Dynamic Reduced Order Models for a Bubbling Fluidized Bed Adsorber

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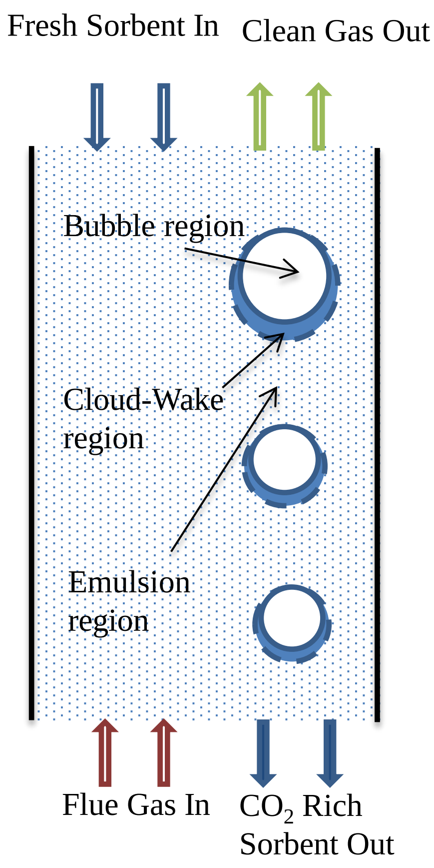
Introduction

Bubbling Fluidized-Bed Adsorber

- Essential component: bubbling fluidized-bed (BFB) adsorber
  - Solid-sorbent-based post-combustion carbon capture system
  - One-dimensional, three region BFB model
  - Described by partial differential and algebraic equations (PDAEs)
  - Differential and algebraic equations (DAEs) (**over 30,000 equations**)



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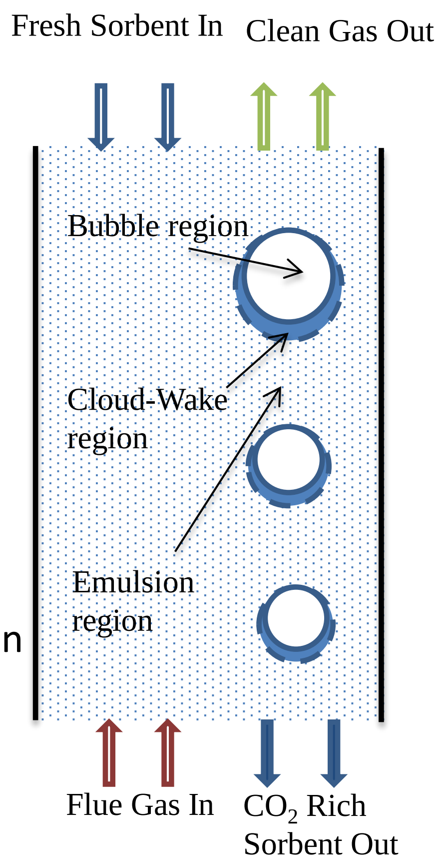
- Why dynamic reduced order models (D-ROM)?
  - BFB adsorber: spatially distributed first-principle model

    + Accurate

    - Computationally expensive

    - For a control case study, the simulation takes **9 hours** for a simulation interval of **1.38 hours**
    - **Too slow** for process control and dynamic optimization tasks



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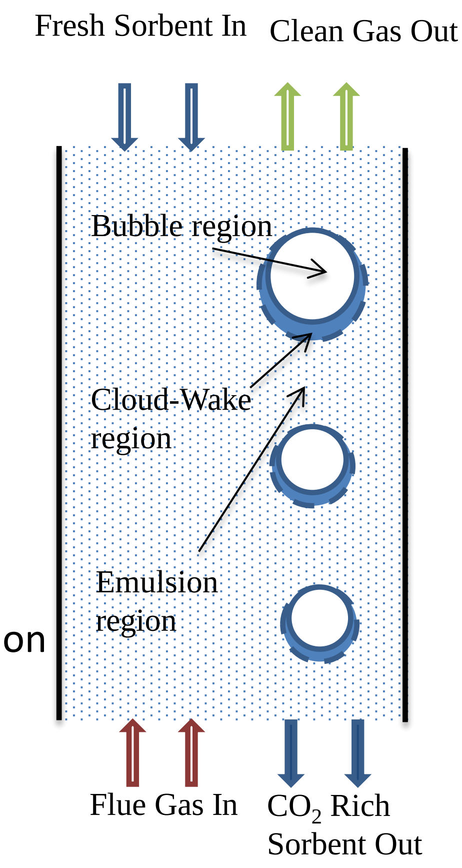
  - Dynamic reduced order model

    + Computationally efficient

    + Capture the dynamics of detailed model



Temporally D-ROM for BFB Adsorber

Time Scale Decomposition Procedures

- Overall procedures

System dynamics ⇔ **Eigenvalue λ**

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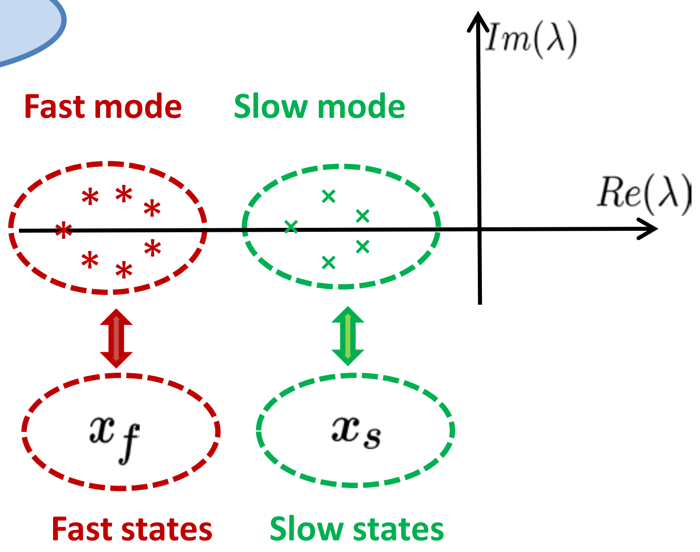
Eigenvalue Analysis

⇩

Eigenvalue-to-State Association



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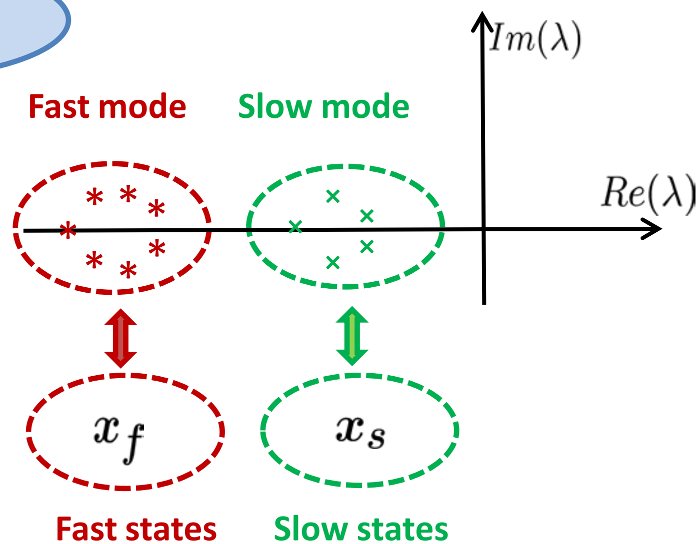
Quasi-steady State Approximation



$$\dot{x}_s = f_s(x_s, x_f)$$
$$\dot{x}_f = f_f(x_s, x_f)$$

$\rightarrow$

$$\dot{x}_s = f_s(x_s, x_f)$$
$$0 = f_f(x_s, x_f)$$

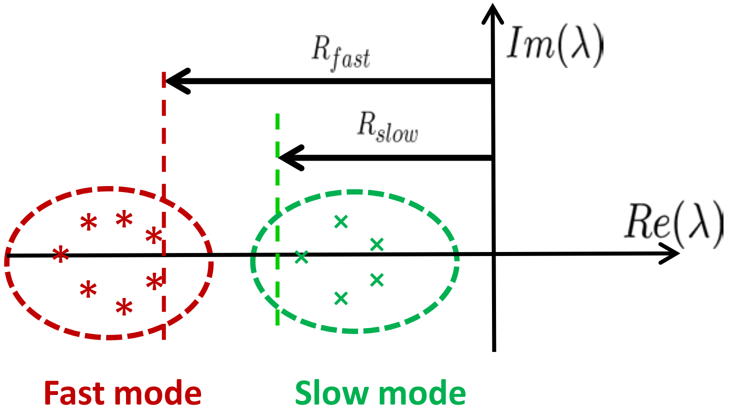
Dynamic reduced model

Temporally D-ROM for BFB Adsorber

Eigenvalue Analysis

- Eigenvalue group separation
  - Separation ratio $\xi = \dfrac{R_{fast}}{R_{slow}}$

  If $\xi \gg 1$, then a fast and a slow mode can be separated



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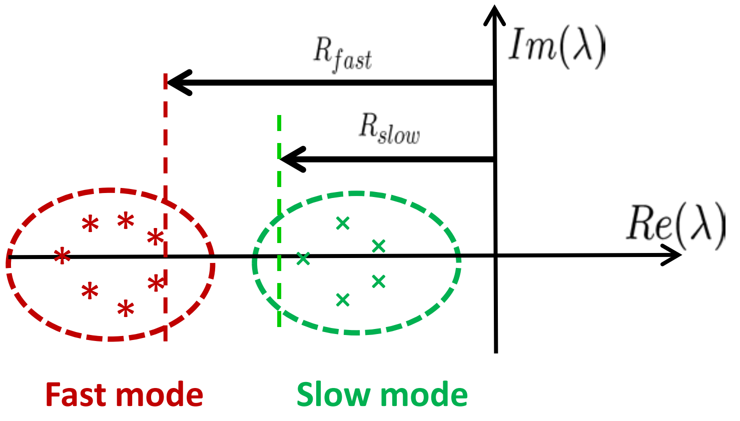
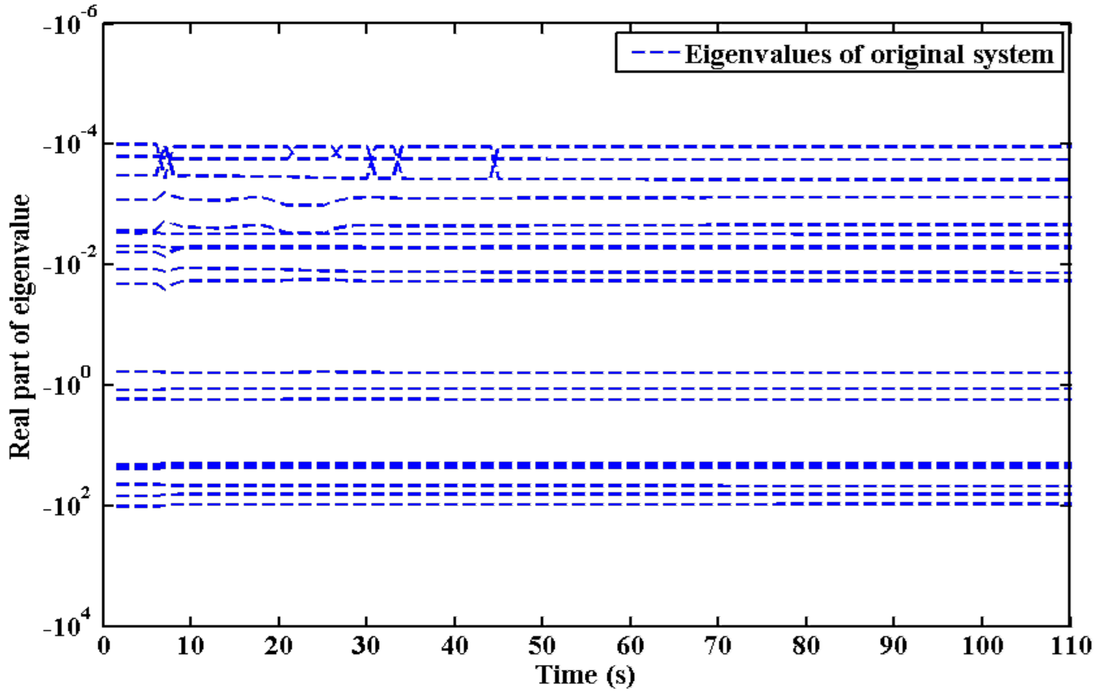


- Eigenvalue variation of original system



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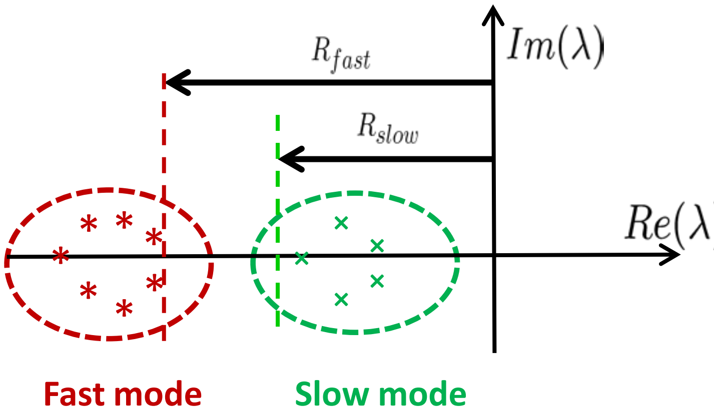

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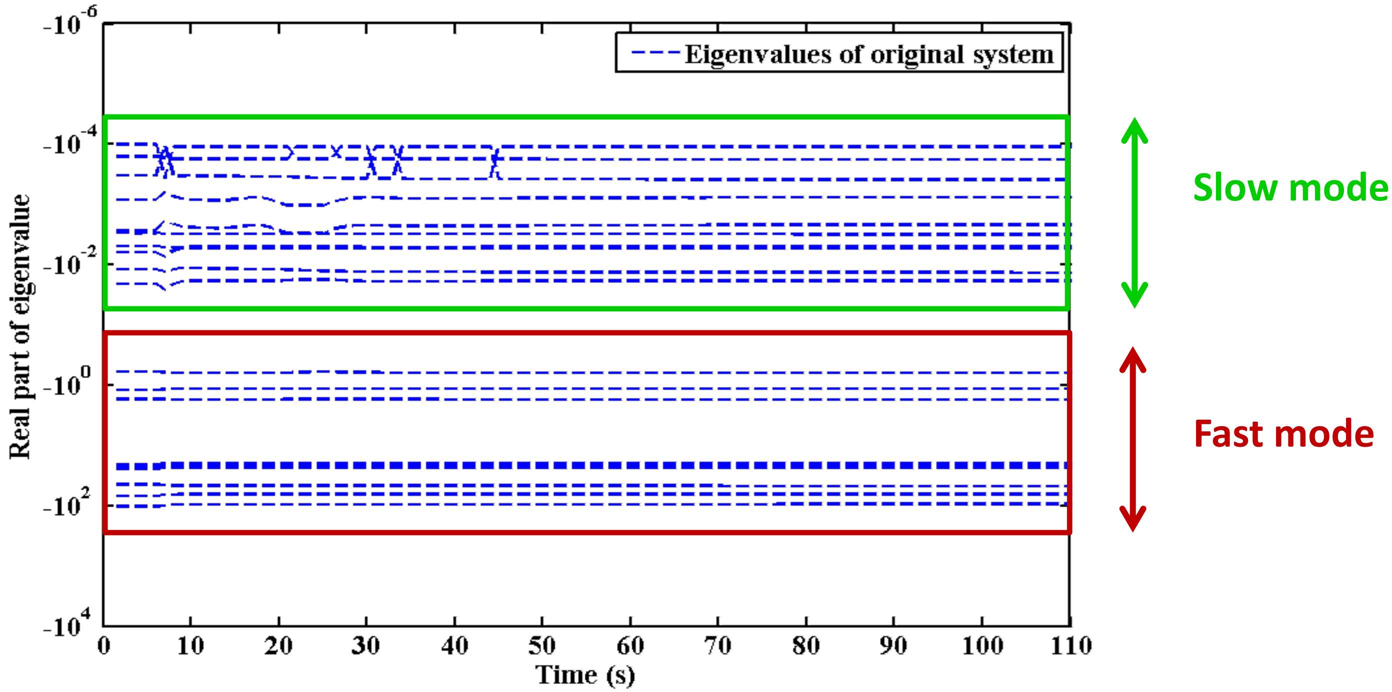

$\xi = \frac{R_{fast}}{R_{slow}} =$ **32**

Temporally D-ROM for BFB Adsorber

Dynamic Reduced Model

- Eigenvalue-to-state association
  - Unit perturbation spectral resolution matrix

    $\boldsymbol{P_{ij}} = \boldsymbol{V_{ij}}(\boldsymbol{V^{-1}})_{\boldsymbol{ji}}$ V is the eigenvector matrix of Jacobian matrix
  - P_{ij} measures the strength of the association between state x_i and eigenvalue λ_j

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  - 9 gas phase states associated with mass balance in all three regions
  - 1 gas phase state associated with heat balance in bubble region

  } **Fast states**

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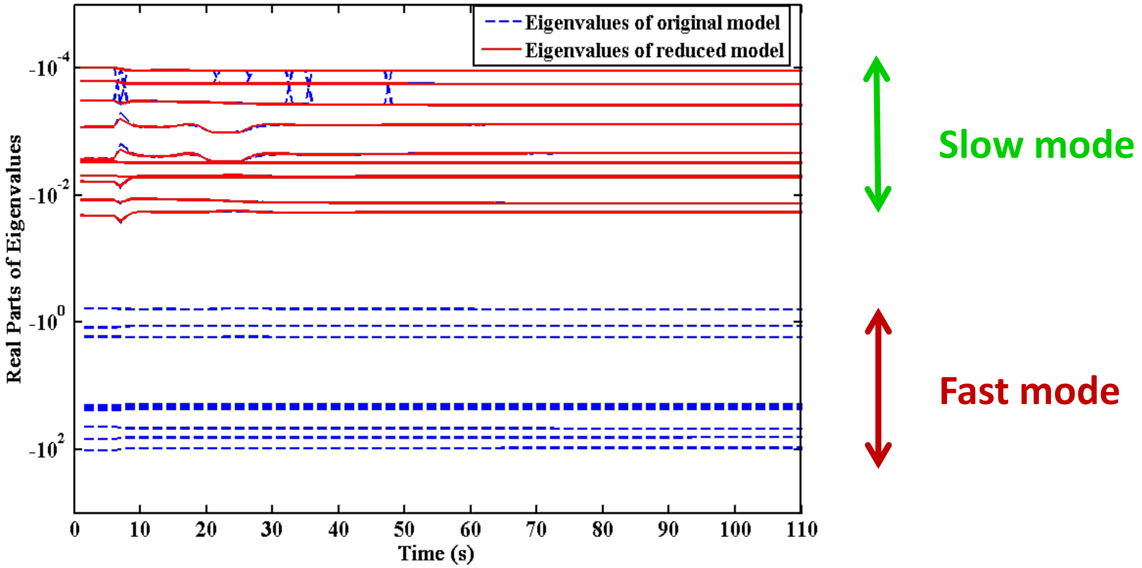
  Fast states

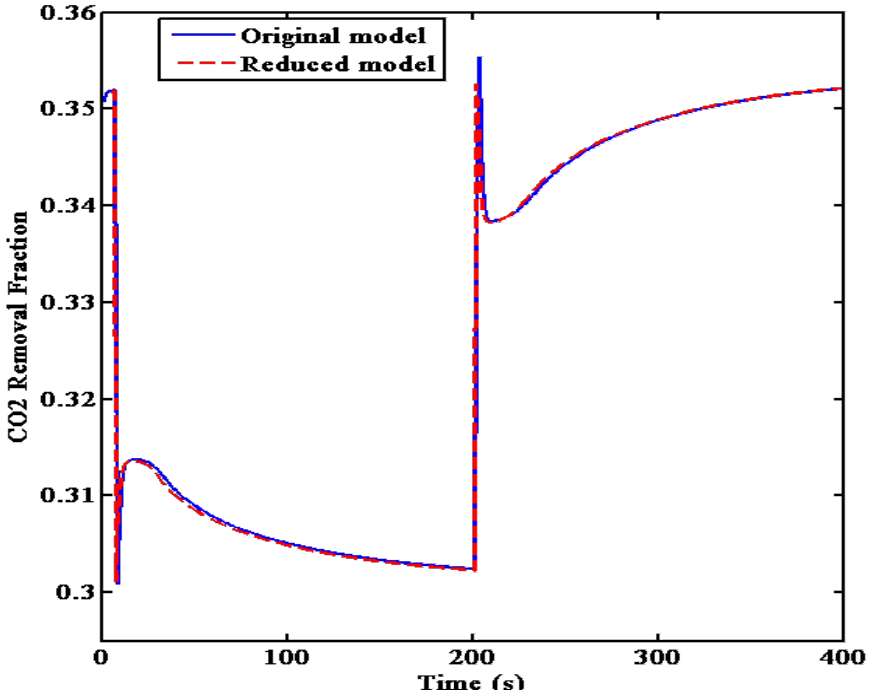
- Eigenvalue variation of original and reduced model

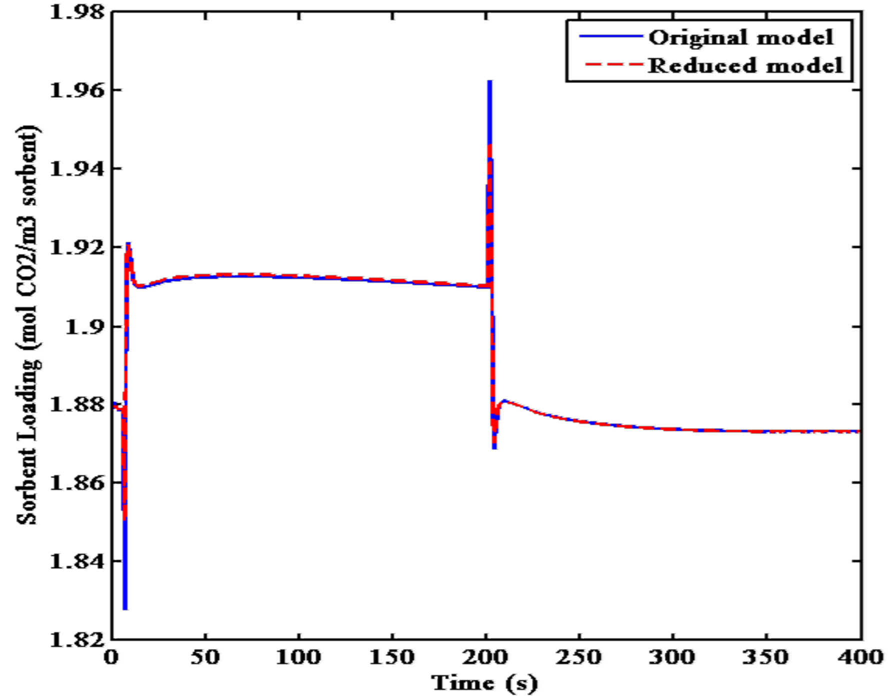


Temporally D-ROM for BFB Adsorber

Case Study: Reduced Model Validation

- Output profiles of the reduced and original BFB model





33% reduction

	Simulation time	MSE1	MSE2	MRE1	MRE2
Original model	427s	-	-	-	-
Reduced model	286s	2.98e-6	2.02e-6	7.2%	1.2%

MSE: mean squared error; MRE: maximum relative error; 1: CO_2 removal fraction; 2: sorbent loading

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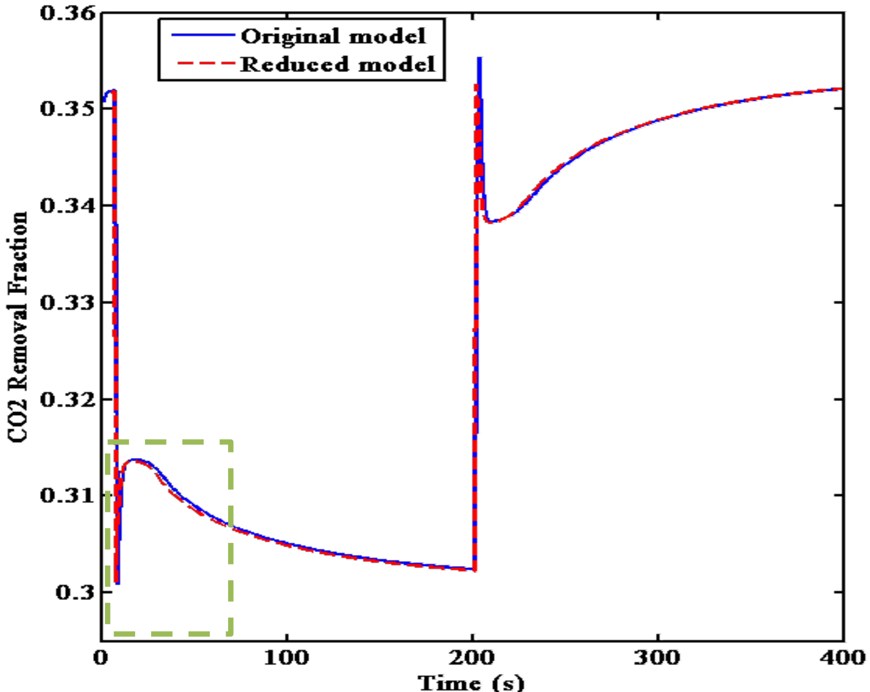

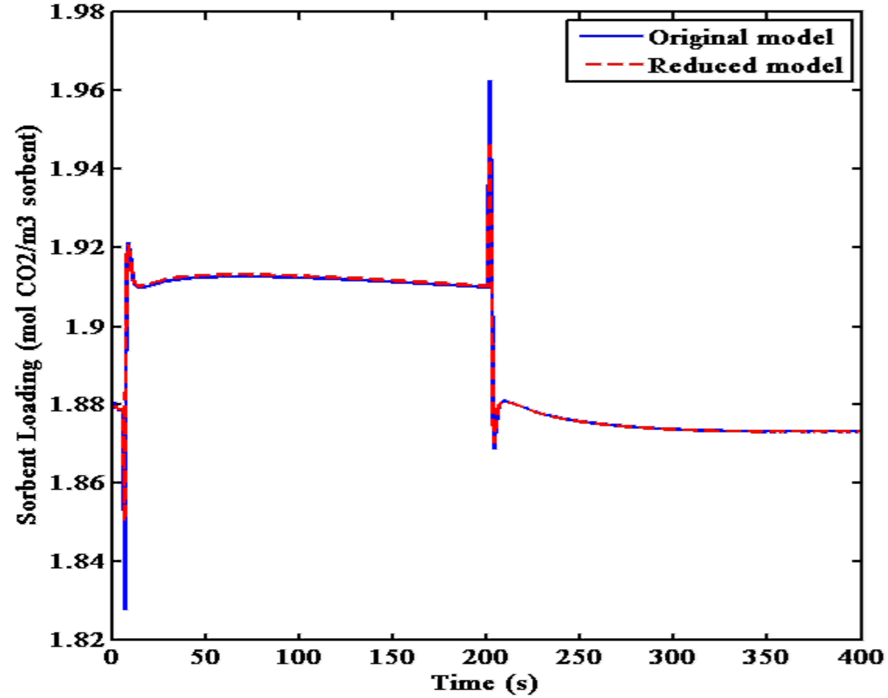

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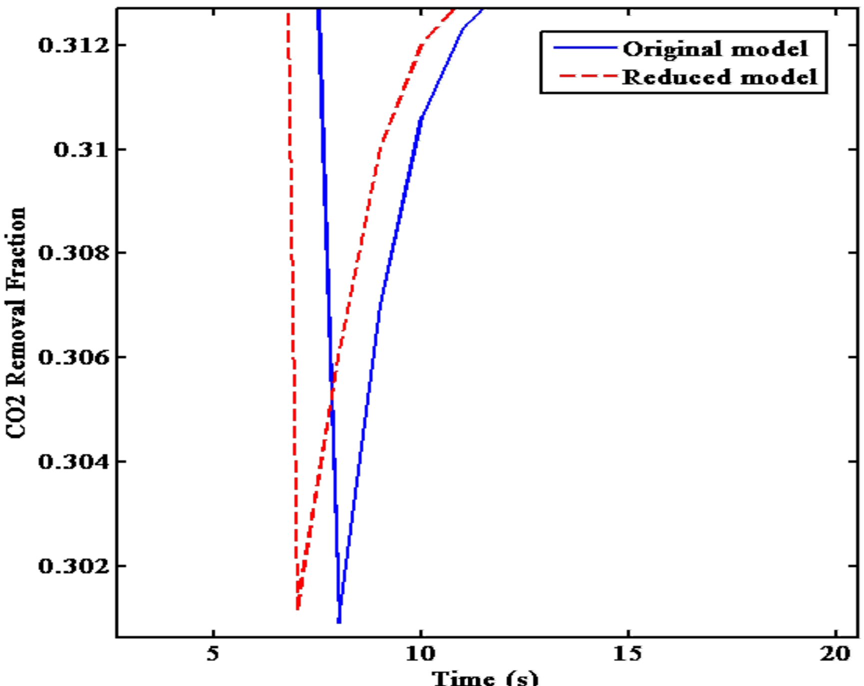

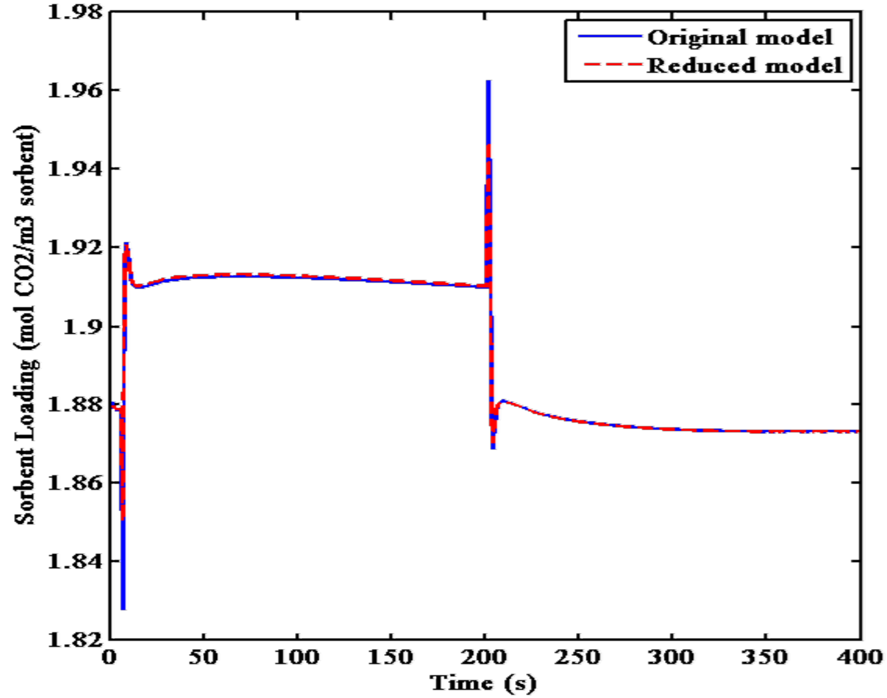

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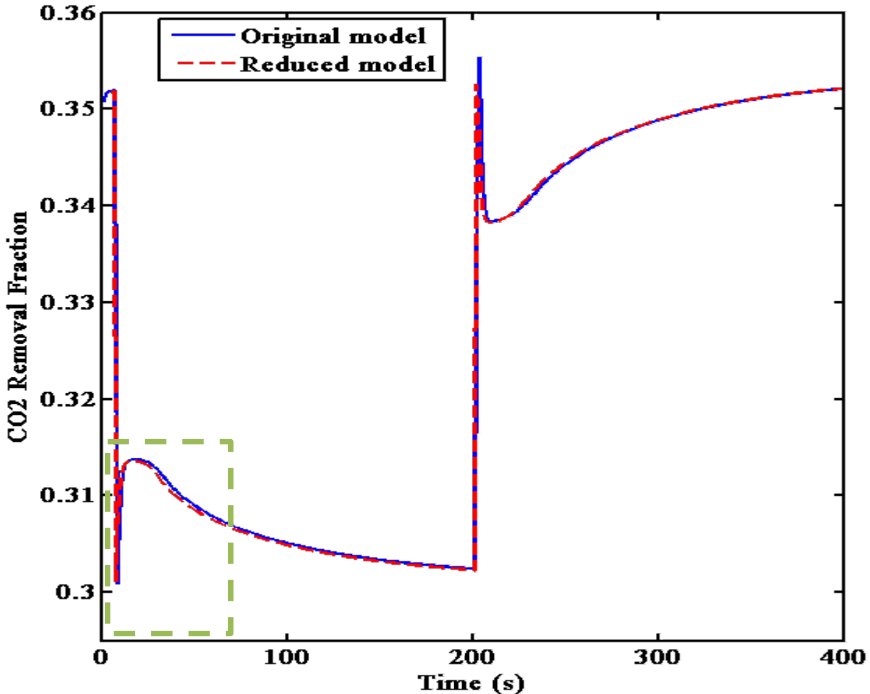

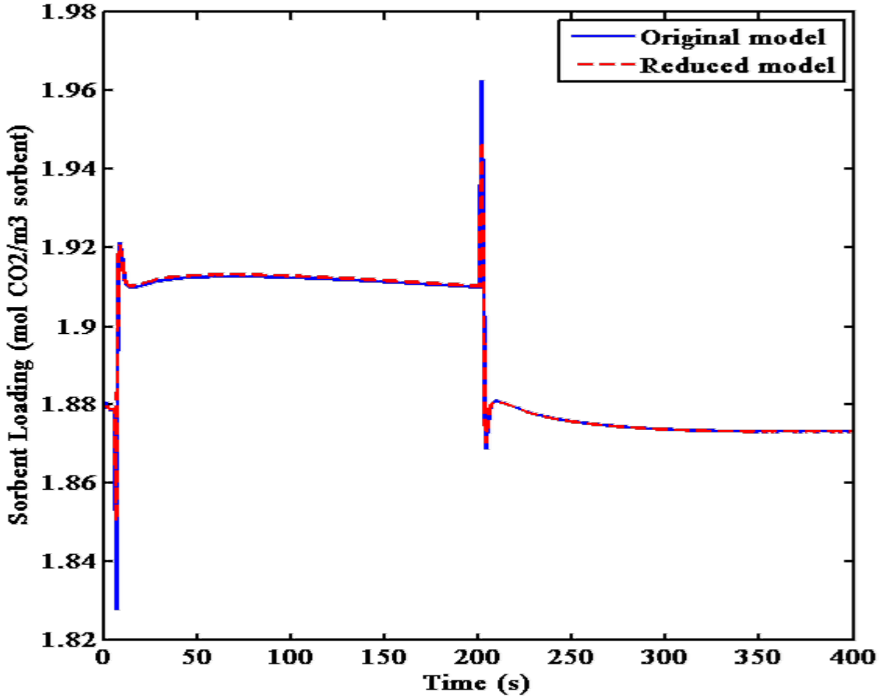

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Spatial Model Reduction

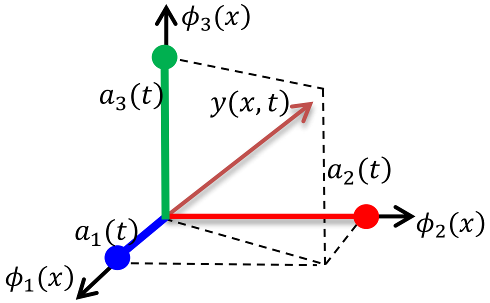
Proper Orthogonal Decomposition (POD)

- Proper orthogonal decomposition

$$y(x,t) \approx \sum_{i=1}^{K} a_i(t)\phi_i(x)$$

$\phi_i(x)$ spatial basis function

$a_i(t)$ time dependent coefficient



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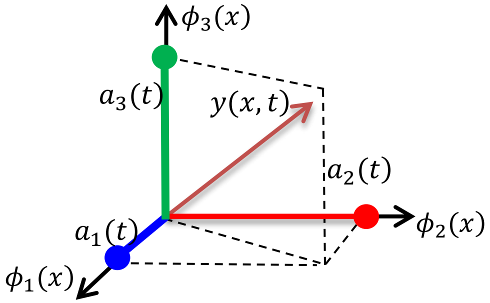


- Method of snapshots
  - Snapshot matrix

$$Y = [y_1, \cdots, y_M]$$

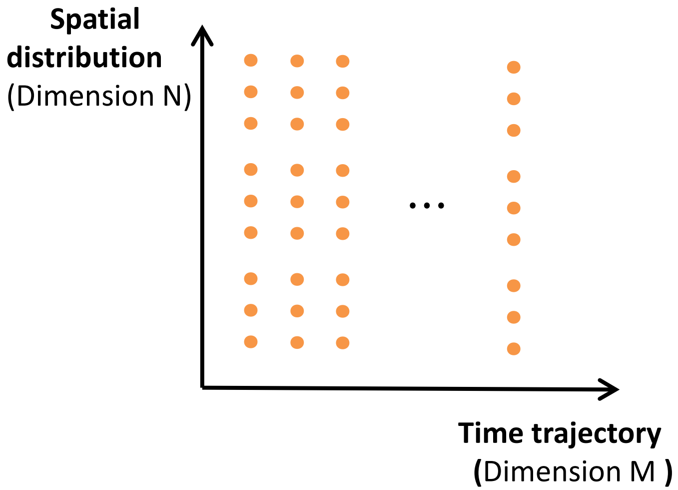
  - Singular value decomposition (SVD) of snapshot matrix

$$Y = UDV^T = \sum_{i=1}^{N} \sigma_i u_i v_i^T \approx \sum_{i=1}^{K} \sigma_i u_i v_i^T \quad K \ll N$$

u_i: basis function, σ_i: amount of projection

  - Projection error:

$$\varepsilon_{norm}^{POD} = 1 - \frac{\sum_{i=1}^{K} \sigma_i^2}{\sum_{i=1}^{N} \sigma_i^2}$$



Snapshot matrix

Spatial Model Reduction

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$$\frac{\partial y}{\partial t} = \mathrm{f}(\mathrm{y}, \mathrm{t})$$

Original model

↓ Spatial discretization

Full discretized system
Dim = N

↓ Simulation

Snapshots $Y = [y_1, \cdots, y_M]$

↓ Method of snapshots

POD basis functions $\varphi_j(x)$

↓ Weighted residual method

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$$y(x,t) = \sum_{i=1}^{K} a_i(t)\varphi_j(x)$$

$$\frac{da_i}{dt} = \mathrm{f}(\mathrm{y}, \mathrm{t}), \mathbf{i} = \mathbf{1} \cdots \boldsymbol{K}$$

Spatial Model Reduction

Preliminary Results

- Preliminary results of POD basis functions:
  - All states can be represented by **6-7** basis functions (instead of **100**)
  - Average projection error is less than **0.1%**

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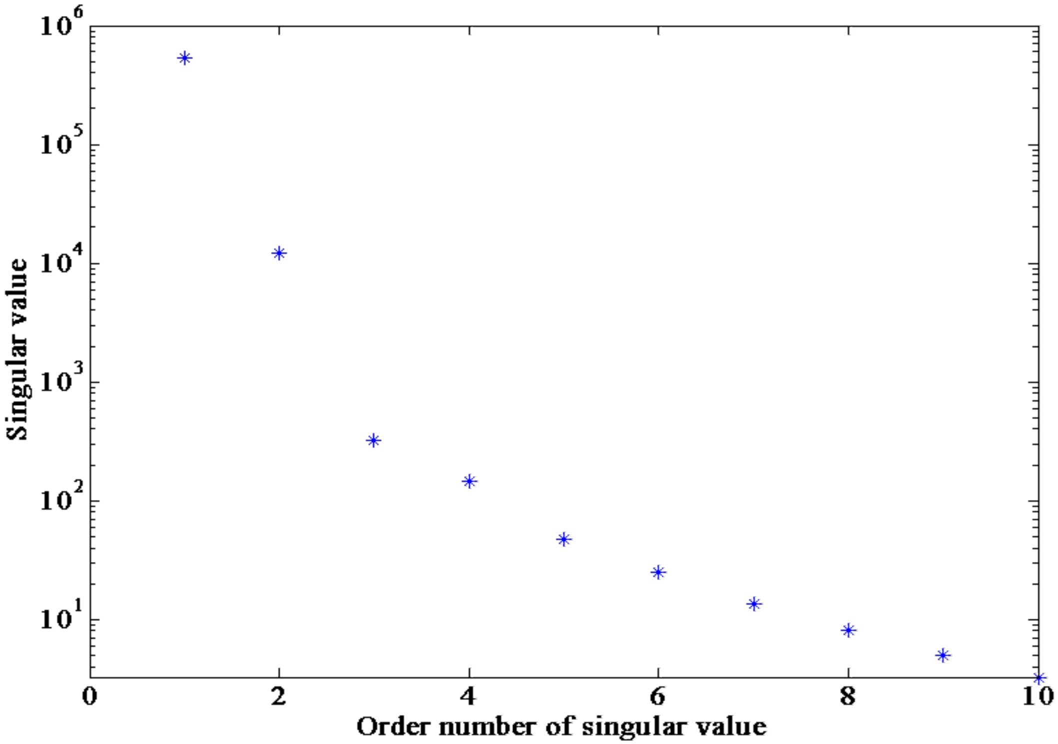

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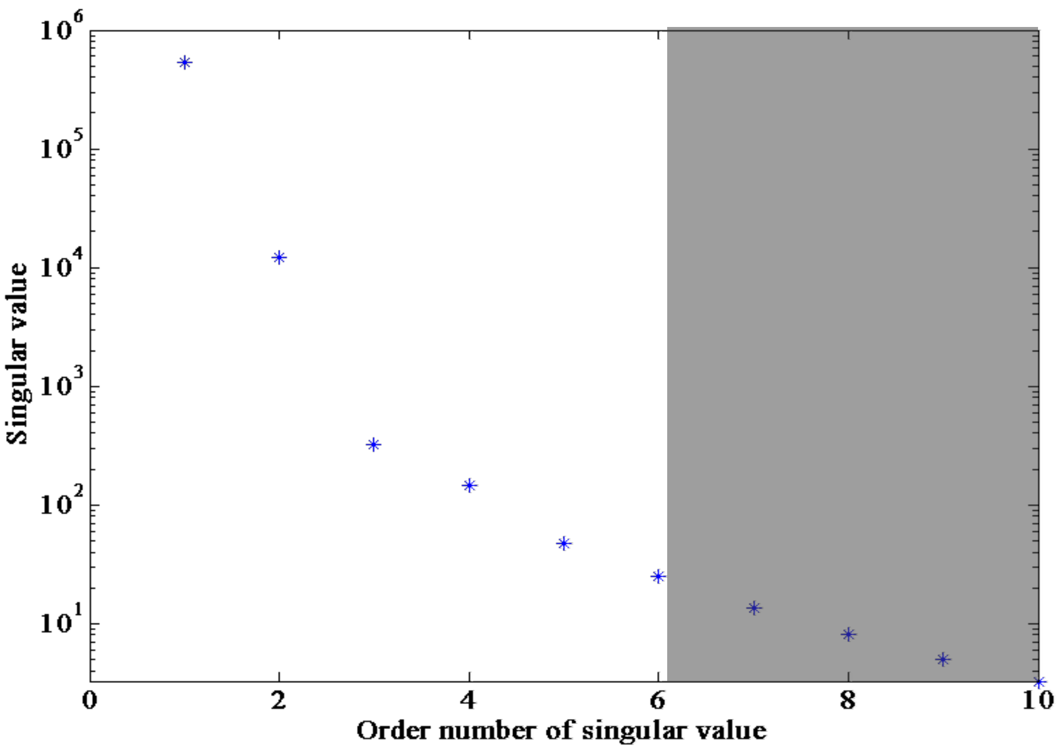

Spatial Model Reduction
Regression model

- Why regression model?
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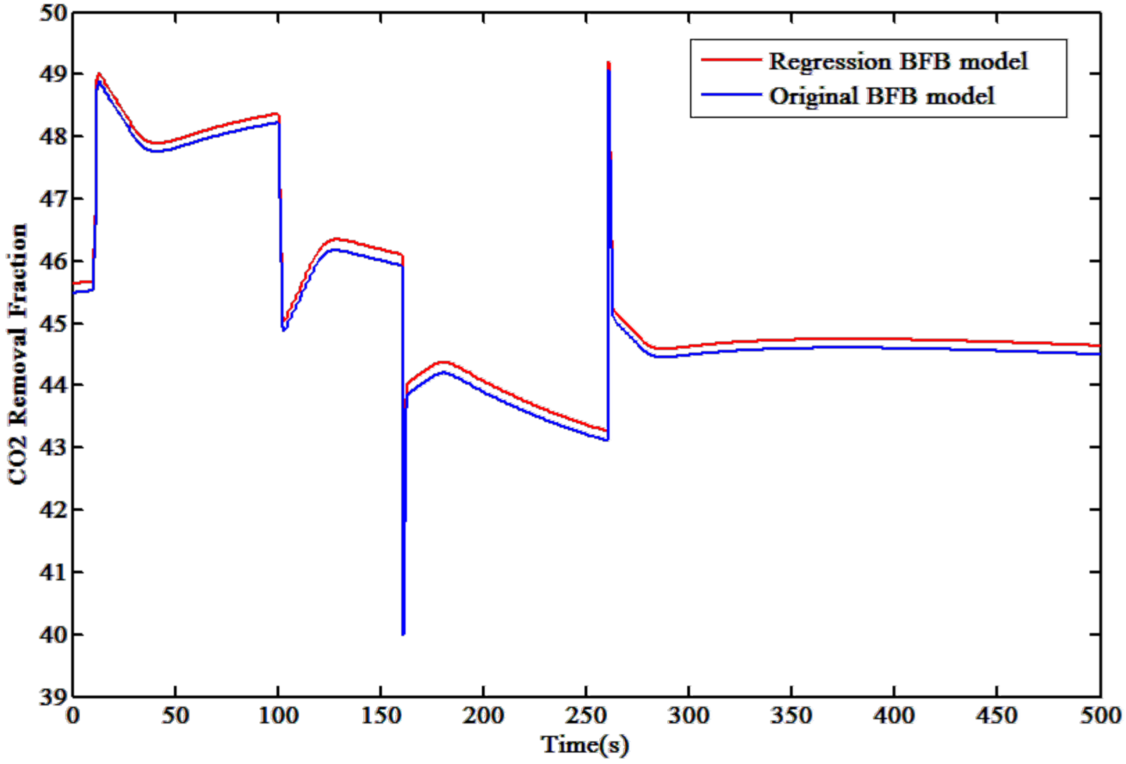
- Model validation



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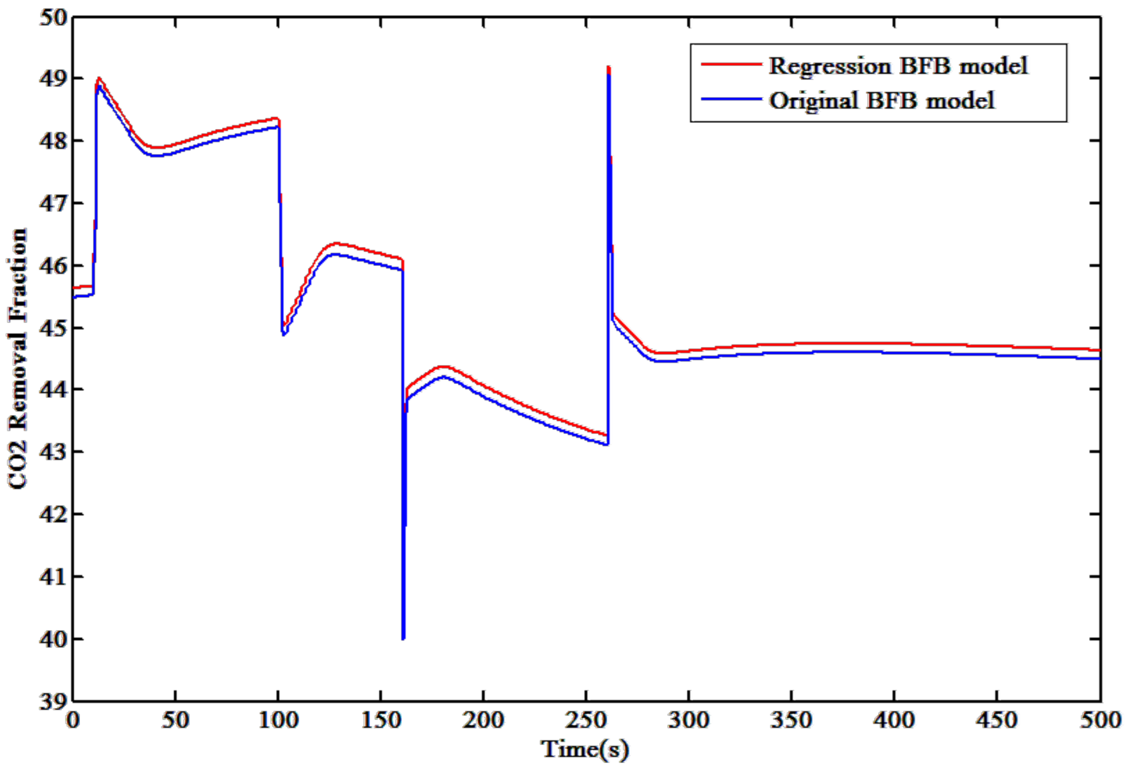

Maximum relative error = 0.41%

Spatial Model Reduction

Potential Analysis

- Only **6-7** spatial basis functions are needed for state y
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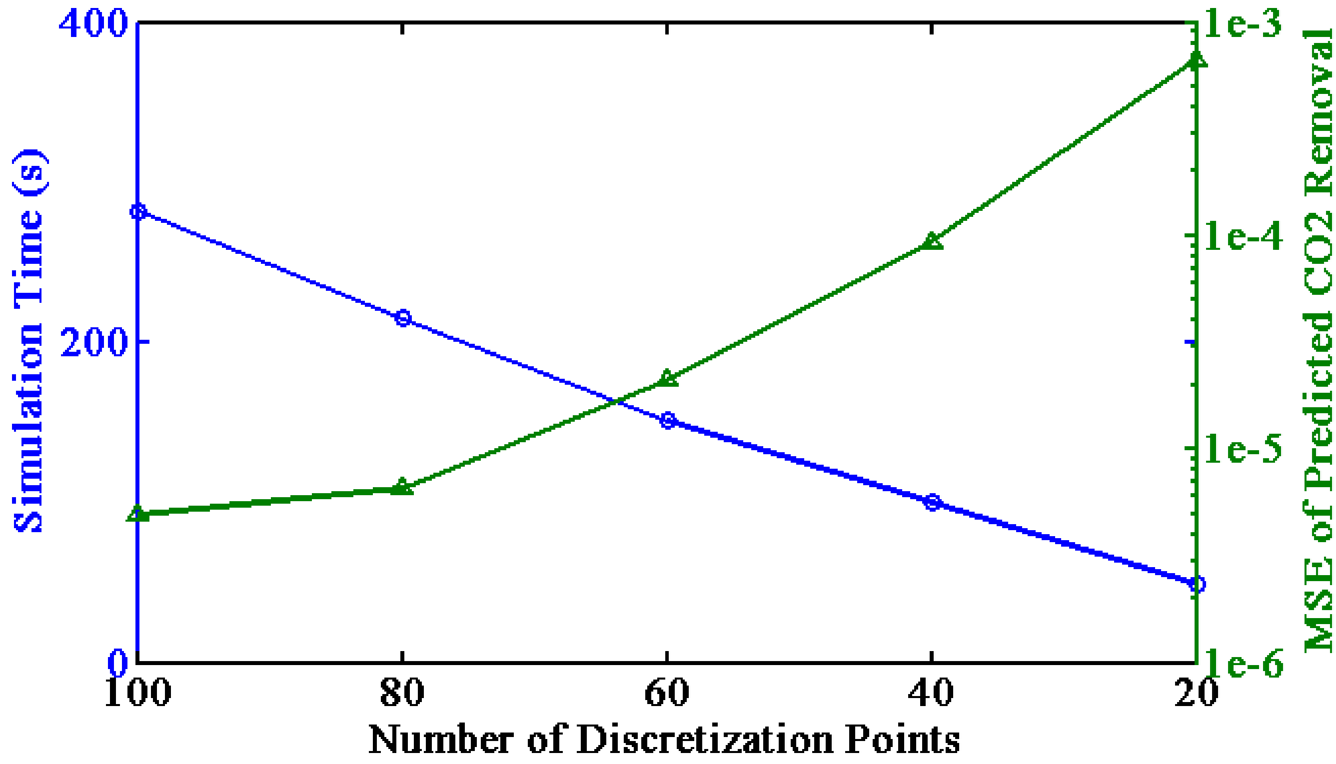
- Only **6-7** spatial basis functions are needed for state y
- The number of model equation is reduced to around **2000** after POD reformulation
- Reduction potential : **5 times faster**



Conclusions & Future Work

- **Conclusions**
  - Developed a **fast and accurate temporally dynamic reduced model** for BFB adsorber
  - Validated the performance of the reduced model in case study (**33% reduction** in simulation time)
  - Generated a small set of basis functions of states with projection errors less than 0.1%
  - Showed the **potential of simulation cost reduction** by POD method

- **Future work**
  - Generate a spatially dynamic reduced model and validate its performance
  - Extend model reduction to the **integrated carbon capture system**
  - Incorporate the **dynamic reduced order models (D-ROM)** into the **dynamic real time optimization (D-RTO)** framework

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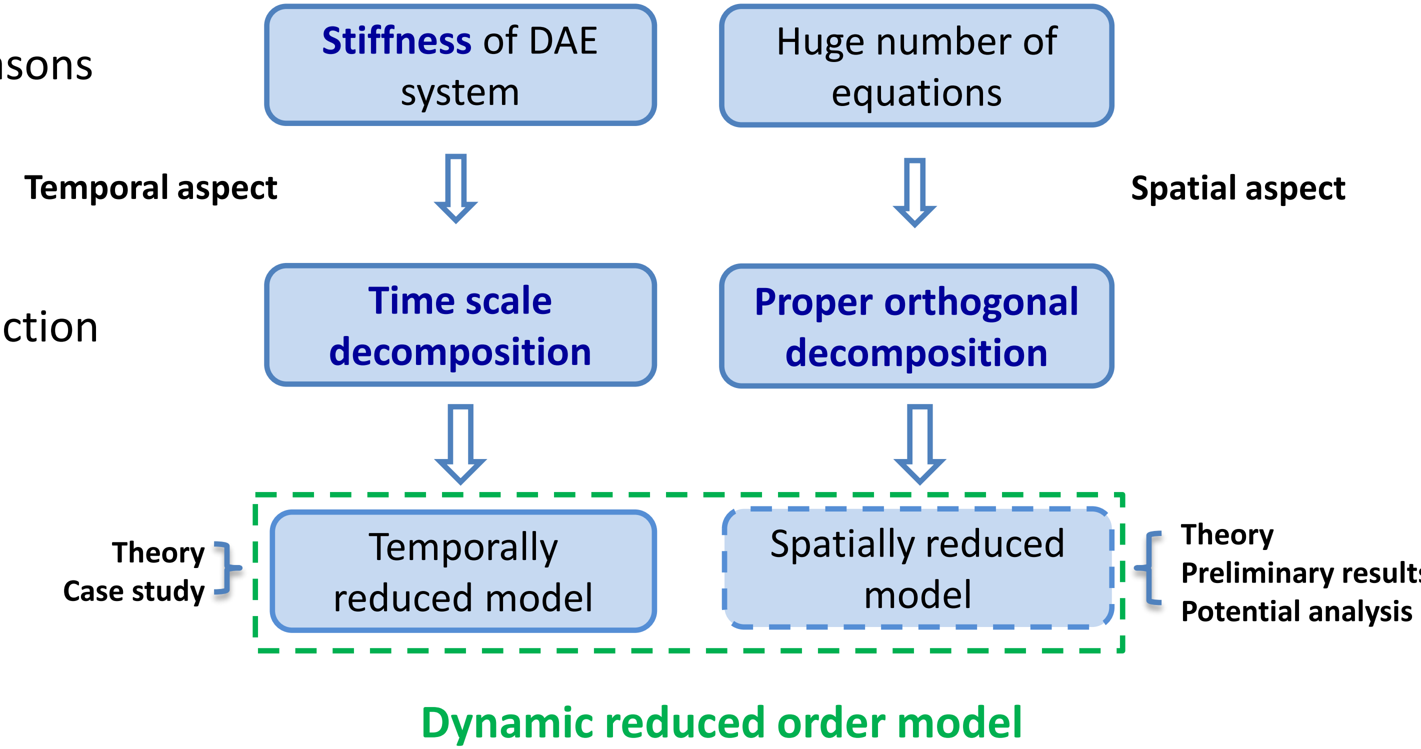
Introduction

Technology Roadmap

- Possible reasons

- Model reduction approaches



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Eigenvalue Analysis

- Jacobian matrix of differential and algebraic equation (DAE) system

$$\dot{x} = f(x, y)$$
$$0 = g(x, y)$$

Perturbation → Schur complement

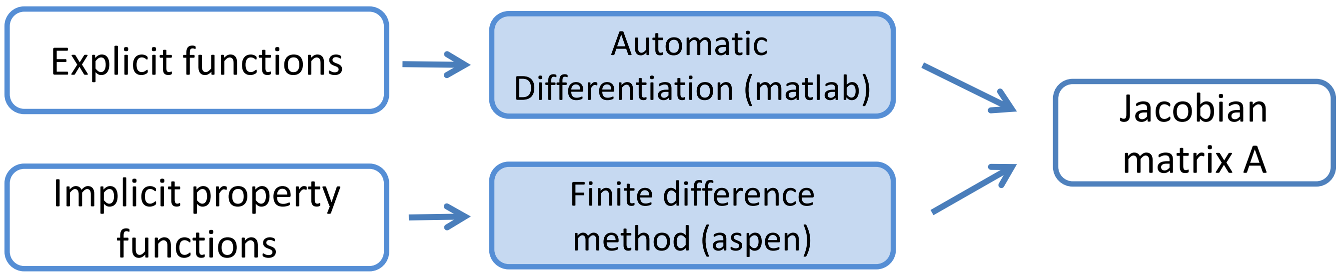
$$\dot{\Delta x} = A\Delta x$$

$$A = \frac{\partial f}{\partial x} - \frac{\partial f}{\partial y} \bullet \frac{\partial g}{\partial y}^{-1} \bullet \frac{\partial g}{\partial x}$$

x – differential variable

y – algebraic variable

- Jacobian Calculation



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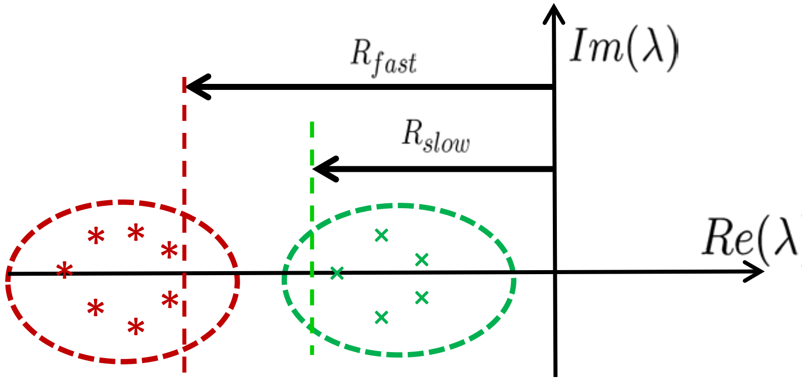
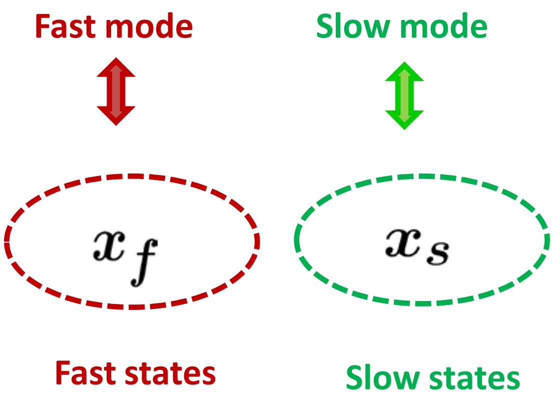
If $\xi \gg 1$, then a fast and a slow mode can be separated





- Eigenvalue-to-state association
  - Unit perturbation spectral resolution matrix

$$\boldsymbol{P}_{ij} = \boldsymbol{V}_{ij}(\boldsymbol{V}^{-1})_{ji}$$

V is the eigenvector matrix of Jacobian matrix

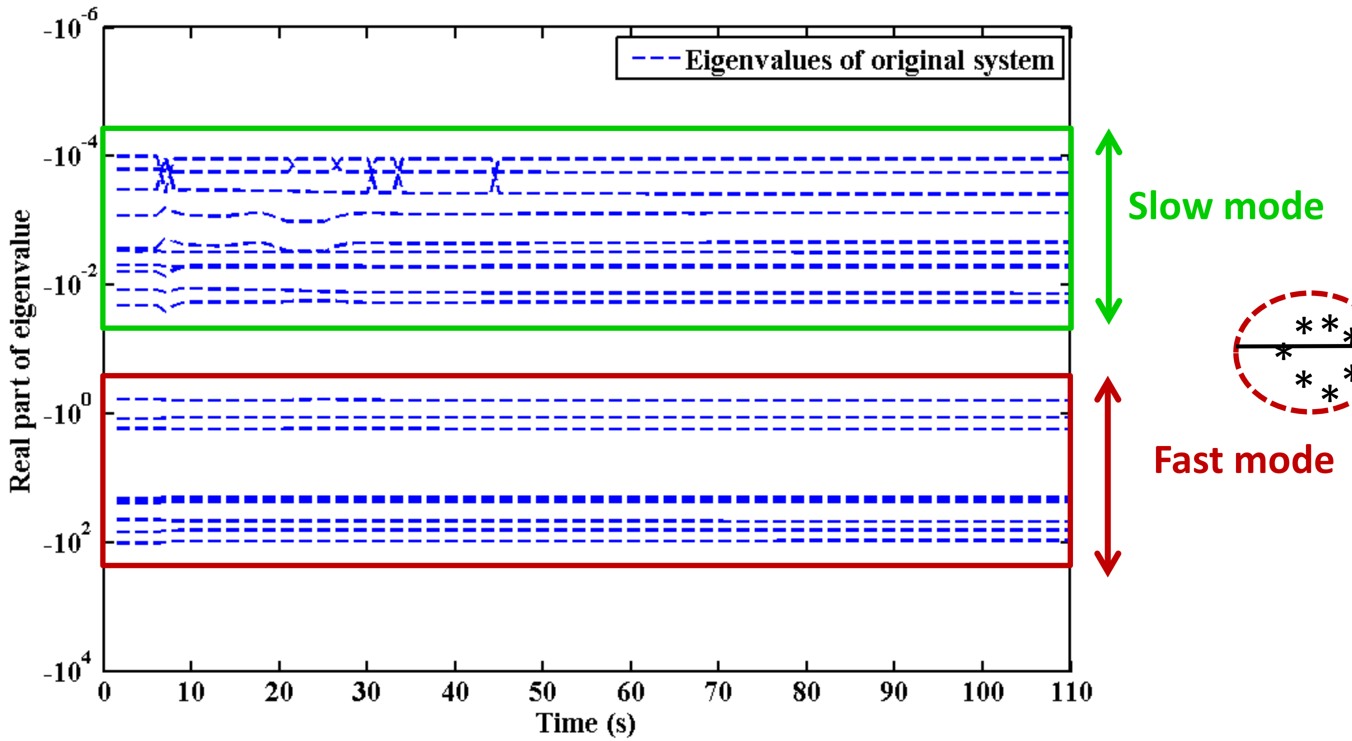
  - P_{ij} measures the strength of the association between state x_i and eigenvalue λ_j

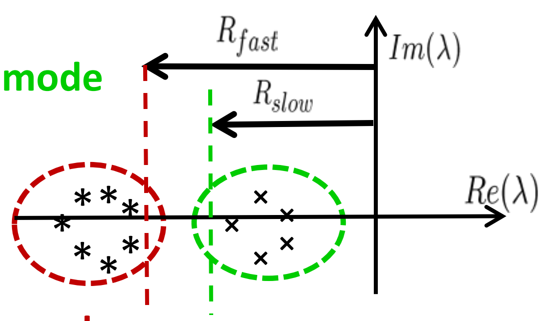
Temporally D-ROM for BFB Adsorber

Time Scale Decomposition Results

- Eigenvalue analysis during the transient response
  - Focus on time scale difference in gas and solid phase
  - Eigenvalue analysis in a single tray model

$$\xi = \frac{R_{fast}}{R_{slow}} = 32$$



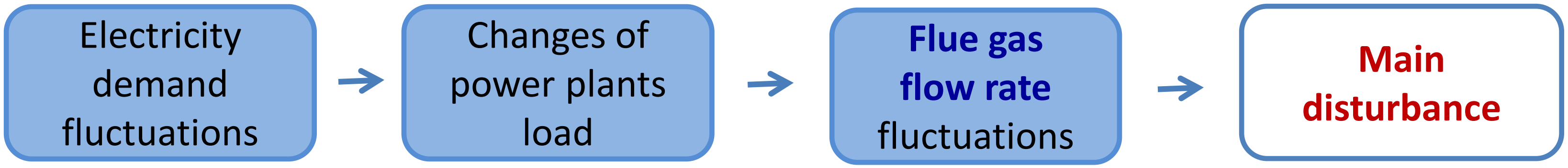


Eigenvalue variation of the original system

Temporally D-ROM for BFB Adsorber

Case Study: Reduced Model Validation

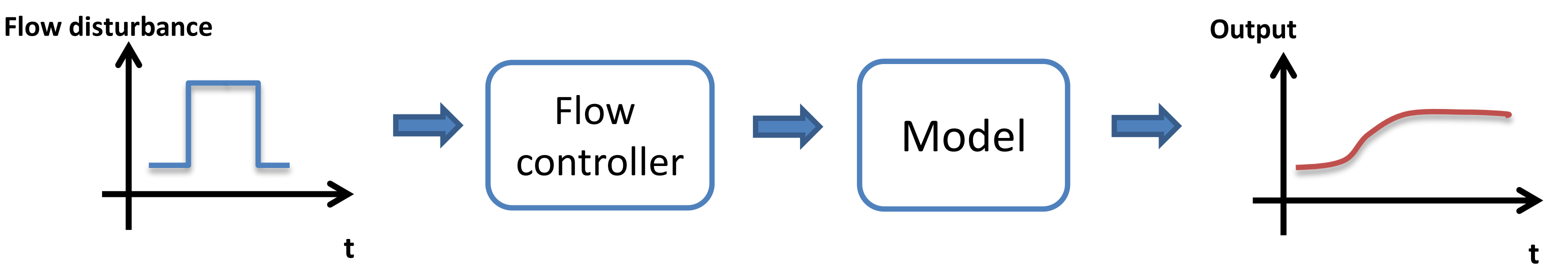
- CO_2 adsorption for fossil fuel power plants



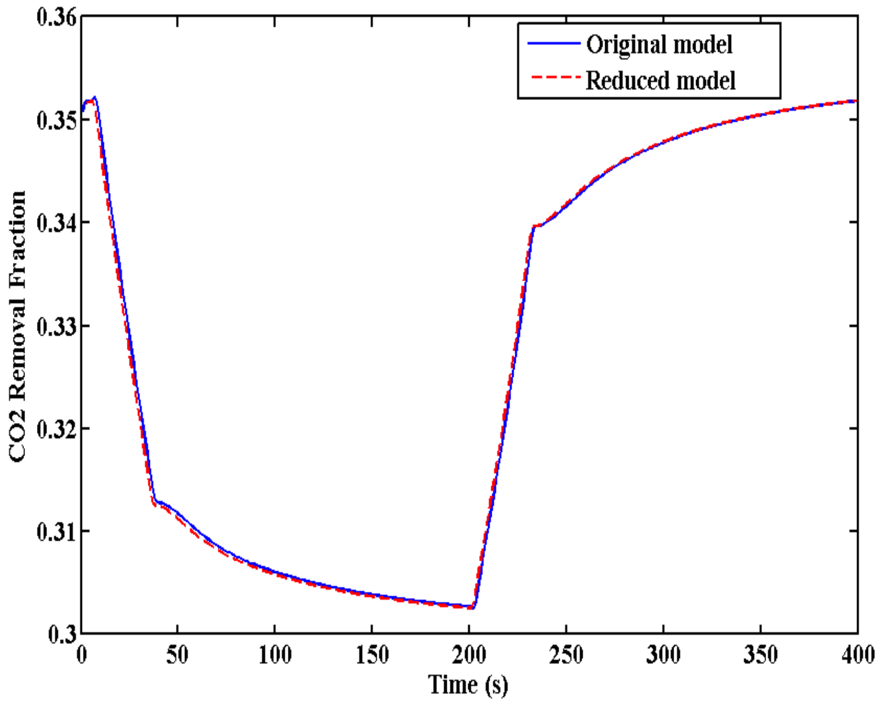
- $\pm 25\%$ step changes in flue gas flow rate are introduced at *t = 5* and *t = 200*

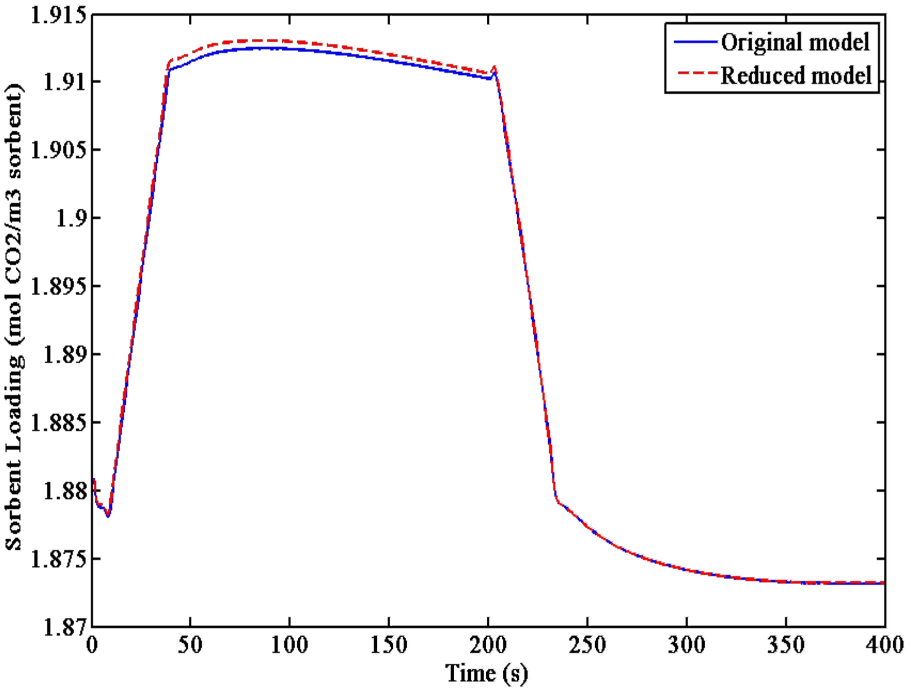
- Two key outputs of the adsorber
  - CO_2 removal fraction
  - Sorbent loading

Step response test:



Back up: Ramp input (25% at 5-35 -25% at 200-230)





Simulation time reduction: 18%

UPSR

GSR matrix

The basis for spectral association is the role played by eigenvalues in describing the dynamics of a linear system. Consider the initial value problem given by:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t),\ \mathbf{x}(0) = \mathbf{x}^0 \tag{1}$$

If the eigenvectors of the matrix $\mathbf{A}$ are linearly independent, the solution has the form:

$$\mathbf{x}(t) = \exp(\mathbf{A}t)\mathbf{x}^0 = \mathbf{V}\exp(\mathbf{\Lambda}t)\mathbf{V}^{-1}\mathbf{x}^0 \tag{2}$$

where $\mathbf{\Lambda}$ and $\mathbf{V}$ are, respectively, the eigenvalues and eigenvectors of $\mathbf{A}$:

$$\begin{aligned} \mathbf{\Lambda} &= \mathbf{V}^{-1}\mathbf{A}\mathbf{V} = diag(\lambda_1, \lambda_2, \ldots, \lambda_n) \\ \exp(\mathbf{\Lambda}t) &= diag\left(e^{\lambda_1 t}, e^{\lambda_2 t}, \ldots, e^{\lambda_n t}\right) \end{aligned} \tag{3}$$

The structure within the solution described by Eq. (2) and Eq. (3) can be expressed as:

$$x_i(t) = \sum_{j=1}^{n}\sum_{k=1}^{n} S_{ij}^{(k)} x_j^0 \exp(\lambda_k t) \tag{4}$$

in which the hyper-matrix $\mathbf{S}$, the *general spectral resolution* (GSR), is given by:

$$S_{ij}^{(k)} = V_{ik}(V^{-1})_{kj} \tag{5}$$

This structure of the GSR is illustrated in Fig. 2. The dynamic response of a system is described in terms of a *source* perturbation x_j^0, a dynamic *pathway* λ_k, and a *response* $x_i(t)$:

$$x_j^0 \xrightarrow{\lambda_k} x_i(t)$$

UPSR

UPSR matrix

3.1. The unit perturbation spectral resolution (UPSR)

Because spectral association seeks to characterise the fundamental dynamics of a state through association with eigenvalues, the response of a state to a *perturbation in itself* can be used as a measure of eigenvalue-to-state association. For example, an initial unit perturbation in the state x_1 is used to calculate the response of that same state x_1:

$$\mathbf{x}^0 = \begin{bmatrix} 1 & 0 & 0 & \cdots \end{bmatrix}^T \Rightarrow x_1(t)$$

The response of each state to such a unit perturbation in itself is described by a diagonal slice through the general spectral resolution matrix $\mathbf{S}$:

$$S_{ii}^{(j)} : x_i^0 \xrightarrow{\lambda_j} x_i(t)$$

which is illustrated in Fig. 3.

The responses can be assembled into the UPSR matrix $\mathbf{P}$ in which the value P_{ij} is a measure of the strength of association between state x_i and eigenvalue λ_j, so that:

$$x_i(t) = \sum_{j=1}^{n} P_{ij}\, e^{\lambda_j t} = \mathbf{P}_{i\bullet} \exp(\boldsymbol{\lambda} t) \qquad (9)$$

Calculation of the UPSR matrix $\mathbf{P}$ follows readily from the general spectral resolution $\mathbf{S}$:

$$P_{ij} = S_{ii}^{(j)} = V_{ij}(V^{-1})_{ji} \qquad (10)$$

Or in matrix notation,

$$\mathbf{P} = \mathbf{V} \otimes (\mathbf{V}^{-1})^T \qquad (11)$$

Where the operator $\otimes$ represents an element by element, or Hadamard, product.