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) \(\text{over 30,000 equations}\)
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  - Differential and algebraic equations (DAEs) (over 30,000 equations)

- 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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    - Computationally expensive
      o For a control case study, the simulation takes 9 hours for a simulation interval of 1.38 hours
      o Too slow for process control and dynamic optimization tasks
  - 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 $\lambda$
Temporally D-ROM for BFB Adsorber
Time Scale Decomposition Procedures

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System dynamics ↔ Eigenvalue \( \lambda \)

Eigenvalue Analysis

Eigenvalue-to-State Association

\begin{align*}
\text{Fast mode} & \quad \text{Slow mode} \\
\text{Fast states} & \quad \text{Slow states}
\end{align*}

\[ \Re(\lambda) \quad \Im(\lambda) \]
Temporally D-ROM for BFB Adsorber

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Eigenvalue-to-State Association

Quasi-steady State Approximation

System dynamics ↔ Eigenvalue $\lambda$

Fast mode

Slow mode

Fast states ↔ Slow states

$x_f = f_f(x_s, x_f)$

$x_s = f_s(x_s, x_f)$

Dynamic reduced model

Energy Systems Initiative (ESI) Meeting
Temporally D-ROM for BFB Adsorber

Eigenvalue Analysis

- Eigenvalue group separation
  - Separation ratio \( \xi = \frac{R_{fast}}{R_{slow}} \)
  
  If \( \xi \gg 1 \), then a fast and a slow mode can be separated
Temporally D-ROM for BFB Adsorber

Eigenvalue Analysis

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- Eigenvalue variation of original system
Temporally D-ROM for BFB Adsorber

Eigenvalue Analysis

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- **Eigenvalue variation of original system**
Temporally D-ROM for BFB Adsorber
Dynamic Reduced Model

- Eigenvalue-to-state association
  - Unit perturbation spectral resolution matrix
    \[ P_{ij} = V_{ij}(V^{-1})_{ji} \]
    \( V \) is the eigenvector matrix of Jacobian matrix
  - \( P_{ij} \) measures the strength of the association between state \( x_i \) and eigenvalue \( \lambda_j \)
Temporally D-ROM for BFB Adsorber
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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
Temporally D-ROM for BFB Adsorber
Dynamic Reduced Model

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- 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

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<tr>
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MSE: mean squared error; MRE: maximum relative error; 1: CO₂ removal fraction; 2: sorbent loading

33% reduction
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33% reduction
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
Spatial Model Reduction

Proper Orthogonal Decomposition (POD)

- Proper orthogonal decomposition

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

- Method of snapshots

  - Snapshot matrix

  \[ Y = [y_1, \ldots, y_M] \]

  - 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, \( \sigma_i \): amount of projection

  - Projection error:

  \[ \varepsilon_{norm}^{POD} = 1 - \frac{\sum_{i=1}^{K} \sigma_i^2}{\sum_{i=1}^{N} \sigma_i^2} \]
Spatial Model Reduction
Proper Orthogonal Decomposition (POD)

- Overall procedures

Original model
    Spatial discretization

Full discretized system
    Dim = \( N \)

Simulation

Snapshots \( Y = [y_1, \ldots, y_M] \)

POD basis functions \( \varphi_j(x) \)

Method of snapshots

Weighted residual method

Reduced discretized system
    Dim = \( K \ll N \)

\( \frac{\partial y}{\partial t} = f(y, t) \)
Spatial Model Reduction
Proper Orthogonal Decomposition (POD)

- Overall procedures

Original model
- Spatial discretization

Full discretized system
Dim = \( N \)

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Snapshots \( Y = [y_1, \ldots, y_M] \)

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Reduced discretized system
Dim = \( K \ll N \)

\[
\frac{\partial y}{\partial t} = f(y, t)
\]

\[
\frac{\partial y_i}{\partial t} = f(y, t), \quad i = 1 \ldots N
\]
Spatial Model Reduction
Proper Orthogonal Decomposition (POD)

- Overall procedures

Original model
  \[ \text{Spatial discretization} \]

Full discretized system
  \[ \text{Dim} = N \]

Simulation

Snapshots \( Y = [y_1, \ldots, y_M] \)

Method of snapshots

POD basis functions \( \varphi_j(x) \)

Weighted residual method

Reduced discretized system
  \[ \text{Dim} = K << N \]

\[ \frac{\partial y}{\partial t} = f(y, t) \]

\[ \frac{\partial y_i}{\partial t} = f(y, t), \quad i = 1 \ldots N \]

\[ y(x, t) = \sum_{i=1}^{K} a_i(t) \varphi_j(x) \]
Spatial Model Reduction
Proper Orthogonal Decomposition (POD)

- Overall procedures

1. Original model
   - Spatial discretization
   - Full discretized system
     \[ \text{Dim} = N \]

2. Simulation
   - Snapshots \( Y = [y_1, \ldots, y_M] \)

3. Method of snapshots
   - POD basis functions \( \varphi_j(x) \)

4. Weighted residual method
   - Reduced discretized system
     \[ \text{Dim} = K \ll N \]

Derivatives:

\[ \frac{\partial y}{\partial t} = f(y, t) \]

\[ \frac{\partial y_i}{\partial t} = f(y, t), i = 1 \ldots N \]

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

\[ \frac{da_i}{dt} = f(y, t), i = 1 \ldots K \]
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%

\[ \varepsilon_{norm}^{POD} = 1 - \frac{\sum_{i=1}^{K} \sigma_i^2}{\sum_{i=1}^{N} \sigma_i^2} \]
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- Examples:

![Graph showing singular values vs. order number of singular values]
Spatial Model Reduction
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Spatial Model Reduction

Regression model

- Why regression model?
  - POD needs to know the **explicit form** of model equation
  - Linear/quadratic regression models are incorporated to replace Aspen property functions
Spatial Model Reduction
Regression model

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- Model validation
Spatial Model Reduction
Regression model

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Maximum relative error = 0.41%
Spatial Model Reduction
Potential Analysis

- Only 6-7 spatial basis functions are needed for state \( y \)
- The number of model equation is reduced to around 2000 after POD reformulation
Spatial Model Reduction
Potential Analysis

- 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
References


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Introduction
Technology Roadmap

- Possible reasons

  Temporal aspect

  Stiffness of DAE system

  Time scale decomposition

  Temporally reduced model

  Dynamic reduced order model

  Theory

  Case study

Spatial aspect

  Huge number of equations

  Proper orthogonal decomposition

  Spatially reduced model

  Theory

  Preliminary results

Potential analysis
Temporally D-ROM for BFB Adsorber

Eigenvalue Analysis

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

\[ \begin{align*}
\dot{x} &= f(x, y) \\
0 &= g(x, y)
\end{align*} \]

- Perturbation

- Schur complement

\[ \Delta x = A \Delta x \]
\[ A = \frac{\partial f}{\partial x} - \frac{\partial f}{\partial y} \frac{\partial g^{-1}}{\partial y} \frac{\partial g}{\partial x} \]

- Jacobian Calculation

- Explicit functions

- Implicit property functions

- Automatic Differentiation (matlab)

- Finite difference method (aspen)

- Jacobian matrix A
**Temporally D-ROM for BFB Adsorber**

**Eigenvalue Analysis**

- Eigenvalue group separation
  - Separation ratio
    \[ \xi = \frac{R_{\text{fast}}}{R_{\text{slow}}} \]

  If \( \xi \gg 1 \), then a fast and a slow mode can be separated.

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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

\[ \xi = \frac{R_{\text{fast}}}{R_{\text{slow}}} = 32 \]

Eigenvalue variation of the original system
Temporally D-ROM for BFB Adsorber
Case Study: Reduced Model Validation

- CO₂ adsorption for fossil fuel power plants

Electricity demand fluctuations → Changes of power plants load → Flue gas flow rate fluctuations → Main disturbance

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

- Two key outputs of the adsorber
  - CO₂ removal fraction
  - Sorbent loading

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

Simulation time reduction: 18%
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:
\[
\frac{d}{dt}x(t) = Ax(t), \quad x(0) = x^0
\]  
(1)

If the eigenvectors of the matrix \( A \) are linearly independent, the solution has the form:
\[
x(t) = \exp(At)x^0 = V \exp(\Lambda t)V^{-1}x^0
\]  
(2)

where \( \Lambda \) and \( V \) are, respectively, the eigenvalues and eigenvectors of \( A \):
\[
\Lambda = V^{-1}AV = diag(\lambda_1, \lambda_2, \ldots, \lambda_n) \nonumber
\]
\[
\exp(\Lambda t) = diag(e^{\lambda_1 t}, e^{\lambda_2 t}, \ldots, e^{\lambda_n t})
\]  
(3)

The structure within the solution described by Eq. (2) and Eq. (3) can be expressed as:
\[
x_i(t) = \sum_{j=1}^{n} \sum_{k=1}^{n} S_{ij}^{(k)} x_j^0 \exp(\lambda_k t)
\]  
(4)

in which the hyper-matrix \( S \), the general spectral resolution (GSR), is given by:
\[
S_{ij}^{(k)} = V_{ik}(V^{-1})_{kj}
\]  
(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 \( \lambda_k \), and a response \( x_i(t) \):
\[
x_j^0 \xrightarrow{\lambda_k} x_i(t)
\]
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 $x_1$:

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

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

$$S^{(j)}_{ii} : x^0_i \xrightarrow{\lambda_j} x_i(t)$$

which is illustrated in Fig. 3.

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

$$x_i(t) = \sum_{j=1}^{n} P_{ij} e^{\lambda_j t} = P_{i*} \exp(\lambda t)$$

(9)

Calculation of the UPSR matrix $P$ follows readily from the general spectral resolution $S$:

$$P_{ij} = S^{(j)}_{ii} = V_{ij}(V^{-1})_{ji}$$

(10)

Or in matrix notation,

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

(11)

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