A comparative study of approximate models for a tubular reactor

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PROMATCH

Outline

Objectives

- Study model reduction strategies at marginally stable operating points
- Perform sensitivity analysis of reduced order model as function of input design
- Evaluation of control quality as function of input design and reduced order model
- Study robustness and stability analysis towards disturbances

Applied to benchmark example of a tubular reactor

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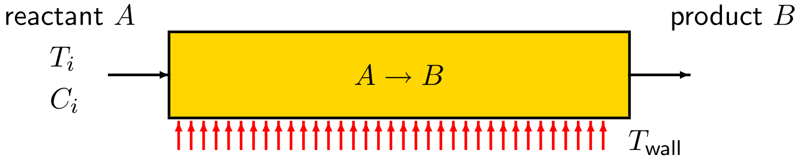
Applied to benchmark example of a tubular reactor

Non-isothermal tubular reactor



Reactor[1] with irreversible exothermic reaction $A \rightarrow B$ described by PDE's:

$$\frac{\partial T}{\partial t} = \frac{1}{P_{\text{eh}}} \frac{\partial^2 T}{\partial z^2} - \frac{1}{L_e} \frac{\partial T}{\partial z} + \nu C e^{\gamma\left(1-\frac{1}{T}\right)} + \mu(T_{\text{wall}} - T)$$

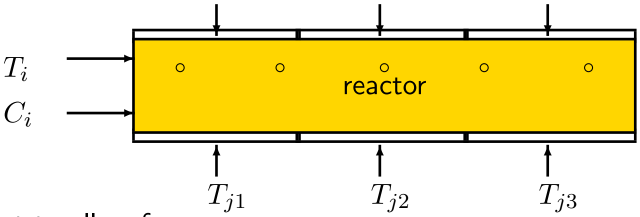
$$\frac{\partial C}{\partial t} = \frac{1}{P_{\text{em}}} \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} - D_{\text{a}} C e^{\gamma\left(1-\frac{1}{T}\right)}$$

subject to boundary conditions:

$$z = 0 \quad \begin{cases} \frac{\partial T}{\partial z} = P_{\text{eh}}(T - T_i) \\ \frac{\partial C}{\partial z} = P_{\text{em}}(C - C_i) \end{cases} \qquad z = 1 \quad \begin{cases} \frac{\partial T}{\partial z} = 0 \\ \frac{\partial C}{\partial z} = 0 \end{cases}$$

[1] K. Hoo et.al. CHemE Sci. 56, 6683–6710,2000

Adjustments to benchmark reactor



Adjustment to allow for

- control at 3 heating/cooling jackets with idealized conditions:

$$
\begin{aligned}
T_w(z,t) &= T_{j1} && 0 \leq z \leq 1/3 \\
T_w(z,t) &= T_{j2} && 1/3 < z \leq 2/3 \\
T_w(z,t) &= T_{j3} && 2/3 < z \leq 1
\end{aligned}
$$

- measurements at 5 temperature sensors inside reactor

$$T_1, \quad T_2, \quad T_3, \quad T_4, \quad T_5$$

Relevant signals

Inputs

- Controls: temperature at 3 heating/cooling jackets T_{j1}, T_{j2}, T_{j3}
- Disturbances:
  - inlet temperature T_i
  - inlet concentration C_i

Outputs

- Temperature at 5 measurement positions $T_1, \dots, T_5$

State variable

- $x(t) = \mathrm{col}(T(z_i, t), C(z_i, t))$ at 100 discrete points in spatial domain.
  - Temperature $T(z_i, t)$ at uniform spatial grid
  - Concentration $C(z_i, t)$ at uniform spatial grid

This brings model in the form:

$$\dot{x} = Ax + \mathcal{B}u + \mathcal{D}d + \mathcal{F}(x)$$

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This brings model in the form:

$$\dot{x} = \mathcal{A}x + \mathcal{B}u + \mathcal{D}d + \mathcal{F}(x)$$

An optimal operating condition

Objectives:

- High production (consumption of reactants)
- Limit maximum temperature inside reactor

Optimization problem:

Optimal steady state problem [2]

$$\begin{aligned} \text{minimize} \quad & C_{ss}(1) \\ \text{subject to} \quad & \mathcal{A}\mathbf{x}_{ss} + \mathcal{B}\mathbf{u}_{ss} + \mathcal{F}(\mathbf{x_{ss}}) + \mathcal{D}\mathbf{d} = 0 \\ & T_{ss}(z) \leq T_{\max} \quad \text{for all points } z \\ & \mathbf{u}_{\min} \leq \mathbf{u}_{ss} \leq \mathbf{u}_{\max} \end{aligned}$$

$C_{ss}(1)$ is steady state concentration at right reactor end

[2] Smets et. al. Optimal Temp. Control of SS Exothermic plug-Flow Reactor, AICHEJ Vol. 48

An optimal operating condition

Included temperature constraint in the objective function

$$\begin{aligned} \text{minimize} \quad & C_{ss}(1) + \gamma \int_0^1 \min(T_{\max} - T_{ss}(z), 0)^2 dz \\ \text{subject to} \quad & \mathcal{A}\mathbf{x} + \mathcal{B}\mathbf{u} + \mathcal{F}(\mathbf{x}) + \mathcal{D}\mathbf{d} = 0 \\ & \mathbf{u}_{\min} \leq \mathbf{u}_{ss} \leq \mathbf{u}_{\max} \end{aligned}$$

specifications

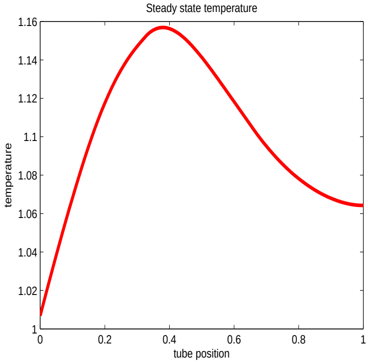
- weighting parameter $\gamma = 200$
- inlet conditions $T_i = 1$ and $C_i = 1$
- input constraints on jacket temperatures: $0.8 < \mathbf{u} < 1.2$.

resulting jacket temperatures:

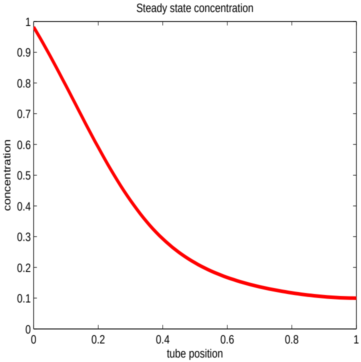
$$\mathbf{u}_{ss} = (0.9970, 1.0475, 1.0353)$$

An optimal operating condition

Steady state operating condition



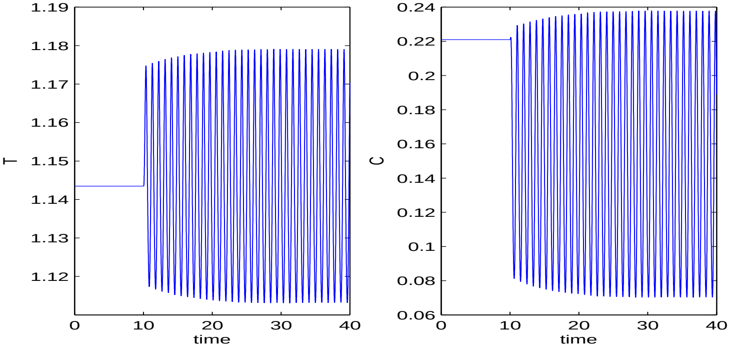
Temperature T_{ss}



Concentration C_{ss}

An optimal operating condition

However, very sensitive to disturbances in T_i and C_i



4% change in inlet temperature T_i at time $t = 10$

Model reduction through Galerkin projections

Most important steps:

- Model

$$\dot{x}(t) = \mathcal{A}x + \mathcal{B}u + \mathcal{D}d + \mathcal{F}(x)$$

- State variable projection

$$x(t) \approx x_r(t) = \sum_{k=1}^{r} c_k(t)\xi_k$$

with ξ_k 'clever' orthonormal basis of state space

- Vector field projection

$$0 = \left\langle \xi_k, \mathcal{A}x + \mathcal{B}u + \mathcal{D}d + \mathcal{F}(x) - \dot{x} \right\rangle, \quad k = 1, \ldots, r$$

- Reduced order model

$$0 = \left\langle \xi_k, \mathcal{A}x_r + \mathcal{B}u + \mathcal{D}d + \mathcal{F}(x_r) - \dot{x}_r \right\rangle, \quad k = 1, \ldots, r$$

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Different spectral decompositions

Distinguish:

- Scalar valued decompositions:

$$T(t) = \sum_{k=1}^{N} a_k(t)\varphi_k, \qquad C(t) = \sum_{k=1}^{N} b_k(t)\psi_k$$

where $\{\varphi_k\}$ and $\{\psi_k\}$ are orthonormal (POD) bases of $\mathbb{R}^N$

- Lumped decompositions:

$$x(t) = \begin{pmatrix} T(t) \\ C(t) \end{pmatrix} = \sum_{k=1}^{2N} c_k(t)\xi_k$$

where $\{\xi_k\}$ is orthonormal (POD) bases of $\mathbb{R}^{2N}$

Computation POD bases

Either case computable by means of SVD of snapshot matrices

$$X_{\text{snap}} := \begin{pmatrix} x(z_1, t_1) & \cdots & x(z_1, t_M) \\ \vdots & \ddots & \vdots \\ x(z_N, t_1) & \cdots & x(z_N, t_M) \end{pmatrix}$$

where N is number of mesh points and M is number of time samples.

- scalar valued basis $\{\varphi_k\}$ and $\{\psi_k\}$:

$$T_{\text{snap}} = \begin{pmatrix} \varphi_1 & \cdots & \varphi_N \end{pmatrix} \Sigma V^*, \quad C_{\text{snap}} = \begin{pmatrix} \psi_1 & \cdots & \psi_N \end{pmatrix} \Sigma V^*$$

- lumped basis $\{\xi_k\}$:

$$X_{\text{snap}} = \begin{pmatrix} \xi_1 & \cdots & \xi_{2N} \end{pmatrix} \Sigma V^*$$

POD and Galerkin projection

Experimental set up:

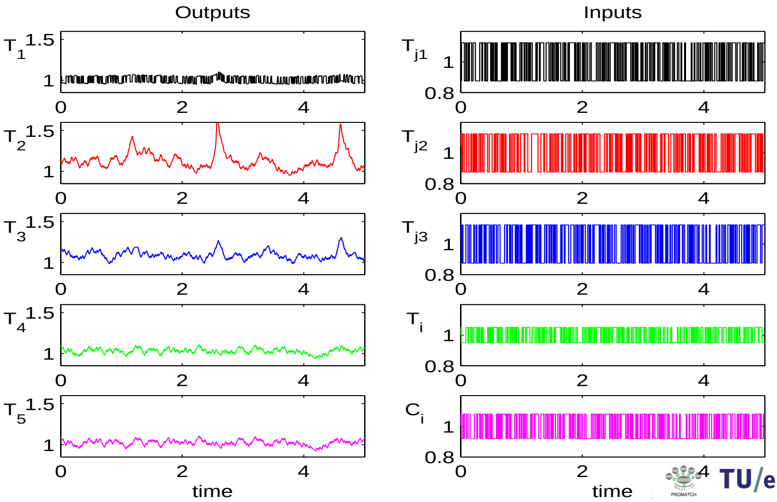
- Apply PRBS signal on $T_{j1}, T_{j2}, T_{j3}, T_{in}, C_{in}$ around steady state operating condition
- Perform model reduction (POD method)
- Validate model for the critical value for C_i
- Validate model for the critical value of T_i

Main question:

? Do reduced order models capture oscillatory behavior ?

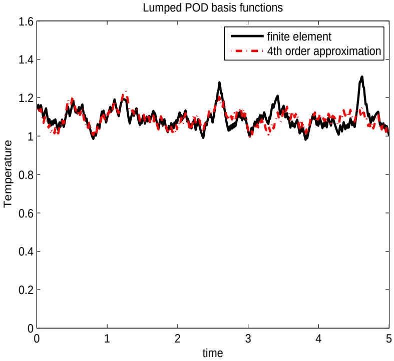
Experiments

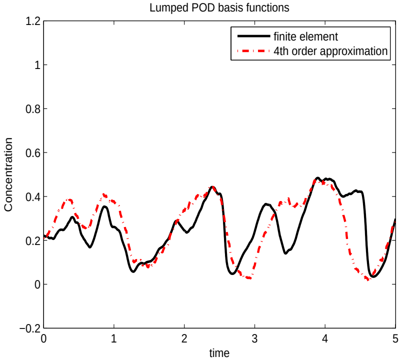
Experiment 1



POD (lumped basis) + Galerkin Projection

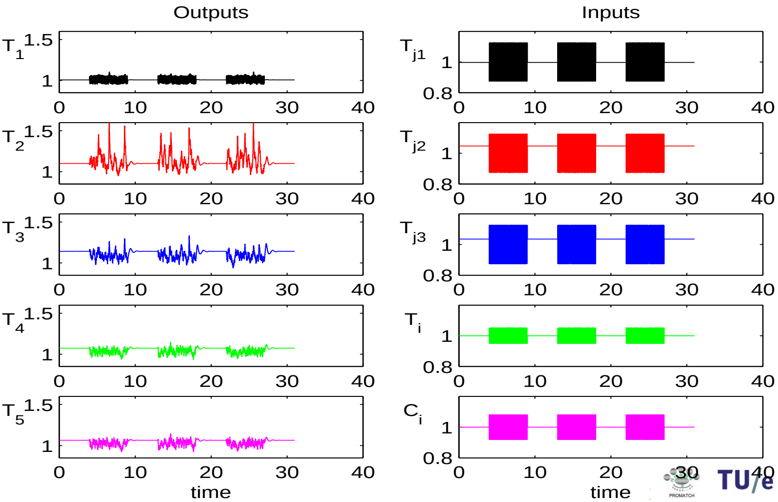
Results of T and C at $z = 0.5$ (middle of reactor), order $r = 4$.





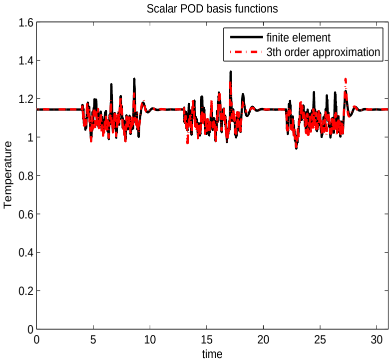
Experiments

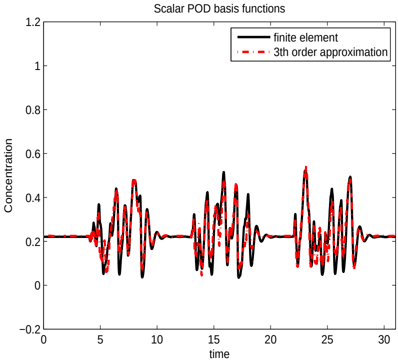
Experiment 2



POD (scalar basis)+ Galerkin Projection

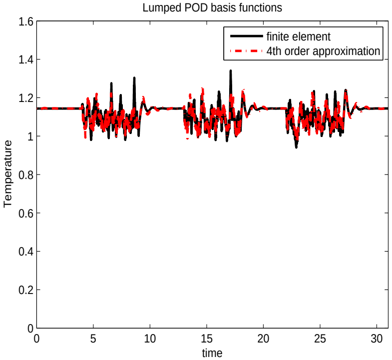
Results of T and C at $z = 0.5$ (middle of reactor), order $r = 3 + 3$.

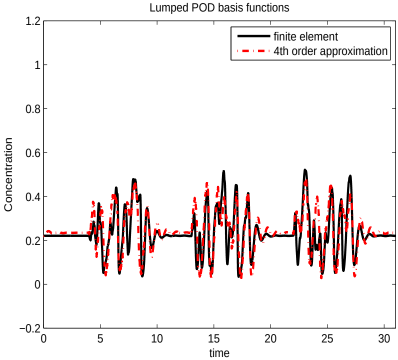




POD (lumped basis) + Galerkin Projection

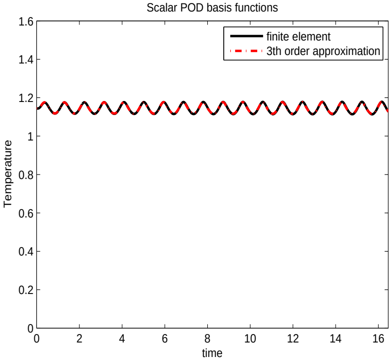
T and C at $z = 0.5$ (middle of reactor), order $r = 4$.

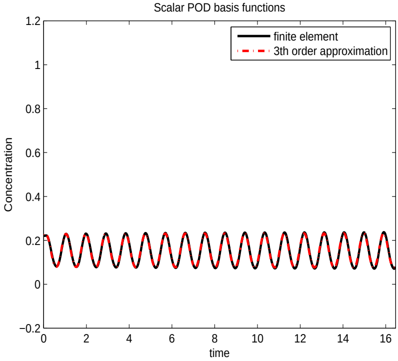




POD (scalar basis) + Galerkin Projection

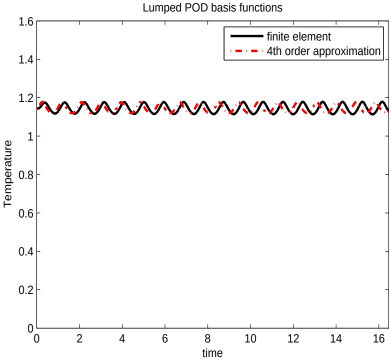
T and C at $z = 0.5$ (middle of reactor), order $r = 3 + 3$ with $T_i = 1.04$

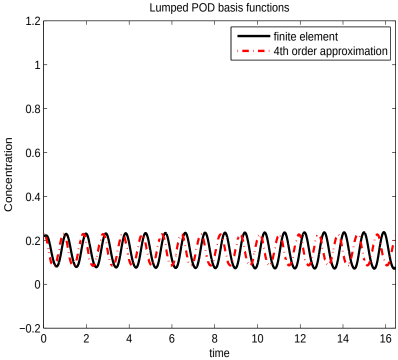




POD (lumped basis) + Galerkin Projection

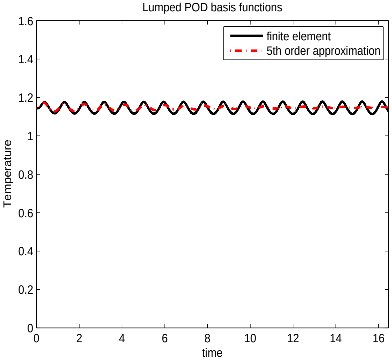
T and C at $z = 0.5$ (middle of reactor), order $r = 4$ with $T_i = 1.04$

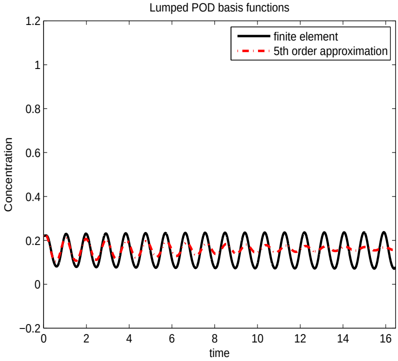




POD (lumped basis) + Galerkin Projection

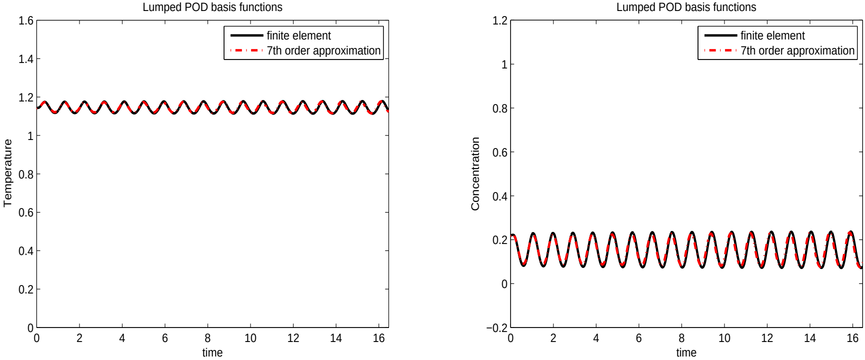
T and C at $z = 0.5$ (middle of reactor), order $r = 3$ with $T_i = 1.04$





POD (lumped basis) + Galerkin Projection

T and C at $z = 0.5$ (middle of reactor), order $r = 7$ with $T_i = 1.04$



Observation: $\frac{\sum_{i=1}^{n} \lambda_i}{\sum_{i=1}^{N} \lambda_i}$ not quite efficient [3].

[3] Bizon et.al, On POD reduced models of tubular reactor with periodic regimes

Conclusions

- This study proved that POD model reduction for this distributed system is able to capture dynamics around marginally stable operating conditions
- Method allows for substantial reductions of complexity
- Multivariable (lumped) POD outperforms single variable (scalar) POD technique
- Currently investigating controller synthesis on basis of these low order models.
- Methods have been implemented in INCA environment of IPCOS

INCA environment