Model Predictive Control of Axial Dispersion Tubular Reactors with Recycle: Addressing State-delay through Transport PDEs*

Behrad Moadeli and Stevan Dubljevic[1]

Abstract— **This paper presents the model predictive control of an axial tubular reactor with a recycle stream, where the intrinsic time delay imposed by the recycle stream—often overlooked in prior studies—is modeled as a transport PDE. This leads to a boundary-controlled system of coupled parabolic and hyperbolic PDEs under Danckwerts boundary conditions, ideal for this reactor type. A discrete-time linear model predictive controller is designed to stabilize the system. Utilizing Caley-Tustin time discretization along with the late lumping approach, the system's infinite-dimensional characteristics are preserved with no need for model reduction or spatial approximation. Numerical simulations demonstrate the controller's effectiveness in stabilizing an unstable system while satisfying input constraints.**

I. Introduction

Many chemical and petrochemical processes involve states that are distributed in space and time. These systems, a.k.a. distributed parameter systems (DPS), are often modeled using partial differential equations (PDEs) to account for distributed states dynamics. Due to the infinite-dimensional nature of DPSs, the control and estimation of these systems becomes inevitably more challenging compared to the well-developed control theories for finite-dimensional systems [1], making this field an active and fertile direction of research. Two primary methods have been proposed to approach the control of DPSs in the literature. The first one is *Early Lumping*, i.e. reducing the infinite-dimensional system to a finite-dimensional one by spatial discretization in the early stages of system modeling [2]. Approximation of the system dynamics at this stage leads to standard control strategies; however, the accuracy of the model is compromised due to potential mismatch between the original system and the reduced-order model [3]. On the contrary, the second method, *Late Lumping*, aims to preserve the infinite-dimensional nature of the system. Approximation may be made only in the final numerical implementation of the controller, resulting in a more accurate yet more complex control strategy.

Numerous studies have utilized a late lumping approach for the purpose of controlling infinite dimensional systems within the field of chemical engineering, focusing on the control of either convection-reaction systems governed by first order hyperbolic PDEs, or diffusion-convection-reaction systems governed by second order parabolic PDEs. In [4], robust control of first order hyperbolic PDEs was addressed, where a plug flow reactor system is stabilized under a distributed input. Boundary feedback stabilization using backstepping method is proposed in [5] for a similar system of first order hyperbolic PDEs. In [6], state feedback regulator design is proposed for a countercurrent heat exchanger system, which is another example of a chemical engineering DPS governed by first order hyperbolic PDEs other than tubular reaction systems. Introducing the effect of dispersion as a prominent aspect of axial dispersion tubular reactors, the robust control of a diffusion-convection-reaction systems governed by second order parabolic PDEs is studied in [7]. A late-lumping based approach is considered in [8] to design a low-dimensional predictive controller for a diffusion-convection-reaction system, where the dominant modes of the system are captured by modal decomposition. Similar approach has been utilized to design an observer-based model predictive controller (MPC) in [9] for an axial dispersion tubular reactor, considering the effects of recycle stream as a well-known feature of industrial chemical reactors.

Delay systems are another class of infinite-dimensional systems that have been studied in the literature [10]. Commonly represented in the form of delay differential equations (DDEs), delay can also be modeled as a transport PDE, showing to be advantageous in more complex scenarios [11]. In the field of control theory for chemical engineering DPSs, input/output delay has been addressed in several works as both output measurement delays and input actuation delays are common in industrial processes. In general, such delays can be addressed by considering a transportation lag block at either the input or output of the system, resulting in a cascade PDE system [12]–[14]. In contrast to input/output delays, state delay is less addressed in the relevant literature, probably since not many applications in this field can be described by state delays. In one of the few attempts, a delayed-state distributed parameter system is addressed in [15], where a full-state and output feedback regulator is designed for a system of heat exchangers. The state delay in this works comes from the time it takes for a stream to leave one pass of the heat exchanger and enter the next pass. Similarly in [16], a tubular reactor system is considered, where the state delay is introduced as a result of the recycle delay in the system, without considering the diffusion term along the reactor. Even in [9] where the recycle stream is considered for a distributed diffusion-convection-reaction system, the recycle is assumed to be instantaneous; a simplifying assumption that leaves a gap in the literature regarding diffusion-convection-reaction systems with a recycle stream imposing state delay.

*This work was not supported by any organization

[1]Behrad Moadeli and Stevan Dubljevic are with the Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB, Canada T6G 1H9 moadeli@ualberta.ca, stevan.dubljevic@ualberta.ca

In this work, an axial dispersion tubular reactor equipped with recycle is addressed as a diffusion-convection-reaction DPS. First, the reactor is modeled by a second order parabolic PDE, where the recycle stream poses a state delay, resulting in a first order hyperbolic transport PDE coupled with the original PDE. Late lumping approach is utilized by obtaining the resolvent of the infinite-dimensional system in a closed operator form, with no need to perform spatial discretization. Then, to enable the implementation of MPC as a digital controller, discrete-time representation of the system is obtained using Caley-Tustin time discretization technique; i.e. a Crank-Nicolson type of discretization that preserves the conservative characteristics of the continuous system, mitigating the need for model reduction [17], [18]. Finally via numerical simulations, the proposed controller is shown to stabilize an unstable system within an optimal framework, given input constraints.

II. Methodology

A. Model representation

The chemical process depicted in Fig. 1 illustrates a first-order irreversible chemical reaction within an axial dispersion tubular reactor [19]. The reactor features a recycle mechanism, allowing a portion of the product stream to re-enter the reactor, ensuring the consumption of any unreacted substrate. 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 [20]. The resulting PDE that describes the reactor model is given by (1), subject to the boundary conditions in (2), obtained by utilizing first-principle modeling through relevant mass balance relations on an infinitesimally small section of the reactor.

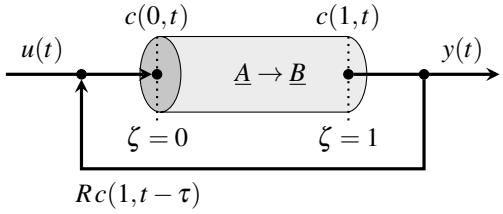

Fig. 1. Axial tubular reactor with recycle stream.

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

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

Here, $c(\zeta,t)$ is the concentration of the product along the reactor, representing the state of the system. The physical parameters D, v, k_r, R, and τ represent the diffusion coefficient, flow velocity along the reactor, reaction constant, recycle ratio, and residence time of the recycle flow, respectively. The coordinate system in space and time is represented by ζ and t, where $\zeta \in [0,1]$ and $t \in [0,\infty)$.

In an attempt to make the model more realistic for common axial dispersion tubular reactors in chemical industry, Dankwerts boundary conditions are chosen as they are known to be suitable for this purpose by accounting for deviations from perfect mixing and piston flow, assuming negligible transport lags in connecting lines [21]. The delayed state resulting from the recycled portion of the flow, occurring τ seconds back in time, is applied at the inlet boundary condition, as shown in (2).

In the case where the problem involves similar forms of PDEs, an effective general practice to address delays in systems is to reformulate the problem such that the notion of delay is replaced with an alternative transport PDE. Therefore, a new state variable $\underline{x}(\zeta,t)$ is defined as a vector of functions $\equiv [x_1(\zeta,t), x_2(\zeta,t)]^T$, where $x_1(\zeta,t)$ represents the concentration within the reactor—analogous to $c(\zeta,t)$—and $x_2(\zeta,t)$ 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 $x_1(\zeta,t)$ is transported from the reactor outlet to the inlet, experiencing a delay of τ time units while in the recycle stream. This makes all state variables expressed explicitly at a specific time instance t, resulting in the standard state-space form for a given infinite-dimensional linear time-invariant (LTI) system as $\dot{\underline{x}} = \mathfrak{A}\underline{x} + \mathfrak{B}u$. Here, $\mathfrak{A}$ is a linear operator $\mathscr{L}(X)$ acting on a Hilbert space $X : L^2[0,1] \times L^2[0,1]$ and $\underline{x}(\zeta,t)$, as defined previously, is the vector of functions describing the states of the system. The operator $\mathfrak{A}$ and its domain are defined in detail as shown in (3). Also, $\mathfrak{B}$ is a linear operator that maps the scalar input from input-space onto the state space, as defined in (4).

$$\begin{aligned} \mathfrak{A} &\equiv \begin{bmatrix} D\partial_{\zeta\zeta} - v\partial_{\zeta} + k_r & 0 \\ 0 & \frac{1}{\tau}\partial_{\zeta} \end{bmatrix} \\ D(\mathfrak{A}) &= \Big\{ \underline{x}(\zeta) = [x_1(\zeta), x_2(\zeta)]^T \in X : \\ &\quad \underline{x}(\zeta), \partial_{\zeta}\underline{x}(\zeta), \partial_{\zeta\zeta}\underline{x}(\zeta) \quad \text{a.c.}, \\ &\quad D\partial_{\zeta}x_1(0) - vx_1(0) = -vRx_2(0), \\ &\quad \partial_{\zeta}x_1(1) = 0, x_1(1) = x_2(1) \Big\} \end{aligned} \tag{3}$$

$$\begin{aligned} \mathfrak{B} &\equiv \begin{bmatrix} \delta(\zeta) \\ 0 \end{bmatrix} v(1-R) \\ D(\mathfrak{B}) &= \Big\{ u \in \mathbb{R} \Big\} \end{aligned} \tag{4}$$

where $\delta(\zeta)$ is dirac delta function. This will enable the derivation of the system's spectrum using the eigenvalue problem. The characteristics equation of the system is obtained by solving the equation $det(\mathfrak{A} - \lambda_i\, I) = 0$ for λ_i, where $\lambda_i \in \mathbb{C}$ is the i^{th} eigenvalue of the system. Attempts to analytically solve this equation has failed; therefore, it is solved numerically using the parameters in Table I. The resulting eigenvalue distribution is depicted in Figure 2 in the complex plane.

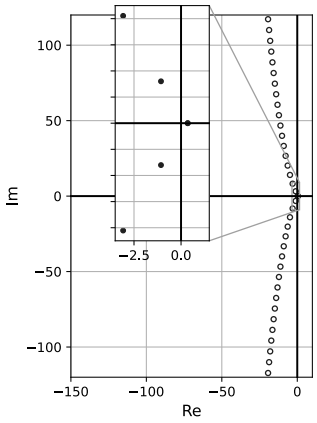

Fig. 2. Eigenvalues of operator $\mathfrak{A}$.

TABLE I

PHYSICAL PARAMETERS FOR THE SYSTEM

Parameter	Symbol	Value	Unit
Diffusivity	D	2×10^{-5}	m^2/s
Velocity	v	0.01	m/s
Reaction Constant	k_r	1.5	s^{-1}
Recycle Residence Time	τ	80	s
Recycle Ratio	R	0.3	–

B. Adjoint system

Next step is to obtain the adjoint system operators $\mathscr{A}^*$ and $\mathscr{B}^*$. Utilizing the relation $\langle \mathfrak{A}\underline{x}+\mathfrak{B}u,\underline{y}\rangle = \langle \underline{x},\mathfrak{A}^*\underline{y}\rangle + \langle u,\mathfrak{B}^*\underline{y}\rangle$, the adjoint operators $\mathfrak{A}^*$ and $\mathfrak{B}^*$ are obtained as shown in (5) and (6), respectively.

$$
\begin{aligned}
\mathfrak{A}^* &= \begin{bmatrix} D\partial_{\zeta\zeta}+v\partial_\zeta+k_r & 0 \\ 0 & -\frac{1}{\tau}\partial_\zeta \end{bmatrix} \\
D(\mathfrak{A}^*) &= \Big\{ \underline{y}=[y_1,y_2]^T \in Y : \\
&\qquad \underline{y}(\zeta),\partial_\zeta\underline{y}(\zeta),\partial_{\zeta\zeta}\underline{y}(\zeta) \quad \text{a.c.}, \\
&\qquad D\partial_\zeta y_1(1)+vy_1(1)=\frac{1}{\tau}y_2(1), \\
&\qquad Rvy_1(0)=\frac{1}{\tau}y_2(0), \partial_\zeta y_1(0)=0 \Big\}
\end{aligned} \tag{5}
$$

$$
\mathfrak{B}^*(\cdot) = \begin{bmatrix} v(1-R)\displaystyle\int_0^1 \delta(\zeta)(\cdot)d\zeta & , & 0 \end{bmatrix} \tag{6}
$$

Once the adjoint operators are determined, the eigenfunctions $\{\underline{\phi_i}(\zeta),\underline{\psi_i}(\zeta)\}$ (for $\mathfrak{A}$ and $\mathfrak{A}^*$, respectively) may be obtained and properly scaled following the calculation of eigenvalues. The set of scaled eigenfunctions will then form a bi-orthonormal basis for the Hilbert space X; which will be later used in the controller design.

C. Resolvent operator

D. Caley-Tustin time discretization

E. Model predictive control design

III. Results and Discussion

IV. Conclusion

Acknowledgment

References

[1] W. H. Ray, *Advanced process control*. McGraw-Hill: New York, NY, USA, 1981.

[2] E. Davison, "The robust control of a servomechanism problem for linear time-invariant multivariable systems," *IEEE transactions on Automatic Control*, vol. 21, no. 1, pp. 25–34, 1976.

[3] A. A. Moghadam, I. Aksikas, S. Dubljevic, and J. F. Forbes, "Infinite-dimensional lq optimal control of a dimethyl ether (dme) catalytic distillation column," *Journal of Process Control*, vol. 22, no. 9, pp. 1655–1669, 2012.

[4] P. D. Christofides and P. Daoutidis, "Feedback control of hyperbolic pde systems," *AIChE Journal*, vol. 42, no. 11, pp. 3063–3086, 1996.

[5] M. Krstic and A. Smyshlyaev, "Backstepping boundary control for first-order hyperbolic pdes and application to systems with actuator and sensor delays," *Systems & Control Letters*, vol. 57, no. 9, pp. 750–758, 2008.

[6] X. Xu and S. Dubljevic, "The state feedback servo-regulator for countercurrent heat-exchanger system modelled by system of hyperbolic pdes," *European Journal of Control*, vol. 29, pp. 51–61, 2016.

[7] P. D. Christofides, "Robust control of parabolic pde systems," *Chemical Engineering Science*, vol. 53, no. 16, pp. 2949–2965, 1998.

[8] S. Dubljevic, N. H. El-Farra, P. Mhaskar, and P. D. Christofides, "Predictive control of parabolic pdes with state and control constraints," *International Journal of Robust and Nonlinear Control: IFAC-Affiliated Journal*, vol. 16, no. 16, pp. 749–772, 2006.

[9] S. Khatibi, G. O. Cassol, and S. Dubljevic, "Model predictive control of a non-isothermal axial dispersion tubular reactor with recycle," *Computers & Chemical Engineering*, vol. 145, p. 107159, 2021.

[10] R. Curtain and H. Zwart, *Introduction to infinite-dimensional systems theory: a state-space approach*. Springer Nature, 2020, vol. 71, ch. 3.2: 'Riesz-spectral operators', pp. 79–108.

[11] M. Krstić, ser. Systems & control. Birkhäuser, 2009, ch. 1.8: 'DDE or Transport PDE Representation', p. 9.

[12] S. Hiratsuka and A. Ichikawa, "Optimal control of systems with transportation lags," *IEEE Transactions on Automatic Control*, vol. 14, no. 3, pp. 237–247, 1969.

[13] L. Mohammadi, I. Aksikas, S. Dubljevic, and J. F. Forbes, "Lq-boundary control of a diffusion-convection-reaction system," *International Journal of Control*, vol. 85, no. 2, pp. 171–181, 2012.

[14] G. O. Cassol and S. Dubljevic, "Discrete output regulator design for a mono-tubular reactor with recycle," in *2019 American Control Conference (ACC)*, 2019, pp. 1262–1267.

[15] G. Ozorio Cassol, D. Ni, and S. Dubljevic, "Heat exchanger system boundary regulation," *AIChE Journal*, vol. 65, no. 8, p. e16623, 2019.

[16] J. Qi, S. Dubljevic, and W. Kong, "Output feedback compensation to state and measurement delays for a first-order hyperbolic pide with recycle," *Automatica*, vol. 128, p. 109565, 2021.

[17] V. Havu and J. Malinen, "The cayley transform as a time discretization scheme," *Numerical Functional Analysis and Optimization*, vol. 28, no. 7-8, pp. 825–851, 2007.

[18] Q. Xu and S. Dubljevic, "Linear model predictive control for transport-reaction processes," *AIChE Journal*, vol. 63, no. 7, pp. 2644–2659, 2017.

[19] O. Levenspiel, *Chemical reaction engineering*. John wiley & sons, 1998.

[20] K. F. Jensen and W. H. Ray, "The bifurcation behavior of tubular reactors," *Chemical Engineering Science*, vol. 37, no. 2, pp. 199–222, 1982.

[21] P. V. Danckwerts, "Continuous flow systems. distribution of residence times," *Chemical engineering science*, vol. 50, no. 24, pp. 3857–3866, 1993.