Delayed recycle Axial Reactor xxx

Behrad Moadeli* Author Two†

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Abstract

This is a brief summary of the paper, usually around 150-250 words.

*Ualberta, Address. Email: moadeli@ualberta.ca

†Affiliation, Address. Email: author2@example.com

1 Introduction

Many chemical, petrochemical, and biochemical unit operation processes are modelled as distributed parameter systems (DPS). When these processes are described using first-principle modeling, they result in a class of partial differential equations (PDEs) to effectively capture diffusion, transport, and reaction phenomena, leading to infinite-dimensional state space representations.[1] This characteristic presents significant challenges, making the control and estimation of DPS inherently more complex than finite-dimensional systems. Two primary methods have emerged for addressing DPS control. One is early lumping, which approximates the infinite-dimensional system with a finite-dimensional model.[2,3] While this method enables the use of standard regulator design techniques, mismatches between the dynamical properties of the original DPS and the approximate lumped parameter model can occur, negatively affecting the performance of the designed regulator.[4] The second method is late lumping, which directly tackles the infinite-dimensional system before applying numerical solutions. This approach introduces a challenging yet fertile direction of research, leading to many meaningful contributions that address various aspects of control and estimation of infinite-dimensional systems.

Among notable studies utilizing late lumping method for control of convection-reaction chemical systems resulting in first order hyperbolic PDEs, Christofides explored the robust control of quasi-linear first-order hyperbolic PDEs, providing explicit controller synthesis formulas for uncertainty decoupling and attenuation.[5] Krstic and Smyshlyaev extended boundary feedback stabilization techniques for first-order hyperbolic PDEs using a backstepping method, converting the unstable PDE into a system for finite-time convergence.[6] Relevant applications of reaction-convection systems other than tubular reactors have also been addressed within this field, resulting in regulator/observer design strategies for chemical systems governed by first order hyperbolic PDEs. Xu and Dubljevic addressed the state feedback regulator problem for a countercurrent heat exchanger system, utilizing an infinite-dimensional approach to ensure that the controlled output tracks a reference signal.[7] Xie and Dubljevic Xie and Dubljevic developed a discrete-time output regulator for gas pipeline networks, emphasizing the transformation of continuous-time models into discrete-time systems while preserving essential continuous-time properties.[8] This work was further extended by Zhang et al., who proposed a tracking model predictive control and moving horizon

estimation design for pipeline systems, addressing the challenges of state and parameter estimation in an infinite-dimensional chemical system governed by first order hyperbolic PDEs.[9] For a similar convection-reaction system, Zhang et al. proposed a model predictive control strategy, incorporating a Luenberger observer to achieve output constrained regulation in a system modeled by nonlinear coupled hyperbolic PDEs.[10]

Additionally, diffusion-convection-reaction systems resulting in parabolic PDEs are also addressed in several works. For example, Christofides addressed order reduction methods for diffusion-convection-reaction type of reactors.[11] Dubljevic et al. utilized modal decomposition to capture dominant modes of a DPS to construct a reduced order finite dimensional system, which enables the design of a low dimensional controller for a diffusion-convection-reaction type reactor described by second order parabolic PDEs.[12] Ozorio Cassol et al. designed and compared the performance of a full-state and output feedback controller for a diffusion-convection heat exchanger system.[13] In Khatibi et al.'s work, an axial dispersion tubular reactor equipped with recycle stream is considered as a second order parabolic DPS, with a predictive controller being utilized to optimally control the reactor.[14] Although the presence of recycle is common in industrial reactor designs, this work is one of the few contributions in this field that addresses a diffusion-convection-reaction system equipped with a recycle stream.

Moreover, continuous-time optimal control design is a well-developed concept for distributed parameter systems, particularly when the system generator is either a self-adjoint operator or can be transformed into one through a proper linear transformation.[15] However, there are distributed parameter systems that do not possess this property. Instead, the system generator belongs to the domain of Riesz-spectral operators. Rather than an orthonormal basis for the function-space, these generators introduce a bi-orthonormal set of eigenfunctions as the basis. Optimal controller design for these systems was initially addressed in Curtain and Zwart.[16] Since then, significant work has been done in this field. For instance, continuous-time optimal control design for a cracking catalytic reactor, another convection-reaction system governed by first-order hyperbolic PDEs, has been achieved by solving an operator Riccati equation (ORE).[17] This work has been further extended to time-varying PDEs of the same class.[18] The same approach has been applied to develop a full-state feedback[19] and output feedback[20] linear quadratic (LQ) optimal regulator for a boundary-controlled convection-reaction system, utilizing the properties of a Riesz-spectral generator for the system.

On top of those dynamic systems that are distributed in space, delay systems are another example of distributed parameter systems.[16] Although delay is commonly represented in the form of delay differential equations (DDEs), it can also be modeled as a transport partial differential equation (PDE), which offers advantages in more complex scenarios or when employing alternative norms on infinite-dimensional states. This approach allows for a smoother transition to problems involving more intricate PDE dynamics while maintaining notational consistency.[21] Input/output delay with relevant applications in chemical engineering has been addressed previously in the field of control theory for DPS. For example, time-delayed boundary observation is considered while addressing an output feedback regulator for a tubular reactor.[22] However, the notion of state-delay (as opposed to delayed-input or delayed-output) seems to be less addressed in this field compared to other relevant fields like signal processing, self-driving cars, or network control theory (NCT). This is probably because not much application in the field of distributed parameter chemical engineering systems can be introduced in the first place. Ozorio Cassol et al.'s work is one of the few instances that addressed a delayed-state distributed parameter chemical engineering system,[13] where they designed a full-state and output feedback regulator for a system of heat exchangers. The notion of state-delay comes from the time it takes for a stream to leave one pass of the heat exchanger and enter the next pass. As stated previously, not much work is published addressing chemical reactors equipped with recycle as distributed parameter systems. Even in Khatibi et al.'s work, the recycle is assumed to be instantaneous; a simplifying assumption that does not resonate well with reality. In fact, taking the time it takes for the recycle stream to re-enter the reactor input can be another instance for the rare concept of a delayed state DPS in the field of chemical engineering.

The present work focuses on the control of an axial tubular reactor equipped with a recycle stream, a configuration common in industrial processes but inadequately addressed in the literature. Unlike previous studies that assumed instantaneous recycle, this work incorporates the time delay associated with the recycle stream re-entering the reactor, presenting a rare example of state-delay in the field of chemical engineering DPS. The model comprises a second-order parabolic PDE to capture the diffusion-convection-reaction nature of the reactor, coupled with a first-order hyperbolic PDE to account for the delay. The boundary conditions are chosen as Danckwerts boundary conditions, which are particularly suitable for this type of reactor. The system results in a non-self-adjoint operator, but by utilizing the bi-orthogonal theorem, given that the gen-

erator is Riesz-spectral, a full-state feedback optimal LQ regulator is developed, followed by an output feedback regulator. The control strategy is derived by solving an operator Riccati equation (ORE) and employs a late lumping approach. Actuation and observation are conducted at the boundaries, making it a boundary-actuated system involving finite-dimensional dynamics for an infinite-dimensional DPS. The paper is structured as follows:

- Open-loop system: Modeled the delay infinite-dimensional system (DPS) and transformed it into a system of coupled PDEs using the delay-transport approach. Explored system dynamics by examining eigenvalues, the adjoint operator, and the bi-orthogonal basis, followed by an assessment of the open-loop response.

- Full-state feedback regulator: Developed the full-state feedback gain by formulating the infinite-time horizon LQ control problem, converting the ORE into matrix Riccati equations (MRE), and studying the resulting closed-loop response.

- Output feedback compensator: Addressed practical limitations of the proposed full-state feedback mechanism by introducing a Luenberger observer for state reconstruction, followed by the design of an output feedback regulator. The closed-loop response of this regulator was also analyzed.

- Numerical simulation: Provided an illustrative numerical example to demonstrate the practical application of the theoretical concepts developed.

2 Open-loop System

2.1 System Model

The chemical process illustrated in Figure 1 represents an axial dispersion tubular reactor, which incorporates diffusion, convection, and a first-order irreversible chemical reaction.[23] The reactor is equipped with a recycle mechanism, allowing a fraction of the product stream to re-enter the reactor to ensure the consumption of any unreacted substrate. By applying first-principle modeling through relevant mass balance relations on an infinitesimally small section of the reactor, the reactor's dynamics can be described by a second-order parabolic PDE, a common class of equations used to characterize diffusion-convection-reaction systems.[24] The resulting PDE that describes the reactor model is given by:

$$\dot{x}(\zeta,t) = D\partial_{\zeta\zeta}c(\zeta,t) - v\partial_{\zeta}c(\zeta,t) + k_r c(\zeta,t) \tag{1}$$

subject to Dankwerts boundary conditions:

$$\begin{cases} D\partial_{\zeta}c(0,t) - vc(0,t) = -v\left[Rc(1,t-\tau) + (1-R)u(t)\right] \\ \partial_{\zeta}c(1,t) = 0 \\ y(t) = c(1,t) \end{cases} \tag{2}$$

Here, $c(\zeta,t)$ denotes the concentration along the reactor, representing the state of the system. The physical parameters D, v, k_r, R, and τ correspond to the diffusion coefficient, flow velocity along the reactor, reaction constant, recycle ratio, and residence time of the recycle stream, respectively. The spatial and temporal coordinates of the system are represented by ζ and t, where $\zeta \in [0,1]$ and $t \in [0,\infty)$.

Dankwerts boundary conditions are particularly suitable for modeling axial tubular reactors, as they account for deviations from perfect mixing and piston flow, assuming negligible transport lags in connecting lines.[25] These conditions make the model more realistic for chemical reactors of this type. The input and the output of the system are also present in the boundary conditions. The system output is measured at the reactor outlet, while the input is applied at the inlet.

Additionally, the delayed state resulting from the recycled portion of the flow, occurring τ time units ago, is incorporated into the inlet; all as shown in Equation 2.

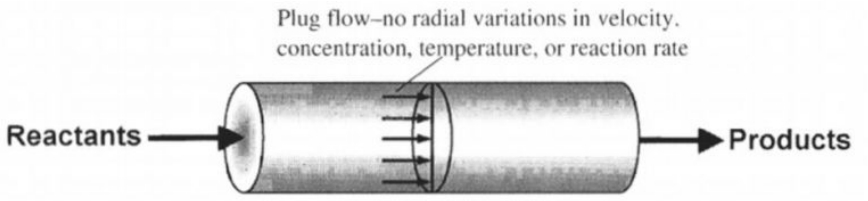

Figure 1: Sample figure.

2.2 PDE Representation of Delay Term

One effective method for addressing delay in systems is to represent the delay using an alternative transport partial differential equation (PDE). This approach is particularly advantageous when the problem already involves similar forms of PDEs, as is the case in the current study. To specifically address the delay in the system under consideration, the state variable $c(\zeta, t)$ is expanded into a vector of functions $C(\zeta, t) \equiv [c_1(\zeta, t), c_2(\zeta, t)]^T$, where $c_1(\zeta, t)$ represents the concentration within the reactor, and $c_2(\zeta, t)$ is introduced as a new state variable to account for the concentration along the recycle stream. The delay is thus modeled as a pure transport process, wherein the first state $c_1(\zeta, t)$ is transported from the reactor outlet to the inlet, experiencing a delay of τ time units while in the recycle stream. As a result, Equations 1 and 2 may be re-formulated as follows:

$$\partial_t \begin{bmatrix} c_1(\zeta,t) \\ c_2(\zeta,t) \end{bmatrix} = \begin{bmatrix} D\partial_{\zeta\zeta} - v\partial_\zeta + k_r & 0 \\ 0 & -\frac{1}{\tau}\partial_\zeta \end{bmatrix} \begin{bmatrix} c_1(\zeta,t) \\ c_2(\zeta,t) \end{bmatrix} \tag{3}$$

$$\begin{cases} D\partial_\zeta c_1(0,t) - v c_1(0,t) = -v\left[R c_2(0,t) + (1-R)u(t)\right] \\ \partial_\zeta c_1(1,t) = 0 \\ c_1(1,t) = c_2(1,t) \\ y(t) = c_1(1,t) \end{cases} \tag{4}$$

With all state variables now expressed explicitly at a specific time instance t—in contrast to the

previous representation where states at t were directly involved with states at $t-\tau$—the system can be described in the standard state-space form of an infinite-dimensional linear time-invariant (LTI) system as $\dot{x} = \mathfrak{A}x$. Here, the state $x(\zeta,t) = [x_1(\zeta,t), x_2(\zeta,t)]^T$ is a vector of functions, and $\mathfrak{A}$ is a linear operator $\mathcal{L}(X)$ acting on a Hilbert space $X : L^2[0,1] \times L^2[0,1]$. The operator $\mathfrak{A}$ and its domain are defined in detail as shown in Equation 5:

$$
\begin{aligned}
\mathfrak{A} \equiv & \begin{bmatrix} D\partial_{\zeta\zeta} - v\partial_\zeta + k_r & 0 \\ 0 & \frac{1}{\tau}\partial_\zeta \end{bmatrix} \\
D(\mathfrak{A}) = & \Big\{ x = [x_1, x_2]^T \in X : x(\zeta), \partial_\zeta x(\zeta), \partial_{\zeta\zeta} x(\zeta) \quad \text{a.c.}, \\
& D\partial_\zeta x_1(0) - v x_1(0) = -v\left[R x_2(0) + (1-R)u\right], \\
& \partial_\zeta x_1(1) = 0, x_1(1) = x_2(1) \Big\}
\end{aligned}
\tag{5}
$$

2.3 Adjoint Operator

Obtaining the adjoint operator $\mathfrak{A}^*$ is a crucial step in analyzing the system's properties, particularly its spectral characteristics. If the operator $\mathfrak{A}$ is shown to be self-adjoint (i.e., $\mathfrak{A} = \mathfrak{A}^*$), the system's eigenmodes can be suitably scaled to form an orthonormal basis for the entire function space, which greatly facilitates the analysis and solution of the system. However, even when the operator $\mathfrak{A}$ is not self-adjoint, the combined set of eigenmodes of $\mathfrak{A}$ and its adjoint $\mathfrak{A}^*$ may still form a bi-orthonormal basis for the given function space. This scenario is typical when $\mathfrak{A}$ is a Riesz-spectral operator.[16] Consequently, determining the adjoint operator $\mathfrak{A}^*$, as represented in Equation 6 is a pivotal step in the spectral analysis of the system.

$$
\begin{aligned}
&\langle \mathfrak{A}\Phi, \Psi \rangle = \langle \Phi, \mathfrak{A}^*\Psi \rangle \Rightarrow \\
&\qquad \mathfrak{A}^* = \begin{bmatrix} D\partial_{\zeta\zeta} + v\partial_\zeta + k_r & 0 \\ 0 & -\frac{1}{\tau}\partial_\zeta \end{bmatrix} \\
&\qquad D(\mathfrak{A}^*) = \Big\{ y = [y_1, y_2]^T \in Y : y(\zeta), \partial_\zeta y(\zeta), \partial_{\zeta\zeta} y(\zeta) \quad \text{a.c.}, \\
&\qquad\qquad D\partial_\zeta y_1(1) + v y_1(1) = \frac{1}{\tau} y_2(1) \\
&\qquad\qquad R v y_1(0) = \frac{1}{\tau} y_2(0) \\
&\qquad\qquad \partial_\zeta y_1(0) = 0 \Big\}
\end{aligned}
\tag{6}
$$

This suggests that the operator $\mathfrak{A}$ is not self-adjoint. To investigate whether $\mathfrak{A}$ is a Riesz-spectral operator, the spectra of both $\mathfrak{A}$ and $\mathfrak{A}^*$ must be determined by solving their characteristic equations, which is done in the upcoming section.

2.4 Eigenvalue Problem

The spectrum of both $\mathfrak{A}$ and $\mathfrak{A}^*$ shall be determined to show whether $\mathfrak{A}$ is a Riesz-spectral operator. In order to obtain the eigenvalues of the system, the eigenvalue problem shall be stated and the characteristic equation needs to be solved once obtained from the equations. Looking back at the state-space representation of the system $\dot{x}(\zeta,t) = \mathfrak{A}x(\zeta,t)$, with $\mathfrak{A}$ defined in Equation 5, spatial part of $x(\zeta,t)$ may be isolated and used to demonstrate the eigenvalue problem[26] as shown in Equation 7:

$$\mathfrak{A}\Phi_i(\zeta) = \lambda_i \Phi_i(\zeta) \tag{7}$$

where $\lambda_i \in \mathcal{C}$ is the i^{th} eigenvalue of the operator $\mathfrak{A}$, with $\Phi_i(\zeta) = [\phi_{i,1}(\zeta), \phi_{i,2}(\zeta)]^T$ being its corresponding eigenfunction. Re-writing the spatial part for the system of PDEs considering the eigenvalues will give Equation 8 for a given i:

$$\begin{cases} \lambda\phi_1 = D\frac{d^2\phi_1}{d\zeta^2} - v\frac{d\phi_1}{d\zeta} + k\phi_1 \\ \lambda\phi_2 = \frac{1}{\tau}\frac{d\phi_2}{d\zeta} \end{cases}$$
$$B.C. \begin{cases} D\ \frac{d\phi_1}{d\zeta}\Big|_{\zeta=0} - v\ \phi_1|_{\zeta=0} = -Rv\ \phi_2|_{\zeta=0} \\ \phi_1|_{\zeta=1} = 0 \\ \phi_1|_{\zeta=1} = \phi_2|_{\zeta=1} \end{cases} \tag{8}$$

The goal is to obtain the set of eigenvalues. To do so, the second order derivative in the operator $\mathfrak{A}$ shall be converted in two first order derivatives to give Equation 9:

$$\partial_\zeta \begin{bmatrix} \phi_1 \\ \partial_\zeta\phi_1 \\ \phi_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ \frac{\lambda - k_r}{D} & \frac{v}{D} & 0 \\ 0 & 0 & \tau\lambda \end{bmatrix} \begin{bmatrix} \phi_1 \\ \partial_\zeta\phi_1 \\ \phi_2 \end{bmatrix} \tag{9}$$

which is a well-known system of ODEs in the form of $\tilde{\Phi}_\zeta = \tilde{\mathfrak{A}}\tilde{\Phi}$, with $\tilde{\Phi} \equiv [\phi_1, \partial_\zeta \phi_1, \phi_2]^T$ and $\tilde{\mathfrak{A}}$ as the 3×3 matrix shown in Equation 9. The obtained system of ODEs has the solution of the form $\tilde{\Phi}(1) = e^{\tilde{\mathfrak{A}}(1-0)}\Phi(0)$. By introducing $\Lambda \equiv e^{\tilde{\mathfrak{A}}}$, Equation 10 may be deduced:

$$\begin{bmatrix} \phi_1 \\ \partial_\zeta \phi_1 \\ \phi_2 \end{bmatrix}_{\zeta=1} = \begin{bmatrix} \Lambda_{1,1} & \Lambda_{1,2} & \Lambda_{1,3} \\ \Lambda_{2,1} & \Lambda_{2,2} & \Lambda_{2,3} \\ \Lambda_{3,1} & \Lambda_{3,2} & \Lambda_{3,3} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \partial_\zeta \phi_1 \\ \phi_2 \end{bmatrix}_{\zeta=0} \tag{10}$$

Next, the boundary conditions may be plugged in Equation 10 accordingly to result a 3×3 algebraic system of equations shown in Equation 11:

$$\begin{bmatrix} -v & D & Rv \\ \Lambda_{2,1} & \Lambda_{2,2} & \Lambda_{2,3} \\ (\Lambda_{1,1} - \Lambda_{3,1}) & (\Lambda_{1,2} - \Lambda_{3,2}) & (\Lambda_{1,3} - \Lambda_{3,3}) \end{bmatrix} \begin{bmatrix} \phi_1 \\ \partial_\zeta \phi_1 \\ \phi_2 \end{bmatrix}_{\zeta=0} = \tilde{\Lambda}\tilde{\Phi}_{\zeta=0} = 0 \tag{11}$$

where $\tilde{\Lambda}$ is defined as the 3×3 matrix shown in Equation 11. The system of algebraic equations shown in Equation 11 suggests that the matrix $\tilde{\Lambda}$ must be rank-deficient for appropriate values of λ_i. Therefore, to solve the characteristic equation means to set $det(\tilde{\Lambda}) = 0$. This will result in the set of eigenvalues of the operator $\mathfrak{A}$. Since an analytical solution may not be feasible, system parameters will be selected to enable numerical calculations. Physical parameters have been selected to reflect realistic values relevant to the application, with their corresponding values provided in Table 1.

Table 1: Physical Parameters for the System

Parameter	**Symbol**	**Value**
Length	L	10 m
Mass	m	5 kg
Damping Coefficient	c	0.1 Ns/m
Spring Constant	k	100 N/m

The eigenvalue distribution in the complex plane is depicted in Figure [XXX], given parameters provided in Table 1.

Following the same procedure for the adjoint operator $\mathfrak{A}^*$ results in the set of adjoint eigenvalues λ_i^*. It can be analytically proven that $\forall i > 0$: $\lambda_i^* = \overline{\lambda_i}$. Therefore, the eigenvalue distribution for $\mathfrak{A}^*$ will be the same as for $\mathfrak{A}$, which is previously shown in Figure [XXX].

2.5 Eigenfunctions Representation

2.6 Open-loop (Zero-input) Response

3 Full-state Feedback Regulator

4 Output Feedback Compensator

5 Conclusion

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