QDMC Using a Reduced-Order SVD-KL Model of a Distributed Parameter System

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Objectives

- ♠ Develop a finite reduced-order model of DPS using plant data
- ♠ Demonstrate the reduction method on a nonlinear reaction system
- ♠ Develop a Quadratic Dynamic Model-based Controller (QDMC) using SVD-KL model
- ♠ Demonstrate the QDMC controller development on a nonlinear reaction system

Input/Output representation

- Input/output characteristics of nonlinear systems may be represented by Volterra series.
- The Volterra series kernels can be identified analytically when the exact mathematical description of the process is known.
- Otherwise kernel must be identified from the data.

For general nonlinear systems: linear models

First-order Volterra model:

$$\mathbf{y(t) = w^0(t,x) + \int_0^t w(\tau)u(t-\tau)d\tau}$$

State space (linear time-invariant) model:

$$\mathbf{y(t) = Ce^{At}x^0 + \int_0^t Ce^{A(\tau)}Bu(t-\tau)d\tau}$$

Kernels from the data

$$\textbf{Inputs} \quad \Delta u(z,t) = \sum_{r=1}^{m} p_r(z) a_r(t)$$

$$\textbf{Outputs} \quad y(z,t) = \sum_{r=1}^{n} q_r(z) b_r(t)$$

Kernel: $k(z,\zeta,\tau)$

Input/Output Model:

$$y(z,t) = \int_0^t \int_\Omega k(z,\zeta,\tau)\Delta u(\zeta, t-\tau)\, d\zeta\, d\tau$$

$$t_0 \le t \le t_f \qquad z \in \Omega$$

Methodology

- ♠ SVD: defines the kernel coefficient matrix
- ♠ Galerkin: solves the kernel coefficient matrix
- ♠ Input/output Model:

  discrete-time, first-order Volterra series approximation

SVD of the kernel in spatial direction

$$
\begin{aligned}
\mathbf{k}(\mathbf{z},\zeta,\tau) &= \sum_{i=1}^{\infty} w_i(z,\tau)\sigma_i(\tau)\overline{\nu_i(\zeta,\tau)} \\
\nu_{\mathbf{i}}(\zeta,\tau) &= \sum_{l=1}^{m} p_l(\zeta)\nu_{li}(\tau) \\
\mathbf{w}_{\mathbf{i}}(\mathbf{z},\tau) &= \sum_{k=1}^{n} q_k(z)w_{ki}(\tau) \\
\mathbf{k}(\mathbf{z},\zeta,\tau) &\simeq \sum_{i=1}^{\min(m,n)} w_i(z,\tau)\sigma_i(\tau)\overline{\nu_i(\zeta,\tau)}
\end{aligned}
$$

$$
\int_{\mathbf{0}}^{\mathbf{t}}\int_{\mathbf{\Omega}} \overbrace{\sum_{r=1}^{N}\left[\sum_{k=1}^{n} q_k(z)w_{kr}(\tau)\sigma_r(\tau)\sum_{l=1}^{m}\overline{\nu_{lr}(\tau)}p_l(\zeta)\right]}^{\textbf{kernel}} \sum_{\mathbf{l=1}}^{\mathbf{m}} \mathbf{p_l}(\zeta)\mathbf{a_l}(\mathbf{t}-\tau)\mathbf{d}\zeta\mathbf{d}\tau
$$

$$
\simeq \sum_{\mathbf{l=1}}^{\mathbf{n}} \mathbf{q_l}(\mathbf{z})\mathbf{b_l}(\mathbf{t})
$$

Galerkin projection

$$\int_{0}^{t} \mathcal{Q}\left(\mathcal{W}(\tau)\boldsymbol{\Sigma}(\tau)\bar{\mathcal{V}}(\tau)\right)\mathcal{P}\mathbf{a}(\mathbf{t}-\tau)\mathbf{d}\tau = \mathcal{Q}\mathbf{b}(\mathbf{t})$$

$$\mathcal{Q} \equiv \int_{\boldsymbol{\Omega}} \mathbf{q}(\zeta)\mathbf{q}^{\mathbf{T}}(\zeta)\mathbf{d}\zeta, \quad \mathcal{P} \equiv \int_{\boldsymbol{\Omega}} \mathbf{p}(\zeta)\mathbf{p}^{\mathbf{T}}(\zeta)\mathbf{d}\zeta$$

$$\mathcal{W} \equiv \{\mathbf{w}_{\mathbf{kl}}(\tau)\}, \quad \mathcal{V} \equiv \{\nu_{\mathbf{rl}}(\tau)\}, \quad \boldsymbol{\Sigma} \equiv \mathrm{diag}\{\sigma_{\mathbf{l}}(\tau)\}$$

Kernel: at time kT

$$\begin{aligned} \mathbf{y}(\mathbf{z},\mathbf{kT}) &= \int_{\boldsymbol{\Omega}} \sum_{\ell=1}^{\infty} \int_{(\ell-1)\mathbf{T}}^{\ell\mathbf{T}} \kappa(\mathbf{z},\zeta,\tau)\mathbf{d}\tau\boldsymbol{\Delta}\mathbf{u}_{\mathbf{k}-\ell}(\zeta)\mathbf{d}\zeta \\ &\approx \sum_{\ell=1}^{\mathbf{N}} \int_{\boldsymbol{\Omega}} \kappa(\mathbf{z},\zeta,\ell)\boldsymbol{\Delta}\mathbf{u}_{\mathbf{k}-\ell}(\zeta)\mathbf{d}\zeta \end{aligned}$$

Kernel from data

$$\sum_{\ell=1}^{\mathbf{N}} \mathcal{Q}\left(\mathcal{W}(\ell)\boldsymbol{\Sigma}(\ell)\bar{\mathcal{V}}(\ell)\right)\mathcal{P}\mathbf{a}_{\mathbf{k}-\ell} = \mathcal{Q}\mathbf{b}(\mathbf{k})$$

Open loop tests: I/O data a and b
Input, Output coefficient matrices: A, B
Least-square approach

$$\bar{\mathbf{K}} \equiv \mathbf{B}\mathbf{A}^{\dagger}$$

$$\mathbf{A} \in \mathbf{mN} \times (\mathbf{P}+\mathbf{1}), \quad \mathbf{B} \in \mathbf{n} \times (\mathbf{P}+\mathbf{1})$$

$\bar{K} = \{K(1), \ldots K(N)\}$ **: Coefficient matrices**

Coefficient Matrix at ℓ

$$\mathbf{K}(\ell) = \mathcal{Q}\left(\mathcal{W}(\ell)\boldsymbol{\Sigma}(\ell)\bar{\mathcal{V}}(\ell)\right)\mathcal{P} \qquad \ell = \mathbf{1}, \ldots, \mathbf{N}$$

$$\mathbf{K}(\ell) \in \mathbf{n} \times \mathbf{m}$$

Methodology

- Dominant spatial effect of the inputs on the outputs: Karhunen-Loève Expansion

  — Identify the dominant empirical eigenfunctions (EEFs): functions of spatial variables

- Project the SVD kernels onto the dominant EEFs: kernel approximation with dominant spatial behavior ($\widehat{\kappa}^{ij}(z,\zeta,t)$)

- Finite input/output model: function of the dominance captured in the kernel

Karhunen-Loève Expansion

Spatial correlation function:

$$\mathcal{R}(\mathbf{z},\zeta) = \lim_{\mathbf{T}\to\infty} \frac{1}{T}\int_{\mathbf{0}}^{\mathbf{T}} \nu(\mathbf{z},\mathbf{t})\nu(\zeta,\mathbf{t})\mathbf{dt}$$

Eigenvalue(λ_j)/ eigenfunction ($\phi_j(z)$) problem

$$\int_{\mathbf{0}}^{\mathbf{1}} \mathcal{R}(\mathbf{z},\zeta)\phi_{\mathbf{j}}(\zeta)\mathbf{d}\zeta = \lambda_{\mathbf{j}}\phi_{\mathbf{j}}(\mathbf{z})$$

Mercer's theorem [Naylor, 1971]

$$\mathcal{R}(\mathbf{z},\zeta) = \sum_{\mathbf{k}=\mathbf{1}}^{\infty} \lambda_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{z})\phi_{\mathbf{k}}(\zeta)$$

Empirical eigenfunction (EEF):

$$\phi_{\mathbf{j}}(\mathbf{z}) = \sum_{\mathbf{k}=\mathbf{1}}^{\mathbf{N}} \alpha_{\mathbf{kj}}\nu_{\mathbf{k}}(\mathbf{z}) \quad \mathbf{j} = \mathbf{1},\ldots$$

Projection

- First few largest eigenvalues represent the dominant behavior.
- The dominant eigenfunctions are the basis functions in an orthogonal projection.

KL expansion to the Dynamic Kernel

$$\hat{\kappa}^{\mathbf{ij}}(\mathbf{z},\zeta,\ell) \simeq \sum_{\mathbf{l}=1}^{\mathbf{n}} \phi_{\mathbf{l}}^{\mathbf{ij}}(\mathbf{z},\zeta)\mathcal{T}_{\mathbf{l}}^{\mathbf{ij}}(\ell) \qquad \mathbf{t_0} \leq \mathbf{t} \leq \mathbf{t_f}$$

$$\mathcal{T}_{\mathbf{l}}^{\mathbf{ij}}(\ell) = \left(\kappa^{\mathbf{ij}}(\mathbf{z},\zeta,\mathbf{t}), \phi_{\mathbf{l}}^{\mathbf{ij}}(\mathbf{z},\zeta)\right)$$

$\mathbf{i}^{th}$ output:

$$\mathbf{y_i}(\mathbf{z},\mathbf{kT}) \simeq \sum_{\ell=1}^{\mathbf{N}} \sum_{\mathbf{j}=1}^{\mathbf{M}} \int_{\Omega} \left[\sum_{\mathbf{l}=1}^{\mathbf{n}} \phi_{\mathbf{l}}^{\mathbf{ij}}(\mathbf{z},\zeta)\mathcal{T}_{\mathbf{l}}^{\mathbf{ij}}(\ell)\right] \Delta\mathbf{u}_{\mathbf{k}-\ell}^{\mathbf{j}}(\zeta)\ \mathbf{d}\zeta$$

Mean value: $\mu^{\mathbf{ij}}(\mathbf{z},\zeta) \qquad \mathbf{j} = 1,\ldots,\mathbf{M},\ \mathbf{i} = 1,\ldots,\mathbf{P},$

Summary of SVD-KL procedure

I/O Tests

Collect data

↓

SVD

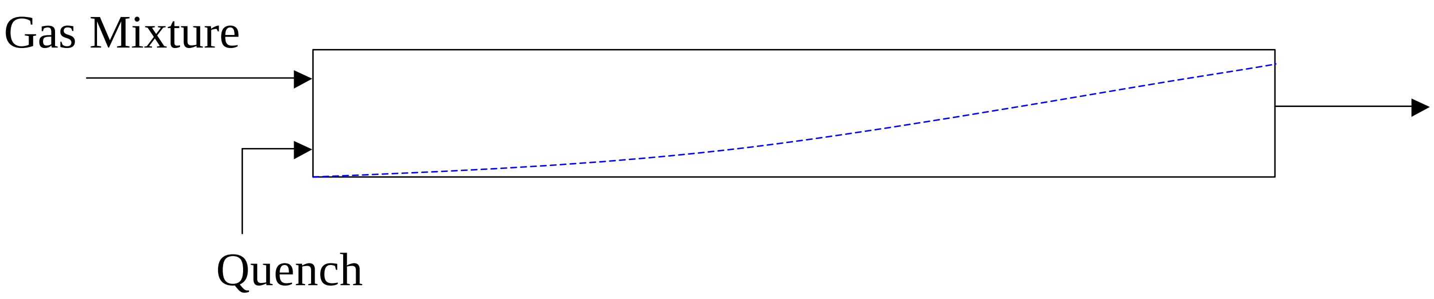
$$y(z,kT) \approx \sum_{\ell=1}^{N} \int_{\Omega} \kappa(z,\zeta,\ell) \Delta u_{k-\ell}(\zeta) d\zeta$$

↓

KL expansion

$$y_i(z,kT) \simeq \sum_{\ell=1}^{N} \sum_{j=1}^{M} \int_{\Omega} \left[\sum_{l=1}^{n} \phi_l^{ij}(z,\zeta) T_l^{ij}(\ell) \right] \Delta u_{k-\ell}^{j}(\zeta)\ d\zeta$$

Hydro-dealkylation of Toluene (HDA)



Two reactions are known to occur,

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$

$$2C_6H_6 \rightleftarrows C_{12}H_{10} + H_2$$

Reactions are exothermic

Temperature between 1150^{o}F$\leq$ T$\leq$ 1300^{o}F

Pressure 500 psia $\pm$ 10%

Five temperature measurements

Concentration measurement at the exit of the reactor

Quench injection

Model of the HDA process

$$\frac{\partial \xi_1}{\partial \tau} = -\nu\left[\frac{\partial \xi_1}{\partial \tau_1} + \frac{\xi_1}{\theta}\frac{\partial \theta}{\partial \tau_1}\right] - \xi_1 \xi_2^{0.5} \theta^{1.5} \mathrm{e}^{\gamma_1 \frac{\theta-1}{\theta}}$$

$$\frac{\partial \xi_2}{\partial \tau} = -\nu\left[\frac{\partial \xi_2}{\partial \tau_1} + \frac{\xi_2}{\theta}\frac{\partial \theta}{\partial \tau_1}\right] - \xi_1 \xi_2^{0.5} \theta^{1.5} \mathrm{e}^{\gamma_1 \frac{\theta-1}{\theta}} + \kappa_2 (\xi_3 \theta)^2 \mathrm{e}^{\gamma_2 \frac{\theta-1}{\theta}} - \kappa_3 \xi_2 \xi_5 \theta^2 \mathrm{e}^{\gamma_3 \frac{\theta-1}{\theta}}$$

$$\frac{\partial \xi_3}{\partial \tau} = -\nu\left[\frac{\partial x_3}{\partial \tau_1} + \frac{\xi_3}{\theta}\frac{\partial \theta}{\partial \tau_1}\right] + \xi_1 \xi_2^{0.5} \theta^{1.5}\, \mathrm{e}^{\gamma_1 \frac{\theta-1}{\theta}} - 2\kappa_2 (\xi_3 \theta)^2 \mathrm{e}^{\gamma_2 \frac{\theta-1}{\theta}} + 2\kappa_3 \xi_2 \xi_5 \theta^2 \mathrm{e}^{\gamma_3 \frac{\theta-1}{\theta}}$$

$$\frac{\partial \xi_4}{\partial \tau} = -\nu\left[\frac{\partial \xi_4}{\partial \tau_1} + \frac{\xi_4}{\theta}\frac{\partial \theta}{\partial \tau_1}\right] + \xi_1 \xi_2^{0.5} \theta^{1.5} \mathrm{e}^{\gamma_1 \frac{\theta-1}{\theta}}$$

$$\frac{\partial \xi_5}{\partial \tau} = -\nu\left[\frac{\partial \xi_5}{\partial \tau_1} + \frac{\xi_5}{\theta}\frac{\partial \theta}{\partial \tau_1}\right] + \kappa_2 (\xi_3 \theta)^2 \mathrm{e}^{\gamma_2 \frac{\theta-1}{\theta}} - \kappa_3 \xi_2 \xi_5 \theta^2 \mathrm{e}^{\gamma_3 \frac{\theta-1}{\theta}}$$

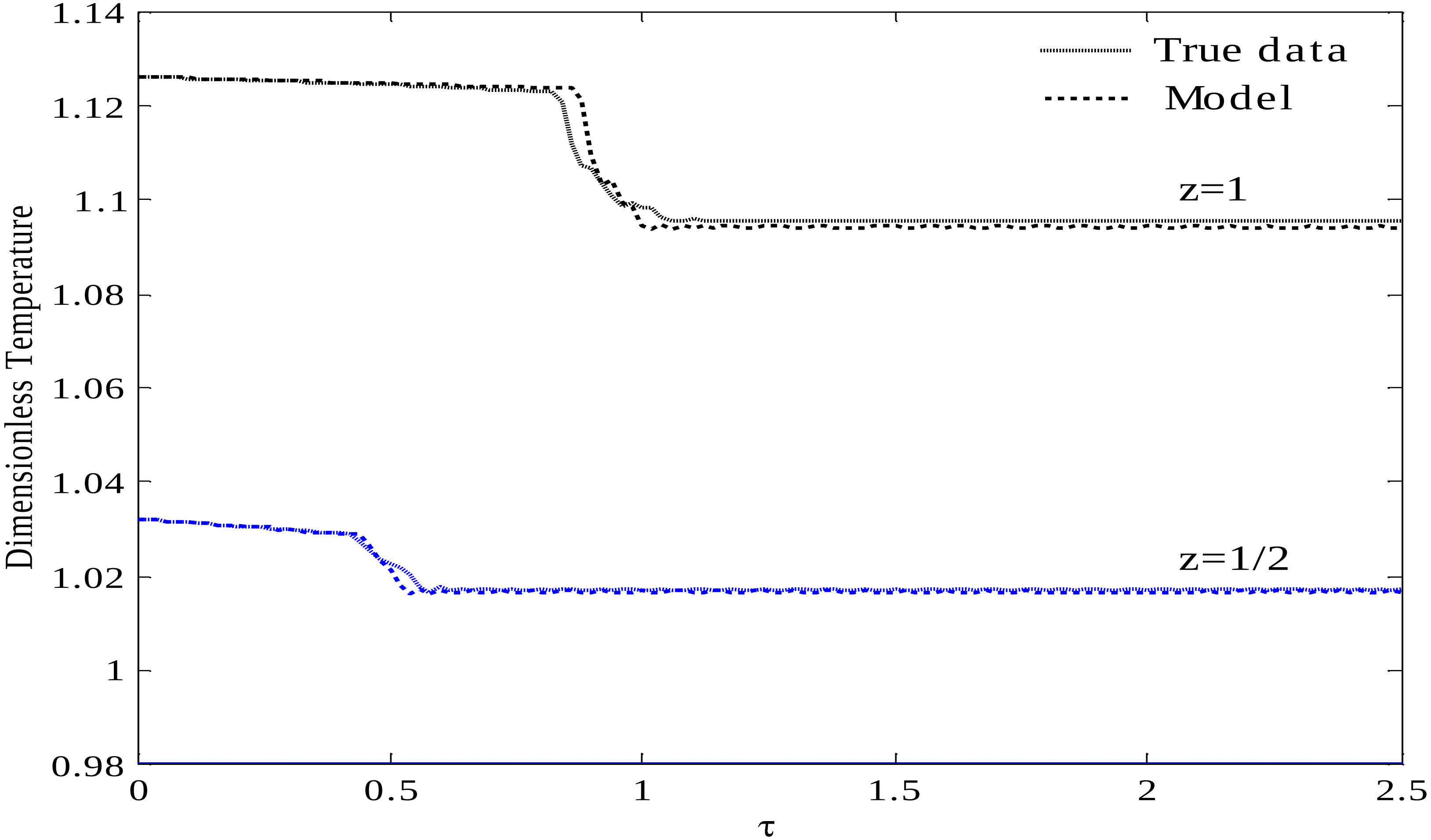
$$\frac{\partial \theta}{\partial \tau} = \frac{1}{\zeta}\left(H_{r_1}\frac{\partial \xi_1}{\partial \tau} - H_{r_2}\frac{\partial \xi_5}{\partial \tau} - \nu\left(\zeta \frac{\partial \theta}{\partial \tau_1} - H_{r_1}\frac{\partial \xi_1}{\partial \tau_1} + H_{r_2}\frac{\partial \xi_5}{\partial \tau_1}\right) - F_{Bm}\zeta_B\right)$$

$$z = 0 \qquad \begin{cases} \xi_j = \xi_j(t=0) & j = 1, \ldots, n_c \\ \theta = \theta(t=0) & \end{cases} \qquad z = 1 \qquad \begin{cases} \dfrac{\partial \xi_j}{\partial z} = 0 & j = 1, \ldots, n_c \\ \dfrac{\partial \theta}{\partial z} = 0 & \end{cases}$$

Model validation at ideal conditions

Temperature

SVD-KL: dashed line, True solution: solid line

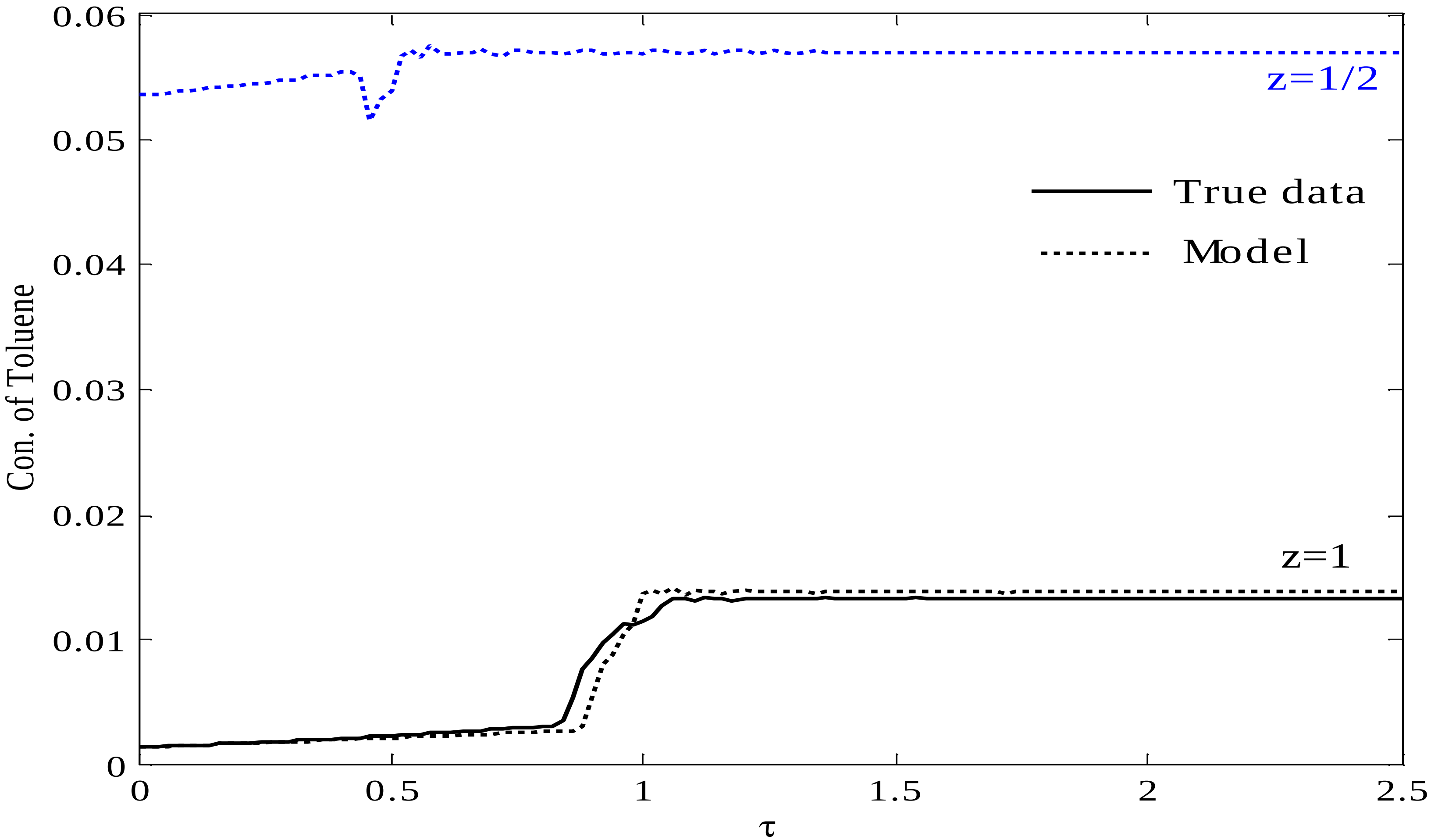


At z=1, time averaged error $= 0.15\%$

Model validation at ideal conditions

Concentration of Toluene

SVD-KL: dashed line, True solution: solid line



At z=1, time averaged error $= 5.25\%$

Controller Design

- ♠ Quadratic Dynamic Matrix Controller (QDMC)
- ♠ Model: Reduced-order SVD-KL
- ♠ Constraints
- ♠ Disturbance rejection:
  - unmeasured feed temperature disturbance
  - unmeasured feed toluene concentration
  - measured feed flow rate disturbance
- ♠ Comparison with other models
  - Lumped model (reactor modelled as one CSTR)
  - QDMC design
    - — NLMPC on nonlinear CSTR model
    - — Linearize ODEs at each sample point kT
    - — Linearize ODEs - use one linear model

Quadratic DMC: Minimize Quadratic objective

$$\min_{U(k)} E = \frac{1}{2}[y^*(k) - \widehat{y}_i(k+\ell|k)]^T \Gamma^T \Gamma [y^*(k) - \widehat{y}_i(k+\ell|k)] + \frac{1}{2} U(k)^T \Lambda^T \Lambda U(k)$$

subject to:

$$\hat{\mathbf{y}}_{\mathbf{i}}(\mathtt{k}+\ell|\mathtt{k}) = \overbrace{y_{i0} + \sum_{r=\ell+1}^{\mathtt{k}} k_{ij}^r \Delta u_j(\mathtt{k}+\ell-r)}^{\textbf{past}} + \overbrace{\sum_{r=1}^{l} k_{ij}^r \Delta u_j(\mathtt{k}+\ell-r)}^{\textbf{future}} + \mathbf{d}(\mathtt{k}+\ell|\mathtt{k})$$

Solve QP problem:

$$\min_{\mathbf{U(k)}} \mathbf{F} = \frac{1}{2}\mathbf{U(k)^T H U(k)} - \mathbf{g}(\mathbf{k}+\ell)^{\mathbf{T}} \mathbf{U(k)}$$

$$\text{s.t.} \quad \mathbf{y_i^{min}} \leq \mathbf{y_i} \leq \mathbf{y_i^{max}}$$

$$\mathbf{U^{min}} \leq \mathbf{U(k)} \leq \mathbf{U^{max}}$$

H : **Hessian**

$g(e(k+\ell))$: **gradient in the direction of** U

Closed-loop stability:

Lemma 1 (Unconstrained case) If the eigenvalue spectrum of the matrix

$$\begin{bmatrix} -\mathbf{A_1 I_u H^{-1} A^T w_y K_y} + \alpha \mathbf{I_{n_y}} & \mathbf{A_1 I_u H^{-1} A^T w_y A_u} - \alpha \mathbf{A_1} + \mathbf{A_2} \\ -\mathbf{I_u H^{-1} A^T w_y K_y} & \mathbf{I_u H^{-1} A^T w_y A_u} \end{bmatrix}$$

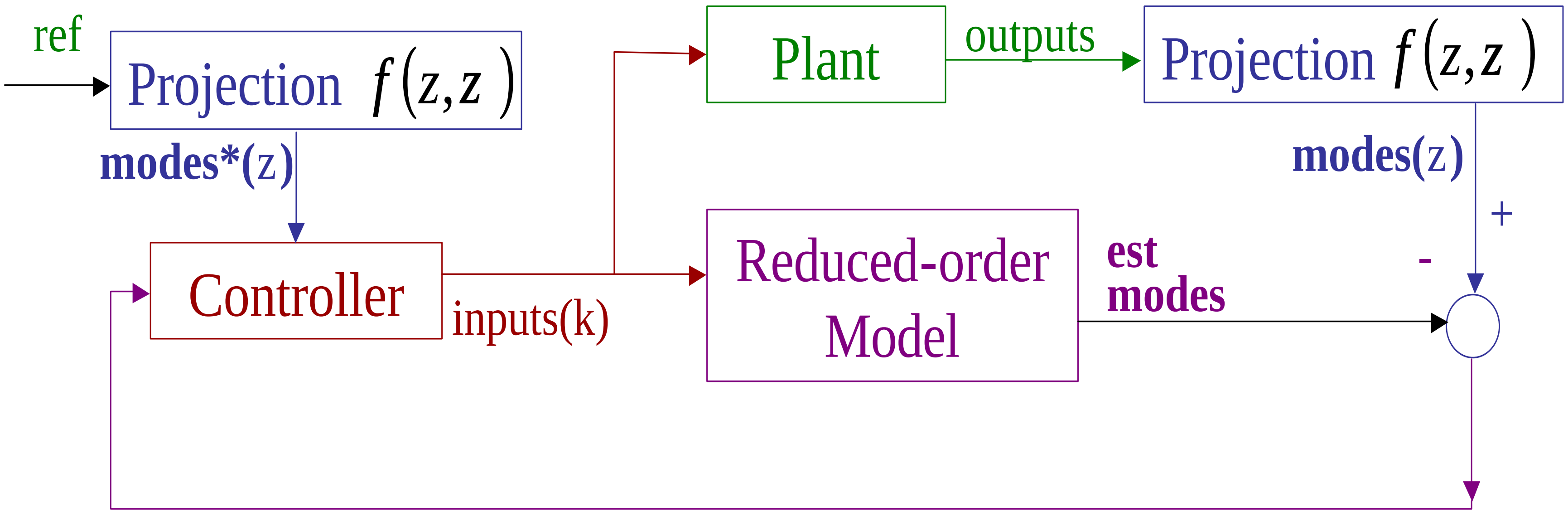
is such that, the largest eigenvalue is less that one, $\max|\lambda_{\mathbf{i}}| < 1$ **then the unconstrained system will be closed-loop asymptotically stable.**

Lemma 2 (Constrained case) For all the possible active constraints combination, if the eigenvalue spectrum of matrix

$$\begin{bmatrix} -\mathbf{A_1 I_u K_u K_y} + \alpha \mathbf{I_{n_y}} & \mathbf{A_1 I_u K_u A_u} - \alpha \mathbf{A_1} + \mathbf{A_2} \\ -\mathbf{I_u K_u K_y} & \mathbf{I_u K_u A_u} \end{bmatrix}$$

has $\max|\lambda_{\mathbf{i}}| < 1$ **then the closed-loop system is asymptotically stable.**

Control Strategy



Input(k) $= \hat{u}_k(\zeta)$

Modes are functions of ζ

QDMC design

QDMC/SVDKL model:

Control horizon $M = 5$

Weight matrices: $\Gamma = 1$ **and** $\Lambda = 40$

QDMC/linear CSTR model:

Control horizon $M = 5$

Weight matrices: $\Gamma = 1$ **and** $\Lambda = 40$

QDMC/nominal linear CSTR model:

Control horizon $M = 5$

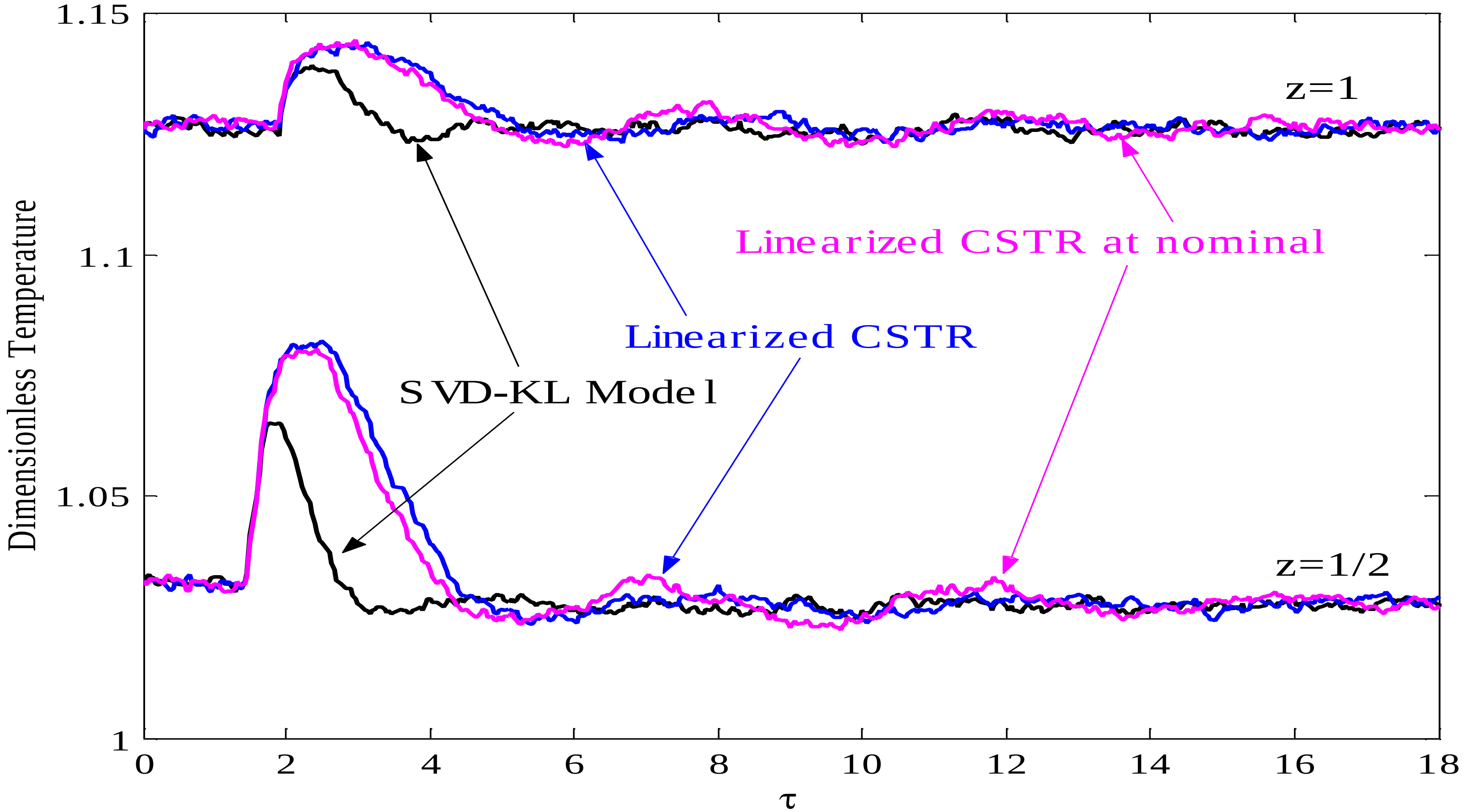
Weight matrices: $\Gamma = 1$ **and** $\Lambda = 40$

Closed-loop performance

Unmeasured disturbance: Feed temperature (+5%)

Unmeasured disturbance: Feed Toluene concentration (+5%)

Temperature response

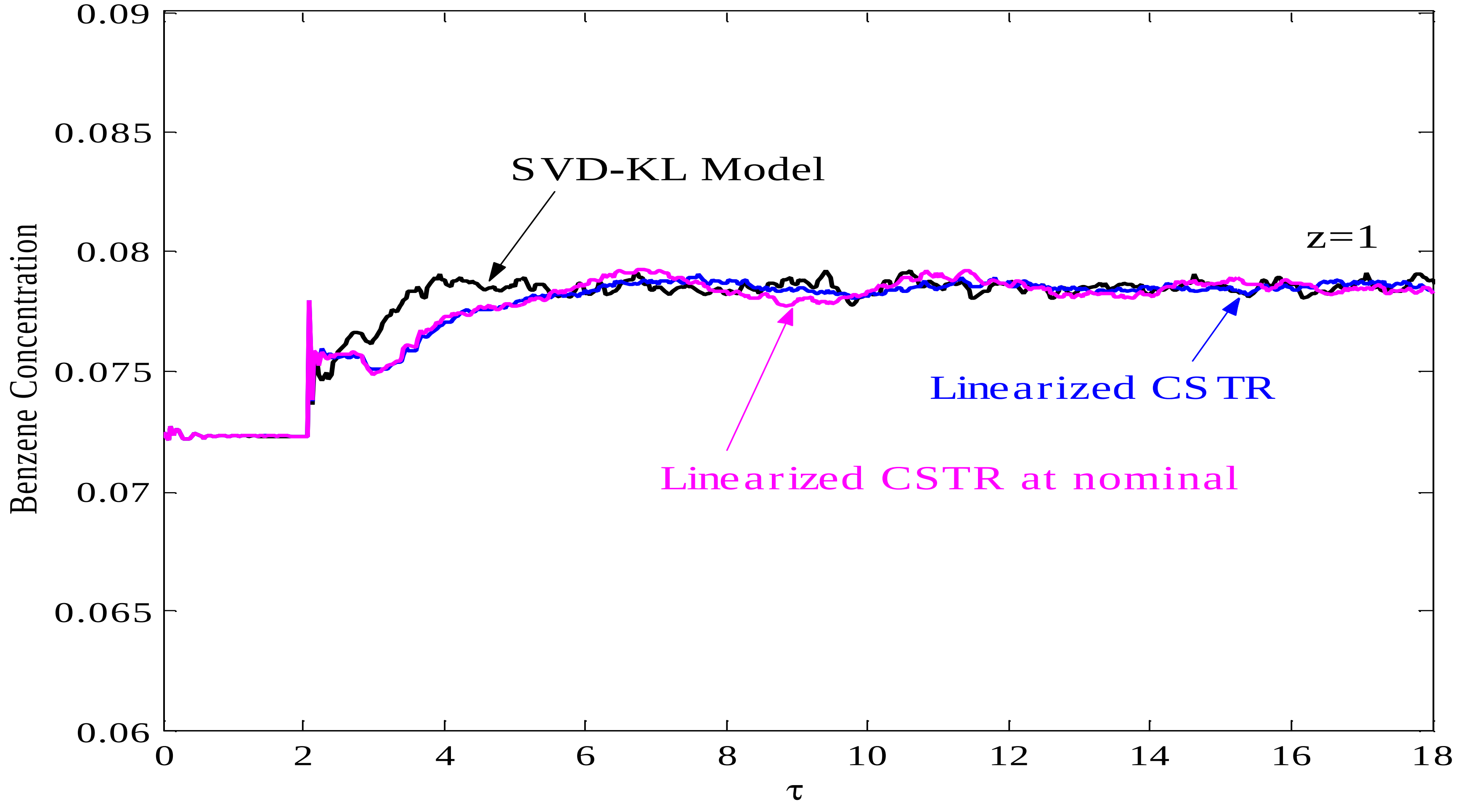


Closed-loop performance

Unmeasured disturbance: Feed temperature (+5%)

Unmeasured disturbance: Feed Toluene concentration (+5%)

Benzene concentration

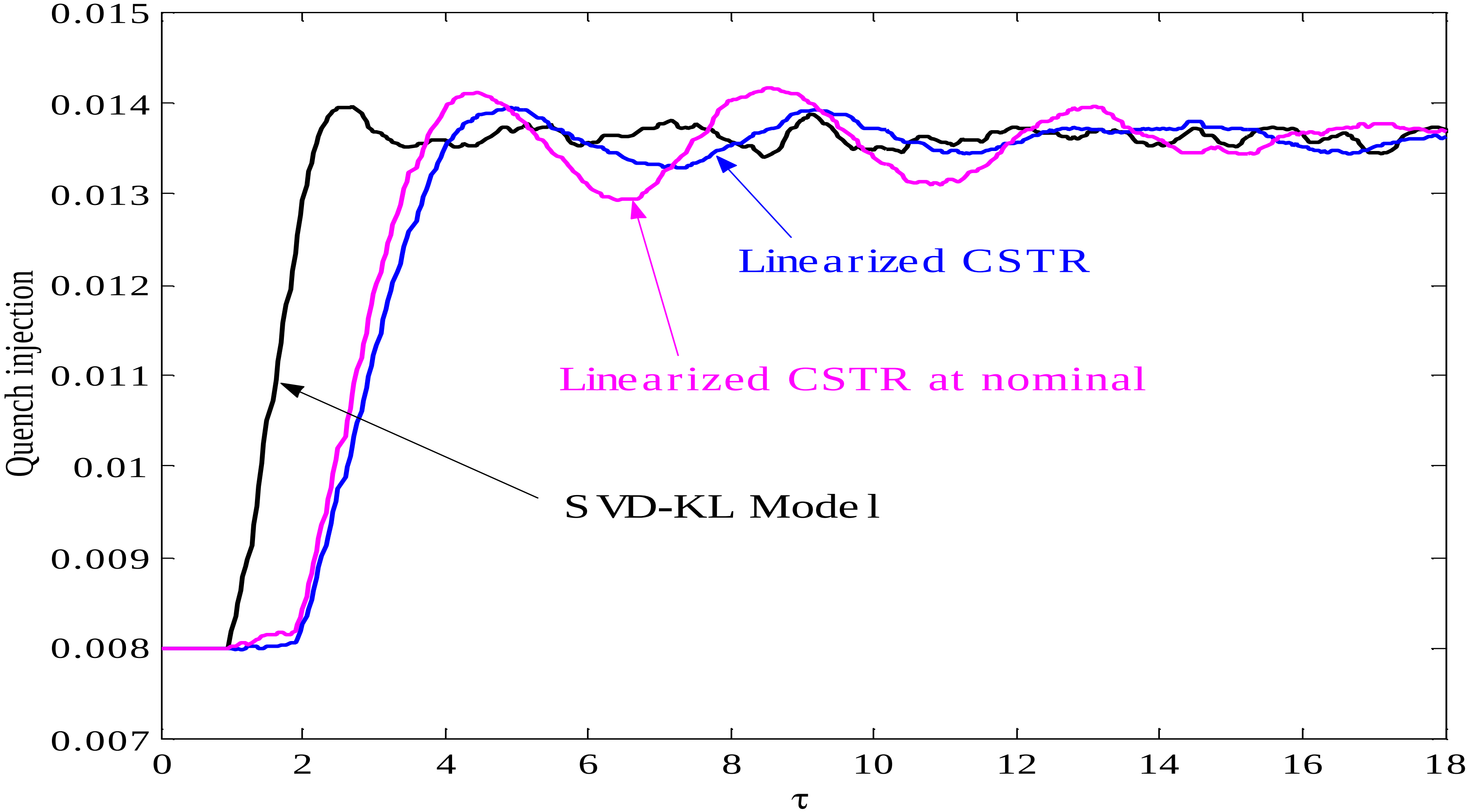


Closed-loop performance

Unmeasured disturbance: Feed temperature (+5%)

Unmeasured disturbance: Feed Toluene concentration (+5%)

Quench

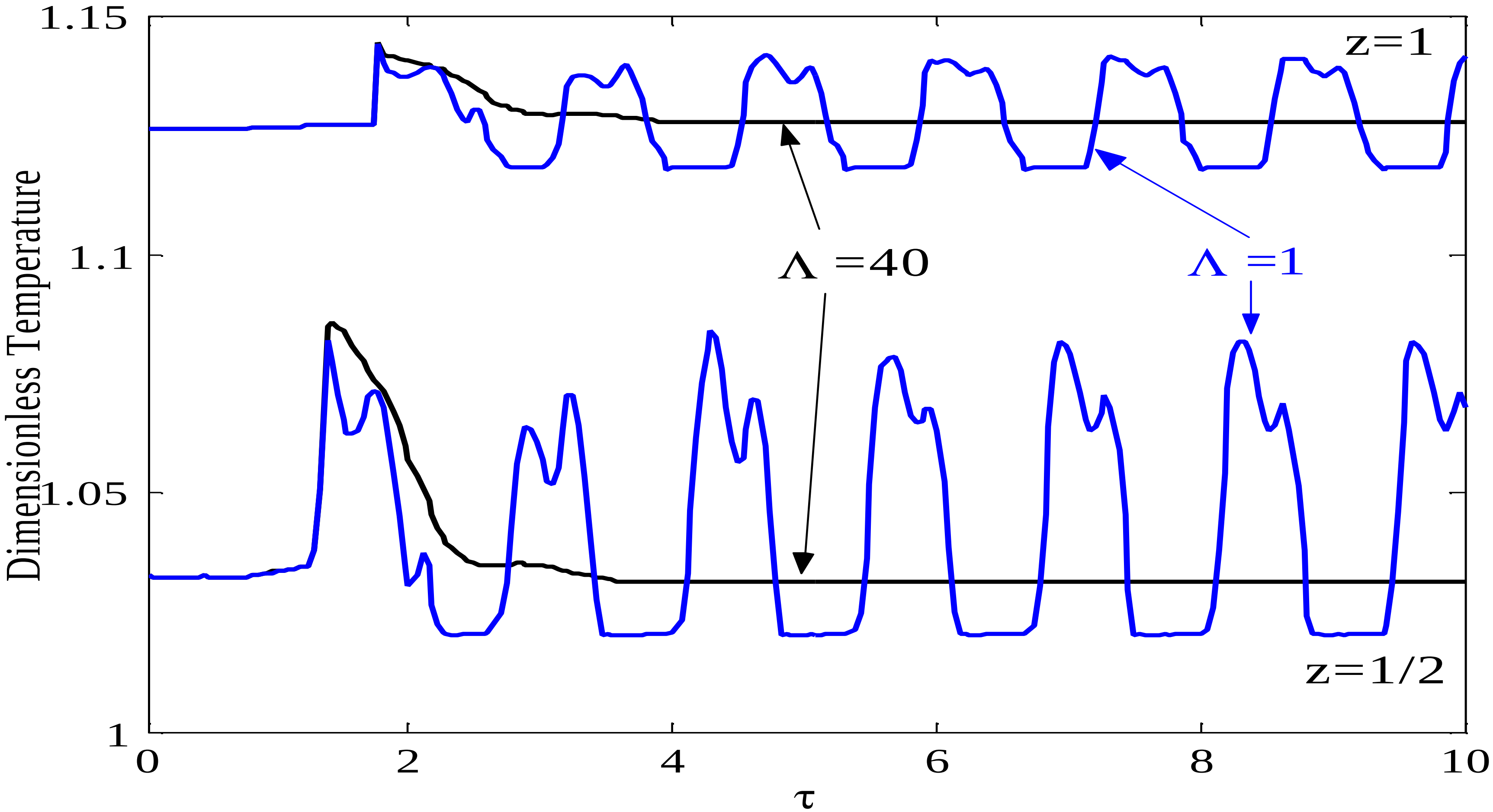


Closed-loop performance

Unmeasured disturbance: Feed temperature (+5%)

Measured disturbance: Feed Flow rate (−3%)

Temperature response

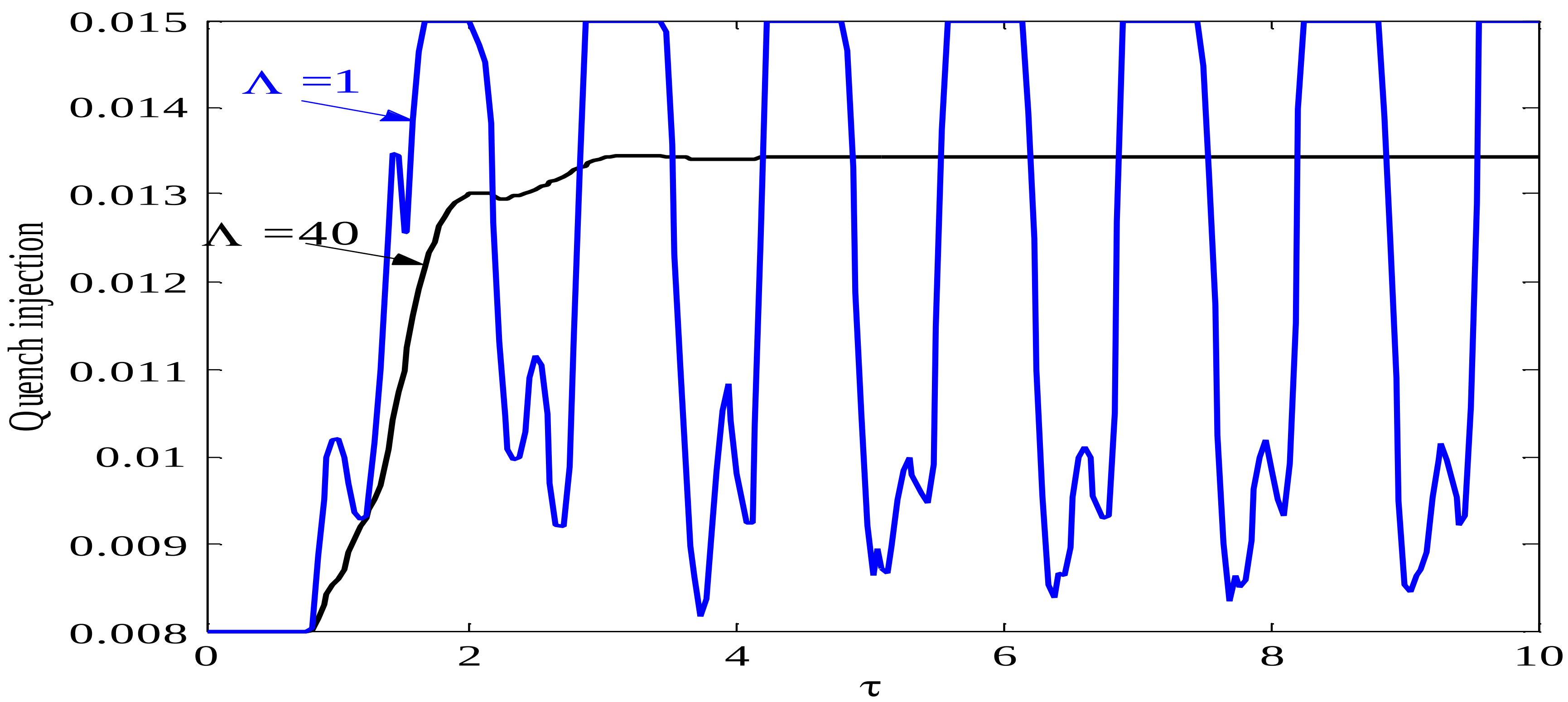


Closed-loop performance

Unmeasured disturbance: Feed temperature (+5%)

Measured disturbance: Feed Flow rate (−3%)

Quench



$\Lambda = 1 \quad |\lambda|_{max} = 1.2015 \quad \Lambda = 5 \quad |\lambda|_{max} = 1.0165$

$\Lambda = 10 \quad |\lambda|_{max} = 1.0011 \quad \Lambda = 40 \quad |\lambda|_{max} = 0.9015$

Summary

- SVD-KL method yields a finite dimension input-output model that captures the dominant behavior.
- The resulting ijth kernel function contains information of how the jth input acts on the ith output.
- Model-based controller (QDMC) based on the SVD-KL model can be designed.
  - HDA reactor system: nonlinear hyperbolic PDEs
  - Concentration measurement is limited to the exit of the reactor.
  - Satisfactory performance: measured and unmeasured disturbances.
- A sufficient condition for closed-loop stability.

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