christofides, "Robust control of parabolic PDE systems with time-dependent spatial domains," Automatica, 1999.*
- *P.K.C.Wang, "Stabilization and control of distributed systems with time-dependent spatial domains," J. Optim. Theor. & Appl., 1990.*

GENERAL MODEL

§ PDE DESCRIPTION

- Let Ω be a bounded open set of $\mathbb{R}^m$ with smooth boundary $\partial\Omega$.
- Consider the initial and boundary value problem of the form:

$$
\begin{aligned}
&\frac{\partial z(\xi,t)}{\partial t} + A(t)z(\xi,t) = f(\xi,t) && \text{in} \quad \Omega \times [0,T] \\
&z(\xi,0) = z_0(\xi) && \text{in} \quad \Omega \\
&\frac{\partial z(\xi,t)}{\partial n} = 0, && \text{on} \quad \partial\Omega \times [0,T]
\end{aligned}
$$

- The family of operators $A(t)$ is defined as:

$$
A(t)z := -\sum_{i,j=1}^{m} a_{ij}(\xi,t)\frac{\partial^2 z}{\partial \xi_i \partial \xi_j} + \sum_{i=1}^{m} b_i(t)\frac{\partial z}{\partial \xi_i} + c(\xi,t)z
$$

(i) $z(\xi,t)$ represents, for example, temperature or concentration, with initial distribution $z_0(\xi)$.

(ii) $a_{ij}(\xi,t)$ describes the heterogeneous thermal conductivity or diffusivity.

(iii) $b_i(t)$ is a convective transport coefficient (e.g. time-dependent fluid superficial velocity).

(iv) $c(\xi,t)$ is a linearized reaction term (e.g. due to catalyst deactivation).

§ PDE OPERATOR PROPERTIES

- Assumptions:

P1. For each $t \in [0, T]$, the operator $A(t)$ is strongly elliptic, i.e.

$$\sum_{i,j=1}^{m} a_{ij}(\xi, t)\boldsymbol{\eta}_i\boldsymbol{\eta}_j \geq \varepsilon|\boldsymbol{\eta}|^2, \qquad \text{for} \qquad \boldsymbol{\eta} \in \mathbb{R}^m$$

P2. The coefficients $c(\xi, t) \in L^2([0, T], L^2(\Omega))$, $b_i(t) \in C^1([0, T])$ and $a_{ij}(\xi, t)$ are sufficiently Hölder continuous, i.e.

$$|a_{ij}(\xi, t) - a_{ij}(\xi, s)| \leq L|t - s|^{\beta}$$

for $s, t \in [0, T]$, $\xi \in \bar{\Omega}$ and constant $L > 0$ and $\beta \in (0, 1]$.

P3. The function $f(\xi, t) \in L^2(\Omega)$ satisfies:

$$\left(\int_{\Omega} |f(\xi, t) - f(\xi, s)|^2 d\xi\right)^{\frac{1}{2}} \leq L|t - s|^{\beta}, \qquad 0 \leq s < t \leq T$$

- $\{A(t)\}_{t\in[0,T]}$ forms a family of strongly elliptic operators which admit a family of eigenfunctions $\{\phi_n(t)\}_{t\in[0,T]}$ with corresponding family of eigenvalues $\{\lambda_n(t)\}_{t\in[0,T]}$.

§ Nonautonomous parabolic evolution system

- Under the properties of: *strong ellipticity* and *continuity* of $a_{ij}(\xi, t)$, $b_i(t)$ and $c(\xi, t)$, the operator $A(t)$ satisfies:
  1. For every $t \in [0, T]$, the resolvent $R(\lambda; A(t))$ exists for all λ with $\mathrm{Re}\lambda \leq 0$ and there exists a constant L_1 such that $\|R(\lambda; A(t))\| \leq L_1/|\lambda|$;
  2. There exists constants L_2 and $\beta \in (0, 1]$ such that $\|(A(t) - A(s))A(\tau)^{-1}\| \leq L_2|t - s|^{\beta}$ for $s, t, \tau \in [0, T]$.
- The initial and boundary value problem is represented as a non-autonomous evolution system on $L^2(\Omega)$:

$$\frac{dz(t)}{dt} = A(t)z(t) + f(t), \qquad z(s) = z_s$$

for $0 \leq s < t \leq T$ and $z_s \in L^2(\Omega)$.

Infinite-dimensional system representation

§ Two-parameter semigroup

- The solution of the nonautonomous evolution system is expressed in the form of:

$$z(t) = U(t,s)z_s + \int_s^t U(t,\tau)f(\tau)d\tau$$

where $U(t,s)$ is the **two-parameter semigroup** generated by the operator $A(t)$.

- The operator $A(t)$ is defined as:

$$A(t) := \sum_{n=1}^{\infty} \lambda_n(t)\langle \cdot , \psi_n(t)\rangle \phi_n(t)$$

- The operator $A(t) : D(A(t)) \subset L^2(\Omega) \to L^2(\Omega)$ is the infinitesimal generator of the two-parameter semigroup:

$$U(t,s)z(s) := \sum_{n=1}^{\infty} e^{\mu_n(t)-\mu_n(s)}\langle z(s), \psi_n(s)\rangle \phi_n(t), \qquad \text{for} \qquad 0 \leq s \leq t \leq T$$

INFINITE-DIMENSIONAL SYSTEM REPRESENTATION

§ TWO-PARAMETER SEMIGROUP

- The operator $U(t,s)$ satisfies the following identities:

  A1. $U(t,t) = I$,

  A2. $U(t,s) = U(t,r)U(r,s)$ for $0 \leq s \leq r \leq t \leq T$

  A3. $U(t,s)$ is continuous on $0 \leq s < t \leq T$, and:

  $$\frac{\partial U(t,s)}{\partial t} = A(t)U(t,s), \qquad \text{and} \qquad \frac{\partial U(t,s)}{\partial s} = -U(t,s)A(s)$$

  A4. $\|U(t,s)\| \leq L_1$,

  A5. $\|A(t)U(t,s)\| \leq L_2(t-s)^{-1}$, and

  A6. $\|A(t)U(t,s)A(s)^{-1}\| \leq L_3$ for constants $L_i > 0$.

INFINITE-DIMENSIONAL SYSTEM REPRESENTATION

§ OPTIMAL CONTROL PROBLEM

- The finite-time horizon optimal control problem is given as the following:

$$\min_u J(u) = \min_u \int_0^T \left(|C(\tau)z(\tau)|^2 + |u(\tau)|^2 \right) d\tau + \langle Qz(T), z(T) \rangle$$

where the functional $J(u)$ is minimized over all trajectories of

$$\begin{cases} \dot{x}(t) & = & A(t)x(t) + B(t)u(t) \\ x(0) & = & x_0 \end{cases} \tag{1}$$

- If $Q \geq 0$, $B(\cdot) \in C([0, T; \mathcal{L}(U; L^2(\Omega)))$ and $C(\cdot) \in C([0, T; \mathcal{L}(Y, L^2(\Omega)))$, then the optimization problem has the unique minimizing solution $u_{\text{min}}(t)$ such that the optimal pair $u^{\min}(t) \in C([0, T]; U)$ and $z^{\min}(t) \in C^1([0, T]; X) \cap C([0, T]; D(A(t))$ are related by the feedback formula,

$$u^{\min}_{t \in [0,T]}(t) = -B^*(t)\Pi(t)z_{\text{min}}(t)$$

- The operator $\Pi(t) \in L(X)$ is the strongly continuous, self adjoint, nonnegative solution of the differential Riccati equation,

$$\dot{\Pi}(t) + A^*(t)\Pi(t) + \Pi(t)A(t) - \Pi(t)B(t)B^*(t)\Pi(t) + C^*(t)C(t) = 0, \quad \Pi(T) = Q$$

EXAMPLE: CRYSTAL GROWTH PROCESS

§ PROCESS MODEL

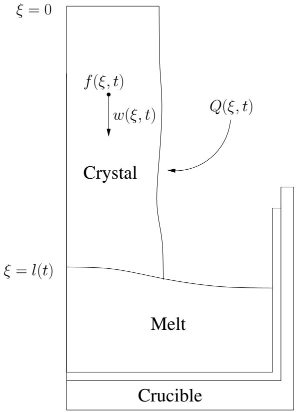
- Model of temperature dynamics:

$$\frac{\partial z(\xi,t)}{\partial t} = \kappa \frac{\partial^2 z}{\partial \xi^2} - v(t)\frac{\partial z}{\partial \xi} + b(\xi)u(t)$$

$$z(\xi,0) = z_0(\xi)$$

$$\frac{\partial z}{\partial \xi}(0,t) = 0, \quad \frac{\partial z}{\partial \xi}(l(t),t) = 0$$

- κ thermal conductivity constant, $v(t)$ is the boundary velocity, and $b(\xi)u(t)$ is the distributed heat input along the length of the rod.
- *The material domain is time-varying due to the motion of the boundary at the material-fluid interface, $\xi = l(t)$.*
- Control objective: Optimally stabilize the temperature around some desired nominal distribution.



EXAMPLE: CRYSTAL GROWTH PROCESS

§ TIME-VARYING SPATIAL DOMAIN AND FUNCTION SPACE DESCRIPTION

- The time-varying spatial domain at some time $t \in [0, T]$ is denoted $\Omega = (0, l(t))$ with $0 < \xi < l(t) \leq l_{\text{max}}$.
- Spatial domain evolution is considered as a sequence of subdomains: $\Omega_j \subset \Omega_{j+1} \subset \cdots \subset \mathbf{\Omega}$
- Let $\phi(\xi, t)$ denote a family of functions defined on the subdomains Ω_j with:

$$\phi(\xi, t) = \begin{cases} \phi(\xi) & \text{for} \quad \xi \in \Omega_j \\ 0 & \text{for} \quad \xi \in \Omega_j^c \cap \mathbb{R} \end{cases}$$

- $L^2(\Omega_j)$ forms a family of function spaces which are precompact in $L^2(\mathbf{\Omega})$ for all $t \in [0, T]$, (see, Adams, 1975):

$$L^2(\Omega_j) \subset L^2(\Omega_{j+1}) \subset \cdots \subset L^2(\mathbf{\Omega})$$

- Enables the use of single inner product $\langle \cdot , \cdot \rangle$ on $L^2(\mathbf{\Omega})$ for functions defined on an arbitrary subdomain Ω:

$$\langle \phi, \phi \rangle_{L^2(\mathbf{\Omega})} = \int_{\mathbf{\Omega}} \phi(\xi, t)\phi(\xi, t) d\xi = \int_{\Omega} \phi(\xi)\phi(\xi) d\xi + \int_{\Omega^c} 0 \, d\xi = \langle \phi, \phi \rangle_{L^2(\Omega)}$$

EXAMPLE: CRYSTAL GROWTH PROCESS

§ PDE OPERATOR PROPERTIES

- The PDE operator $A(t)$ is defined as:

$$A(t) := \kappa \frac{\partial^2 z}{\partial \xi^2} - v(t) \frac{\partial z}{\partial \xi}$$

- The operator $A(t)$ is *strongly elliptic* for each $t \in [0, T]$;

- For each $t \in [0, T]$ the family of eigenfunctions $\{\phi_n(t)\}_{\in [0,T]}$ are:

$$\phi_n(\xi, t) = B_n(t) e^{\frac{1}{2}\kappa^{-1} v(t)\xi} \left(\cos\left(\frac{n\pi}{l(t)} \xi \right) - \frac{1}{2}\kappa^{-1} \frac{v(t)}{(n\pi / l(t))} \sin\left(\frac{n\pi}{l(t)} \xi \right) \right)$$

with coefficients:

$$B_n(t) = \sqrt{\frac{2}{l(t)}} \left(1 + \left(\frac{v(t)}{2\kappa \left(n\pi / l(t) \right)} \right)^2 \right)^{-\frac{1}{2}}$$

- $\phi_n(\xi, t)$ are orthonormal to the eigenfunctions: $\psi_n(\xi, t) = e^{-\kappa^{-1} v(t)\xi} \phi_n(\xi, t)$ of the adjoint operator $A^*(\xi, t)$ for each $t \in [0, T]$.
- The corresponding family of eigenvalues are:

$$\lambda_n(t) = -\kappa \left(\frac{n\pi}{l(t)} \right)^2 - \frac{1}{2}\kappa^{-1} \frac{v(t)^2}{2}$$

EXAMPLE: CRYSTAL GROWTH PROCESS

§ INFINITE-DIMENSIONAL SYSTEM REPRESENTATION

- The associated family of linear operators $A(t)$ in $L^2(\mathbf{\Omega})$ is defined as:

$$A(t)z = A(\xi, t)z \qquad \text{for} \qquad z \in D(A(t))$$

with domain $D(A(t))$:

$$D(A(t)) := \left\{ \phi \in L^2(\mathbf{\Omega}) : \ \phi, \ \frac{\partial \phi}{\partial \xi} \text{ are a.c.}, \ A(t)\phi \in L^2(\mathbf{\Omega}), \right.$$
$$\left. \text{and } \ \frac{\partial \phi}{\partial \xi}(0,t) = 0, \ \frac{\partial \phi}{\partial \xi}(l(t),t) = 0 \right\}$$

- Initial and boundary value control problem is represented as the nonautonomous parabolic initial value problem:

$$\frac{dz}{dt} = A(t)z(t) + B(t)u(t), \qquad z(0) = z_0, \qquad 0 \leq s \leq t < T$$

- The solution of the initial value problem is expressed in terms of the two parameter semigroup $U(t,s)$,

$$z(t) = U(t,0)z_0 + \int_0^t U(t,\tau)B(\tau)u(\tau)d\tau$$

with $z(s) \in L^2(\mathbf{\Omega})$.

EXAMPLE: CRYSTAL GROWTH PROCESS

§ INFINITE-DIMENSIONAL SYSTEM REPRESENTATION

- The operator $A(t) : D(A(t)) \subset L^2(\mathbf{\Omega}) \to L^2(\mathbf{\Omega})$ generates the two-parameter semigroup $U(t,s)$, $0 \le s \le t \le T$ expressed as:

$$U(t,s)z(s) = \sum_{n=1}^{\infty} \exp\left\{ -\kappa_0 (n\pi)^2 \left(\frac{t}{l(t)^2} - \frac{s}{l(s)^2} \right) - \frac{1}{4\kappa_0} \left(tv(t)^2 - sv(s)^2 \right) \right\} \langle z(s), \psi_n(s) \rangle \phi_n(t)$$

- One can note that in the case where the boundary motion ceases and Ω is constant, i.e. $l(t) = l$, $v(t) = 0$, the expression for $U(t,s)$ becomes:

$$U(t,s)z(s) = \sum_{n=1}^{\infty} \exp\left\{ -\kappa_0 \left(\frac{n\pi}{l} \right)^2 (t-s) \right\} \langle z(s), \phi \rangle \phi = T(t-s)z(s)$$

where $T(t)$, $t \ge 0$ is the C_0-semigroup of operators on $L^2(\Omega)$ which is generated by the standard heat equation.

EXAMPLE: CRYSTAL GROWTH PROCESS

§ CONTROLLER FORMULATION

- Let consider the weighted inner product on $L^2(\Omega)$, for $z_1, z_2 \in D(A(t))$,

$$\langle z_1, z_2 \rangle_r = \int_\Omega r(\xi,t) z_1(\xi,t) z_2(\xi,t) d\xi$$

with weight function $r(\xi,t) := \exp(-(v(t)/\kappa_0)\xi)$.

- Note that $\langle \phi_n, \phi_m \rangle_r = \delta_{nm}$ where $\delta_{nm} = 1$ if $n = m$ and 0 otherwise.

- The differential Riccati equation can be written under the form:

$$\langle \phi_n(t), \dot{\Pi}(t)\phi_m(t)\rangle_r + \langle A(t)\phi_n(t), \Pi(t)\phi_m(t)\rangle_r + \langle \phi_n(t), \Pi(t)A(t)\phi_m(t)\rangle_r$$

$$-\langle \Pi(t)B(t)B^*(t)\Pi(t)\phi_n(t), \phi_m(t)\rangle_r + \langle C(t)\phi_n(t), C(t)\phi_m(t)\rangle_r = 0$$

with $\langle \phi_n(T), \Pi(T)\phi_m(T)\rangle_r = \langle \phi_n(T), Q\phi_m(T)\rangle_r$.

EXAMPLE: CRYSTAL GROWTH PROCESS

§ CONTROLLER FORMULATION

- In the case where $B(t) = I$ and $C(t) = I$ the differential Riccati equation becomes the system of infinitely many ordinary differential equations:

$$\dot{\Pi}_{nn}(t) + 2\lambda_n(t)\Pi_{nn}(t) + 1 - \Pi_{nn}^2(t) = 0, \qquad \Pi_{nn}(T) = Q$$

- The input $u_{t\in[0,T]}^{\min}$ is determined from the solution of the system of ODEs, and the optimal state trajectory is the mild solution of the state feedback system

$$\dot{z} = (A(t) - B(t)B^*(t)\Pi(t))z(t), \quad z(0) = z_0$$

and is expressed as:

$$z(t) = \sum_{n=1}^{\infty} e^{\mu_n(t)} \langle z_0, \psi_n(0)\rangle \phi_n(t) - \int_0^t U(t,\tau) \sum_n \Pi_{nn}(t) \langle z_0(\tau), \psi_n(\tau)\rangle \phi_n(\tau) d\tau$$

NUMERICAL RESULTS

§ HEAT INPUT AND TEMPERATURE DISTRIBUTION

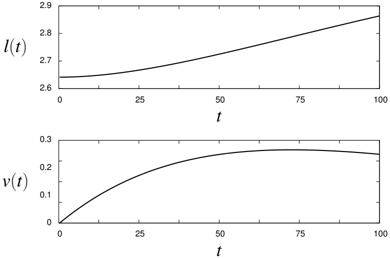


Figure: Slab domain length $l(t)$ and boundary velocity $v(t)$.

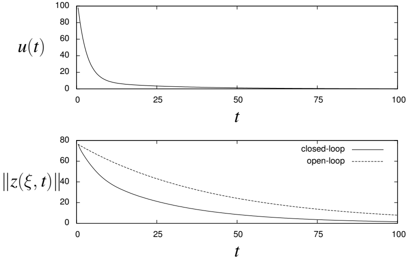


Figure: (Top) Optimal input profile $u^{\min}(t)$ applied to the slab at input location $\xi_c = 0.875$. (Bottom) Total open and closed loop system energy.

NUMERICAL RESULTS

§ CLOSED LOOP SYSTEM

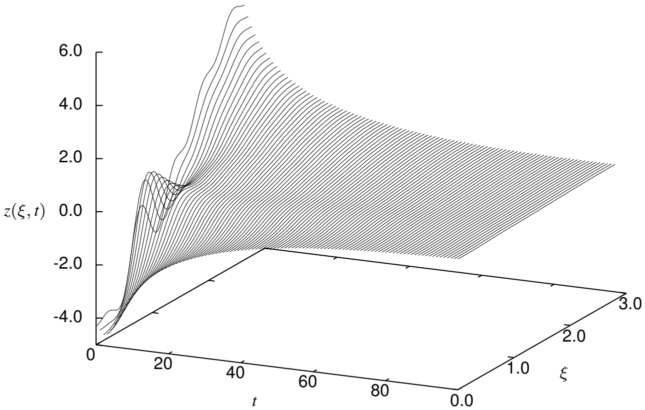


Figure: Slab temperature evolution in the time-dependent spatial domain with diffusivity $\kappa_0 = 1.75$. Input applied at $\xi_c = 0.875$.

§ CONCLUDING REMARKS

- The general two-parameter semigroup representation of a class of nonautonomous parabolic PDE has been presented.
- The optimal control formulation for the infinite-dimensional system representation is considered.
- A practical example of an crystal growth process is considered with PDE model defined on time-varying spatial domain.
- The infinite-dimensional system representation of the PDE is determined, and the explicit two-parameter semigroup expression is provided.
- The corresponding optimal control problem is considered and numerical results demonstrate the stabilization of the temperature distribution in the time-dependent region.