OPTIMAL CONTROL OF AN AXIAL DISPERSION TUBULAR REACTOR WITH DELAYED RECYCLE

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Presentation Outline

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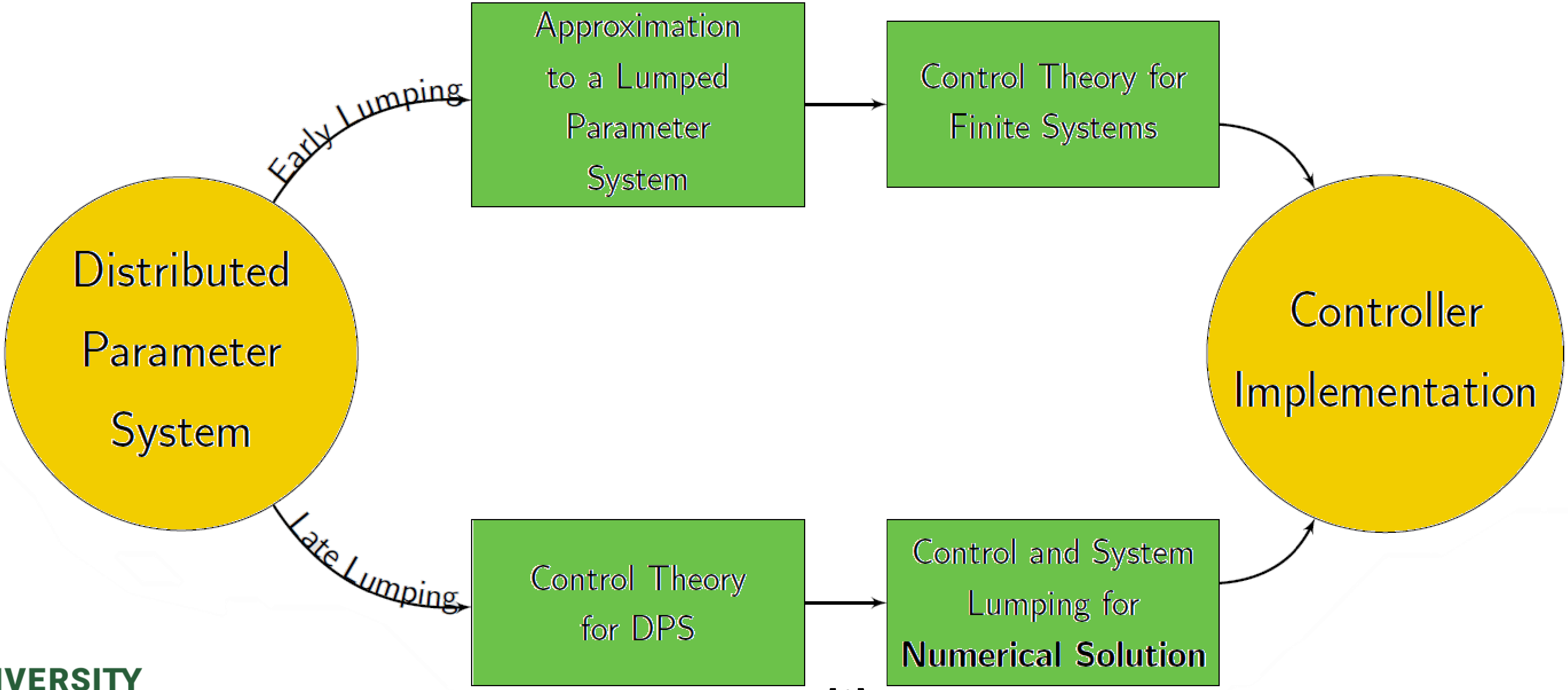
1- Introduction and Literature Review

- Distributed Parameters System
- Axial Dispersion Tubular Reactor with Recycle
- Notion of Delay in Recycle Flow
- Problem Statement
- Literature Review

Distributed Parameter Systems (DPS)

- Spatially varying states in model
- Partial Differential Equations (PDE)
- Infinite-dimensional systems
- Regulator / Observer design becomes challenging

DPS: Early Lumping vs. Late Lumping



[1]

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Axial Dispersion Tubular Reactor

In general:

$$x = x(\zeta, t),\ \zeta \in \Omega \text{ and } t \in \Re^+ \tag{1}$$

A linear PDE:

$$\frac{\partial x}{\partial t}(\zeta, t) = A(\zeta, t)x(\zeta, t) + B(\zeta, t)u(t) \tag{2}$$

with:

$$A(\zeta, t) = \frac{\partial}{\partial \zeta}\underbrace{\left(D(\zeta, t)\frac{\partial}{\partial \zeta}\right)}_{Diffusion} + \underbrace{v(\zeta, t)\frac{\partial}{\partial \zeta}}_{Convection} + \underbrace{k(\zeta, t)}_{Gen./Cons.} \tag{3}$$

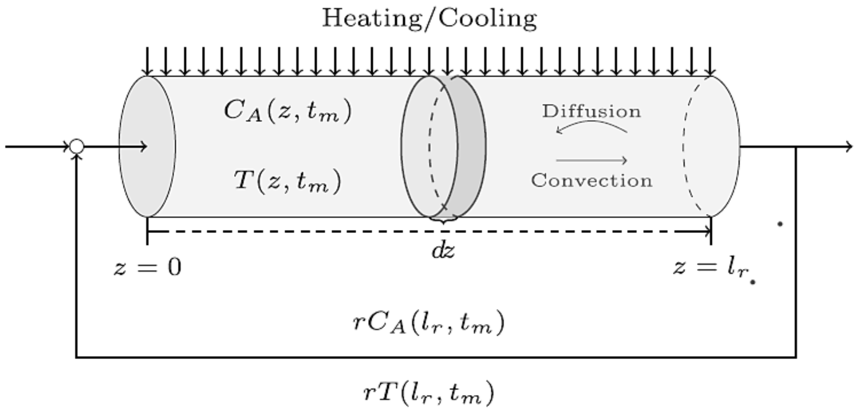

Figure 1 - Schematic view an axial dispersion tubular reactor with recycle [2]

Notion of Delay

- Recycle flow: Pure Transport (Plug Flow)

- Equivalent to Notion of Delay:

$$
\frac{\partial x}{\partial t}(\zeta, t) = -v\frac{\partial}{\partial \zeta}x(\zeta, t)
$$

$$
\text{with: } \begin{cases} x(\zeta = 0, t) & = u(t) \quad \textbf{B.C} \\ x(\zeta, t = 0) & = x_0(\zeta) \quad \textbf{I.C} \\ y(t) & = x(\zeta = l, t) \end{cases} \overset{\tau_d = \frac{l}{v}}{\Longrightarrow} y(t) = u(t - \tau_d) \tag{4}
$$

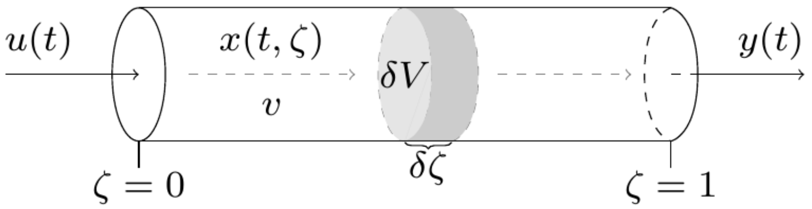

Figure 2 – Pure Transport Representation

Problem Statement: Model

- Dispersion Tubular Reactor: Second Order Parabolic PDE
- Recycle Flow: First Order PDE
  - Considering Danckwerts boundary conditions
  - Input applied at the Boundary (Boundary-Control Problem)

$$\begin{cases} \partial_t x(\zeta,t) = D\partial_{\zeta\zeta}x(\zeta,t) - v\partial_\zeta x(\zeta,t) + kx(\zeta,t) \\ D\partial_\zeta x(0,t) - vx(0,t) = -v[Rx(1,t-\tau) + (1-R)u(t)] \\ \partial_\zeta x(1,t) = 0 \\ y(t) = x(1,t) \end{cases} \tag{5}$$

Problem Statement: Methodology and Goals

- Open-loop modeling using Late Lumping Methods
- Spectrum (Eigenvalue) Analysis
- Determining Dominant Modes
- Continuous Infinite-dimensional Optimal Controller
- Confirm Stability of the Closed-loop System

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Literature Review

- Optimal in-domain Control of Scalar Infinite-dimensional Systems [3]
- Optimal Boundary Control of Infinite-dimensional Spectral Systems [4]
- Model Predictive Control of Axial Dispersion Tubular Reactors with Instantaneous Recycle [2]
- Optimal Boundary Control of First-order Hyperbolic Systems [5]

2- Open-loop System Design

- Eigenvalue Problem
- Adjoint Operator
- Characteristic Equation
- Eigenvalue Distribution (Spectrum Analysis)
- Eigenfunctions (Bi-orthogonal Basis)
- Dominant Modes

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Eigenvalue Problem

$$\begin{cases} \lambda\phi = D\partial_{\zeta\zeta}\phi - v\partial_\zeta\phi + k\phi \\ \lambda\psi = \dfrac{1}{\tau}\partial_\zeta\psi \\ D\partial_\zeta\phi(0) - v\phi(0) = -Rv\psi(0) \\ \partial_\zeta\phi(1) = 0 \\ \psi(1) = \phi(1) \end{cases} \tag{6}$$

$$\begin{cases} \partial_\zeta X = \begin{bmatrix} 0 & 1 & 0 \\ \frac{\lambda-k}{D} & \frac{v}{D} & 0 \\ 0 & 0 & \tau\lambda \end{bmatrix} X = \Lambda X \\ DX_2(0) - vX_1(0) = -RvX_3(0) \\ X_2(1) = 0 \\ X_3(1) = X_1(1) \end{cases} \tag{7}$$

where $X = [\phi,\ \partial_\zeta\phi,\ \psi]^T$

Finding the Adjoint Operator

$$\begin{cases} \hat{A}(.) = & \begin{bmatrix} D\partial_{\zeta\zeta}(.) - v\partial_{\zeta}(.) + k(.) & 0 \\ 0 & \frac{1}{\tau}\partial_{\zeta}(.) \end{bmatrix} \\ B.C. \quad : & \begin{cases} D\partial_{\zeta}\phi(0) - v\phi(0) = -Rv\psi(0) \\ \partial_{\zeta}\phi(1) = 0 \\ \psi(1) = \phi(1) \end{cases} \end{cases} \tag{8}$$

$$< \hat{A}\Phi, \Psi > = < \Phi, \hat{A}^{*}\Psi > \Rightarrow \begin{cases} \hat{A}^{*}(.) = & \begin{bmatrix} D\partial_{\zeta\zeta}(.) + v\partial_{\zeta}(.) + k(.) & 0 \\ 0 & -\frac{1}{\tau}\partial_{\zeta}(.) \end{bmatrix} \\ B.C. \quad : & \begin{cases} D\partial_{\zeta}\phi^{*}(1) + v\phi^{*}(1) = Rv\psi^{*}(1) \\ \partial_{\zeta}\phi^{*}(0) = 0 \\ \psi^{*}(0) = \phi^{*}(0) \end{cases} \end{cases} \Rightarrow \hat{A} \neq \hat{A}^{*}$$

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Characteristic Equation

- Breaking 2nd order PDE in a system of two 1st order PDEs
- Solving for the eigenvalues:

$$det(\bar{A}) = det\left(\begin{bmatrix} -v & D & Rv \\ q_4 & q_5 & 0 \\ q_1 & q_2 & -q_9 \end{bmatrix}\right) = 0 \quad \text{where} \begin{bmatrix} q_1 & q_2 & q_3 \\ q_4 & q_5 & q_6 \\ q_7 & q_8 & q_9 \end{bmatrix} = e^{\Lambda} \tag{9}$$

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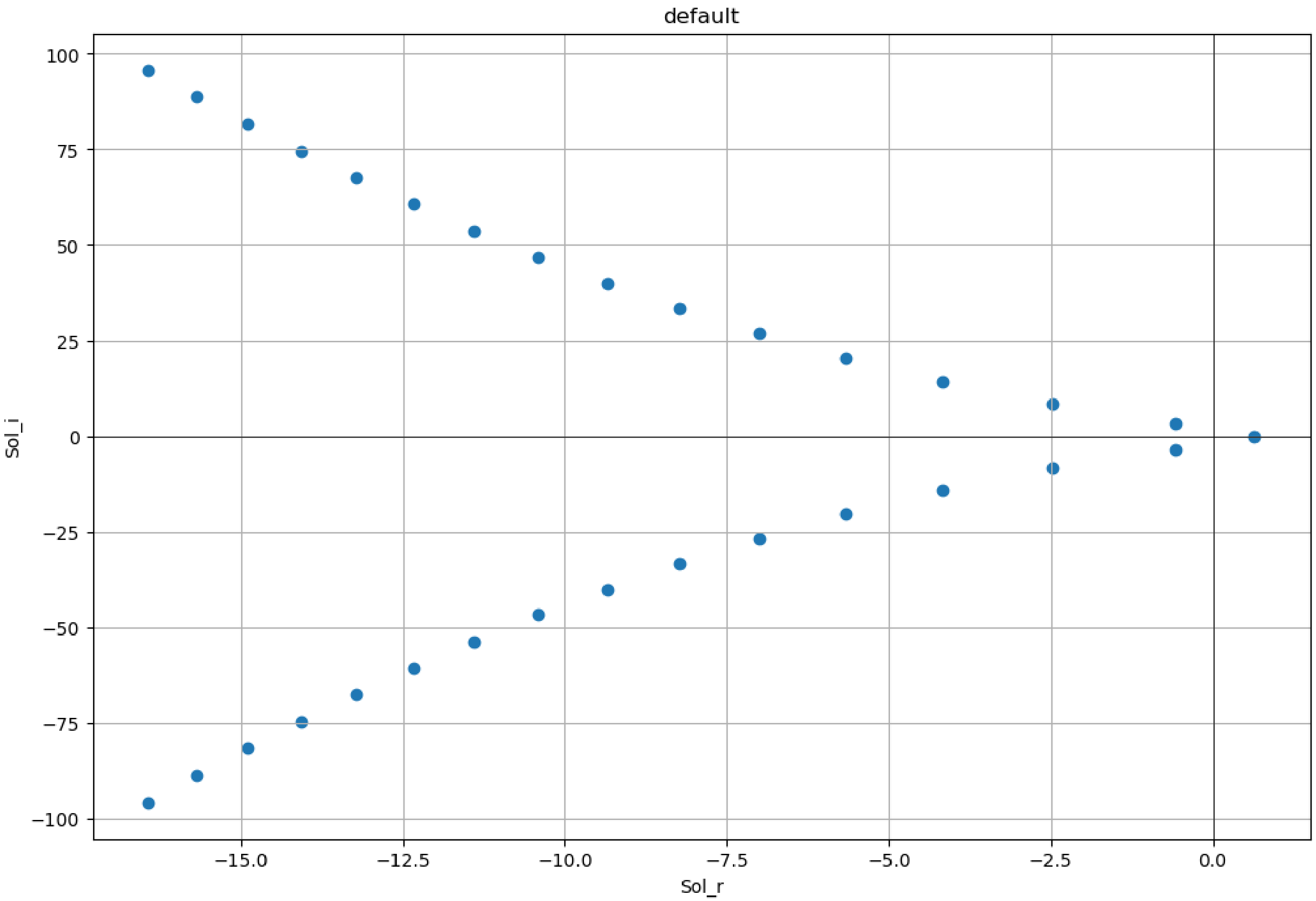
Eigenvalue Distribution



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Eigenfunctions (Bi-orthogonal Basis)

$$\begin{cases} \phi_i(\zeta) = & b_i\left[\left(-\frac{r_{i,2}e^{r_{i,2}}}{r_{i,1}e^{r_{i,1}}}\right)e^{r_{i,1}\zeta} + e^{r_{i,2}\zeta}\right] \\ \psi_i(\zeta) = & b_i(1 - \frac{r_{i,2}}{r_{i,1}})e^{r_{i,2}-\tau\lambda}e^{\tau\lambda\zeta} \end{cases}$$

$$\begin{cases} \phi_i^*(\zeta) = & b_i^*\left[-\frac{r_{i,2}^*}{r_{i,1}^*}e^{r_{i,1}^*\zeta} + e^{r_{i,2}^*\zeta}\right] \\ \psi_i^*(\zeta) = & b_i^*\left(1 - \frac{r_{i,2}^*}{r_{i,1}^*}\right)e^{-\tau\lambda\zeta} \end{cases}$$

$$r_{1,2_i} = \frac{v \pm \sqrt{v^2 + 4D\left(\lambda_i - k\right)}}{2D} \tag{10}$$

- Normalizing coefficients may be found utilizing **Bi-orthogonality Theorem** [2] as follows:

If $\{\Phi_n^*, n \geq 1\}$ are the eigenvectors of the adjoint of A corresponding to the eigenvalues $\{\lambda_n, n \geq 1\}$, then the eigenvectors can be suitably scaled such that $< \Phi_n, \Phi_m^* >= \delta_{mn}$

Dominant Modes (Eigenvalues)

- Using the following Corollary [2] of the previous Theorem makes way for determining the **Dominant Modes** of the system dynamics, by trying to reconstruct any arbitrary function that belongs to our function space with sufficient accuracy using a finite sum, instead of the infinite sum:

Every function $z \in Z$ can be represented by the following infinite sum:

$$z = \sum_{n=1}^{\infty} < z, \Phi_n^* > \Phi_n \tag{11}$$

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Dominant Modes (Eigenvalues)

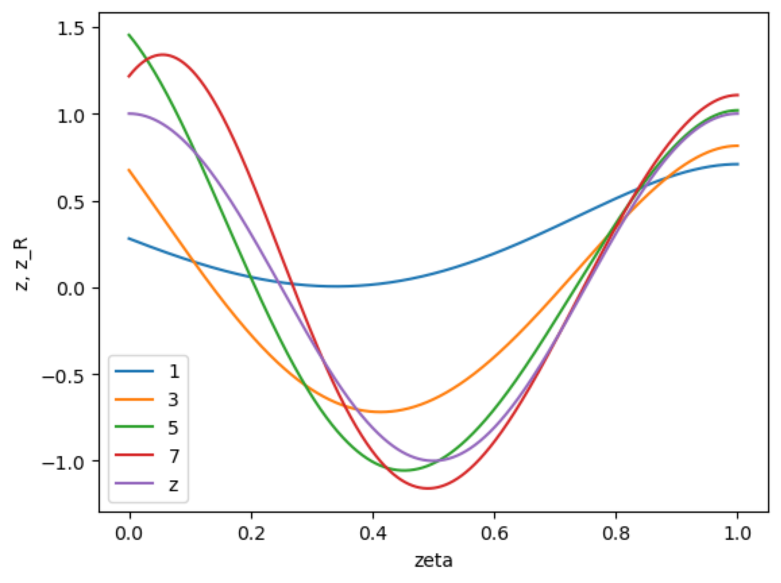

Figure 3 – Arbitrarily chosen function $z(\zeta)$ and its reconstructed approximations $z_R(\zeta)$

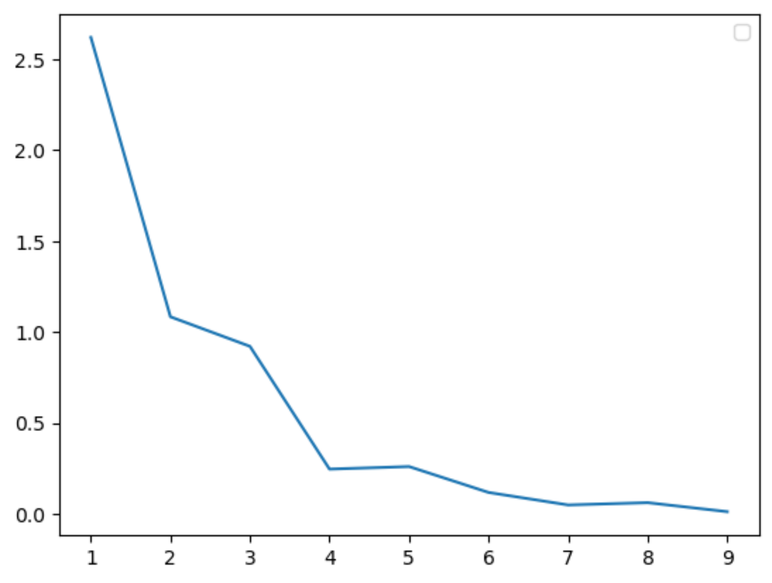

Figure 4 – Reconstruction error $[z(\zeta)- z_R(\zeta))^2$ against the number of modes used

7 modes chosen: (λ_i *for* $i = 1, \ldots, 7$)

3- Controller Design

- Linear Quadratic (LQ) State Feedback Optimal Controller
- Continuous Algebraic Riccati Equation (ARE)

LQ State Feedback Optimal Controller

- The goal is to find the input that minimizes the following cost function:

$$\mathbf{J}(u) = \int_0^\infty < \mathbf{x}, Q\mathbf{x} > + < u, Ru > dt \qquad (12)$$

- The solution of this optimal control problem can be obtained by solving **Algebraic Riccati Equation (ARE)**:

$$< A^* P\mathbf{x}, \mathbf{y} > + < PA\mathbf{x}, \mathbf{y} > + < R^{-1}B^*P\mathbf{x}, B^*P\mathbf{y} > + < Q\mathbf{x}, \mathbf{y} >= 0 \quad (13)$$

- The quadratic cost function is minimized by the following optimal control law:

$$K\mathbf{x} = R^{-1}B^*P\mathbf{x} = R^{-1}\int_0^1 [k_1(\zeta), k_2(\zeta)] \cdot \mathbf{x}(\zeta)d\zeta \qquad (14)$$

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Continuous Algebraic Riccati Equation

- For this system with boundary control, we can write:

$$\hat{B} = v(1-R)[\delta_0(\zeta), 0]^T \tag{15}$$

$$\hat{B}^* = v(1-R)\int_0^1 [\delta_0(\zeta), 0] \cdot \begin{bmatrix} (.) \\ (.) \end{bmatrix} \tag{16}$$

- ***Q*** and ***R*** are also assumed to be as follows:

$$\mathbf{Q} = \begin{bmatrix} R & 0 \\ 0 & 1-(1-R)\zeta \end{bmatrix}; \qquad \mathbf{R} = \mathbf{R}^{-1} = 1 \tag{17}$$

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4- Results and Discussion

- Infinite Dimensional Feedback Gain
- Closed-loop System Input
- Input Response of the System (Stability)

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Infinite Dimensional Feedback Gain

- **ARE** is solved numerically to get **P**
- **K(ζ) = [k_1(ζ), k_2(ζ)]** will be obtained accordingly as functions of space
- u(t) = <**K(ζ) . X(ζ,t)**>
- Feedback Gain shown in Figure 5:

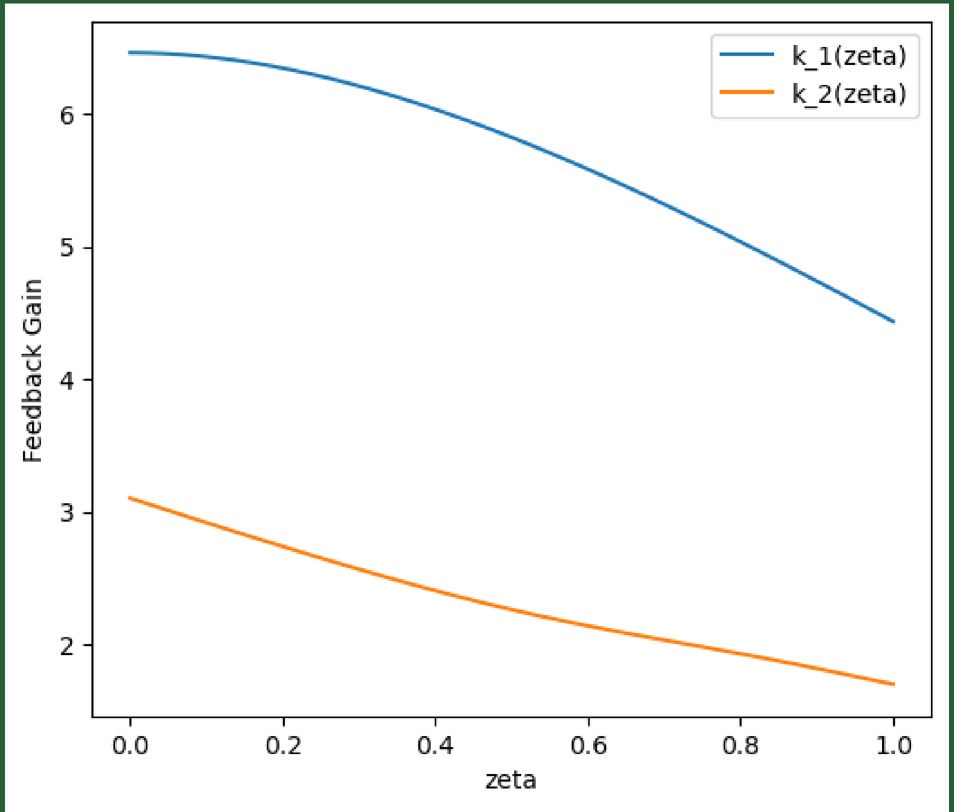

Figure 5 – Feedback Gain K(ζ) = [k_1(ζ), k_2(ζ)] versus zeta

Input Response (Stability)

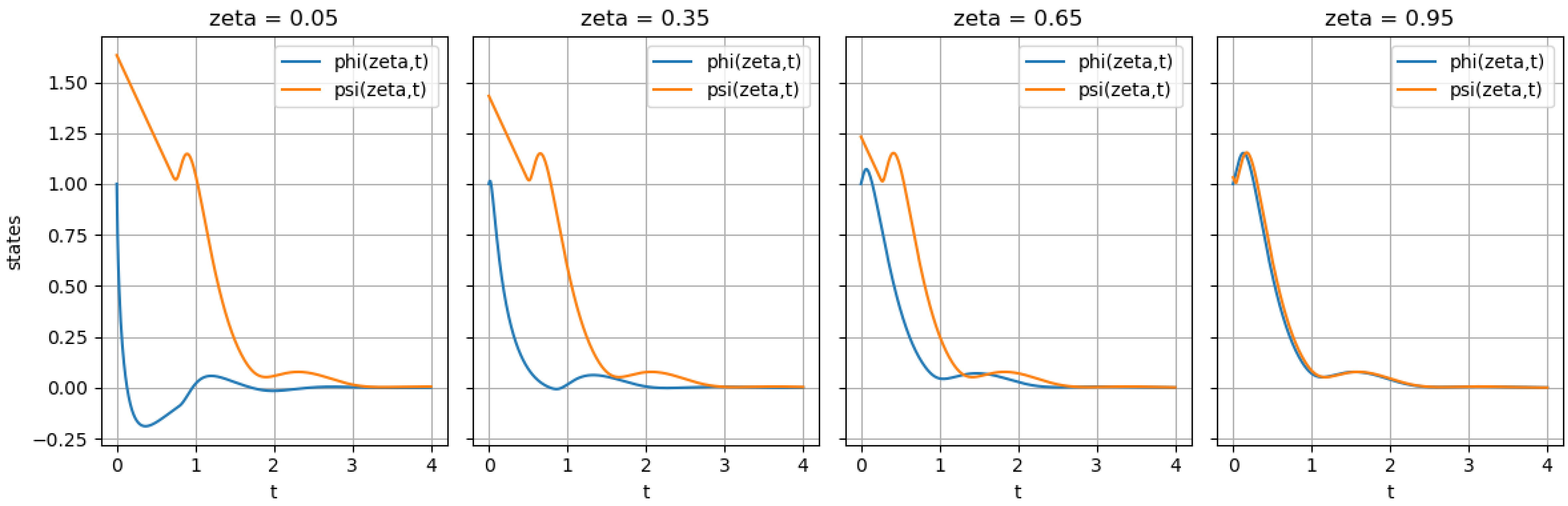

Figure 6 – Input response vs. time at four different locations of the reactor and the recycle stream – i.e. phi(zeta,t) and psi(zeta,t), respectively

Input Response (Stability)

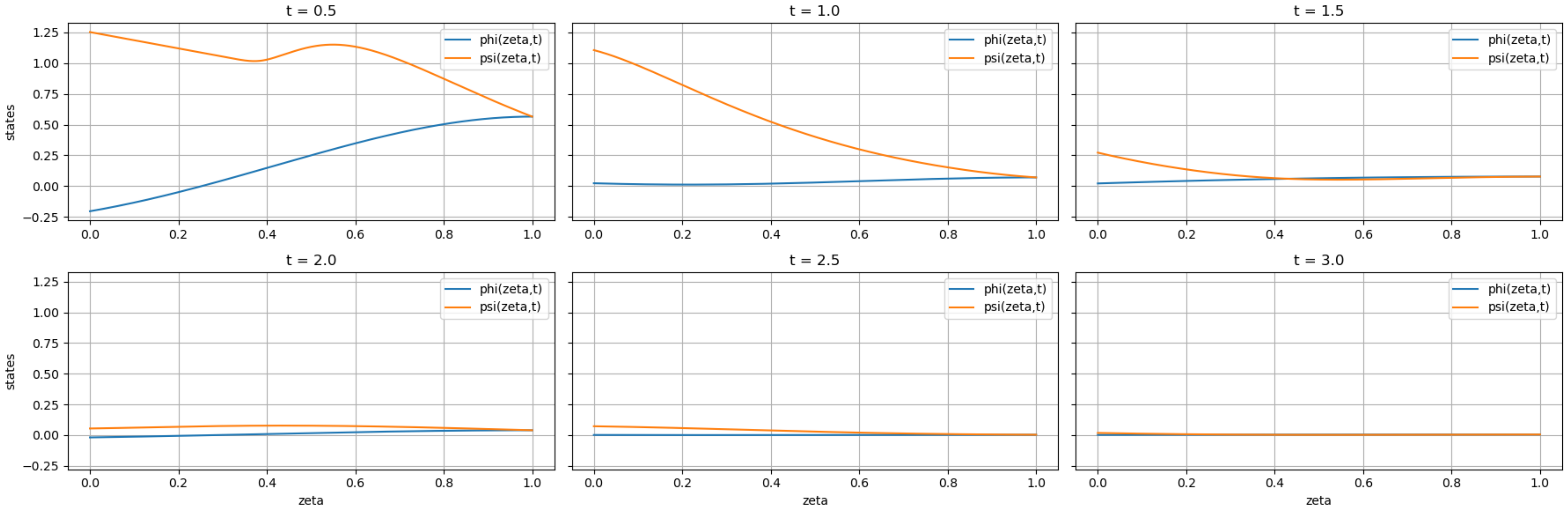

Figure 7 – Input response vs. zeta at six different times for phi(zeta,t) and psi(zeta,t)

Conclusion

- **Open-loop System:**
  - Notion of Delay and Pure Transport
  - Axial Dispersion Tubular Reactor with Delayed Recycle
  - A 3x3 system of coupled PDEs
  - Late Lumping
- **Closed-loop System:**
  - Infinite-horizon Linear Quadratic State Feedback Optimal Control
  - Boundary Control
  - Stability is achieved

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Further Considerations and Future Work

- Study the effect of Parameters on Eigenvalue Distribution
- State Reconstruction to address Full State Feedback issue
- Study the limitations of addressing the system through Early Lumping Methods
- Considering Constraints and Designing MPC

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THANK YOU!

Any Questions?

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