A Trust-region Algorithm for the Optimization of PSA Processes using Reduced-order Modeling

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CAPD Annual Review Meeting
March 7, 2010
Pressure Swing Adsorption Process

Pressure Swing Adsorption is an adsorption based gas separation technique.

A two-bed four-step PSA process
Computational Challenges with PSA Optimization

- PSA processes governed by stiff PDAEs
- Profiles characterized by steep adsorption fronts
- $O(1000)$ DAEs after spatial discretization
- Jiang et al.* solved a 5-bed 11-step PSA optimization problem in 50-200 CPU hrs.

Develop a reduced-order model (ROM)

\[
\begin{align*}
\text{min} & \quad \Phi(y(t), z(t), q) \\
\text{s.t.} & \quad \frac{dy}{dt} = f(y(t), z(t), q) \\
& \quad w(y(t), z(t), q) \leq 0 \\
& \quad h(y(t), z(t), q) = 0
\end{align*}
\]

\[
\begin{align*}
\text{min} & \quad \Phi(y^{ROM}(t), z^{ROM}(t), q) \\
\text{s.t.} & \quad \frac{dy^{ROM}}{dt} = f(y^{ROM}(t), z^{ROM}(t), q) \\
& \quad w(y^{ROM}(t), z^{ROM}(t), q) \leq 0 \\
& \quad h(y^{ROM}(t), z^{ROM}(t), q) = 0
\end{align*}
\]

Reduced-order Modeling

- Solve the DAE system for a particular set of parameters
- Store the solution in a snapshot matrix
- Obtain new set of basis functions using proper orthogonal decomposition (POD)

\[
\min_{\varphi_1, \varphi_2, \ldots, \varphi_n} \varepsilon^{POD}(m) = \sum_{i=1}^{p} \left\| y^i - \sum_{j=1}^{m} (y^i, \varphi^j)\varphi^j \right\|^2
\]

\[
s.t. \quad \| \varphi^i \| = 1 \quad (\varphi^i, \varphi^i) = 1 \quad i = 1, 2, \ldots, n
\]
\[
(\varphi^i, \varphi^j) = 0 \quad i = 1, 2, \ldots, n \quad i \neq j
\]

Original Rigorous Model

\[
y(x, t) = \sum_{j=1}^{n} y_j(t)e_j(x)
\]

\[
\frac{dy_i}{dt} = f(y, t) \quad i = 1\ldots n
\]

\[n \sim O(1000s)\]

\[m \sim O(10s \text{ or } 100s)\]

Galerkin-type projection

Reduced Order Model

\[
y(x, t) = \sum_{j=1}^{m} a_j(t)\varphi_j(x)
\]

\[
\frac{da_i}{dt} = f(a, t) \quad i = 1\ldots m
\]
ROM-based Optimization

ROM depends on snapshots taken at current value of parameters

Trust region based optimization*

Contours of objective function

Constraints

optimum

ROM shows error

Accurate ROM


For convergence to first order critical point

\[ f(x_k) = f_k^R(x_k) \]
\[ c(x_k) = c_k^R(x_k) \]
\[ \nabla f(x_k) = \nabla f_k^R(x_k) \]
\[ \nabla c(x_k) = \nabla c_k^R(x_k) \]

Zero-order correction*

\[ \tilde{f}_k(x) = f_k^R(x) + (f(x_k) - f_k^R(x_k)) \]
\[ \tilde{c}_k(x) = c_k^R(x) + (c(x_k) - c_k^R(x_k)) \]

Ensures

\[ f(x_k) = \tilde{f}_k(x_k) \]
\[ c(x_k) = \tilde{c}_k(x_k) \]

First-order correction*

\[ \tilde{f}_k(x) = f_k^R(x) + (f(x_k) - f_k^R(x_k)) + (\nabla f(x_k) - \nabla f_k^R(x_k))^T (x - x_k) \]
\[ \tilde{c}_k(x) = c_k^R(x) + (c(x_k) - c_k^R(x_k)) + (\nabla c(x_k) - \nabla c_k^R(x_k))^T (x - x_k) \]

Ensures

\[ f(x_k) = \tilde{f}_k(x_k) \]
\[ c(x_k) = \tilde{c}_k(x_k) \]
\[ \nabla f(x_k) = \nabla \tilde{f}_k(x_k) \]
\[ \nabla c(x_k) = \nabla \tilde{c}_k(x_k) \]

Inequalities

Exact penalty function

Original optimization problem

\[
\min_x F(x) = f(x) + p \sum_j \max(0, c_j(x))
\]

Corresponding TR subproblem with ROM

\[
\begin{align*}
\min_s M(x_k + s) &= \tilde{f}_k(x_k + s) + p \sum_j \max(0, \tilde{c}_{k,j}(x_k + s)) \\
\text{s.t.} &\quad \|s\| \leq \Delta_k
\end{align*}
\]

Filter-based approach

- Either reduce objective or infeasibility or both
- \(x_k\) dominates other points in the shaded region
- \(x_k, x_l,\) and \(x_m\) do not dominate each other, and form the filter
- Keep adding points to filter until convergence
Trust-region algorithm (with penalty approach)

\[
\min_{x} F(x) = f(x) + p \sum_{j} \max(0, c_j(x))
\]

\[
\min_{s} M(x_k + s) = \tilde{f}_k(x_k + s) + p \sum_{j} \max(0, \tilde{c}_{k,j}(x_k + s))
\]

s.t. \( \|s\| \leq \Delta_k \)

TR Algorithm*

Choose \( \Delta_0, x_0 \). Compute \( F(x_0) \). Set \( k = 0 \)

Obtain POD basis set at \( x_k \). Construct ROM for TR subproblem

Compute step \( s_k \) which satisfies following sufficient decrease condition

\[
M(x_k) - M(x_k + s_k) \geq \kappa \|g(x_k)\| \min(\delta, \Delta_k)
\]

or a weaker condition

\[
M(x_k) - M(x_k + s_k) \geq \kappa \min(v_1, v_2 \Delta_k)
\]

Calculate \( F(x_k + s_k) \), and \( \rho_k = \frac{ared}{pred} = \frac{F(x_k) - F(x_k + s_k)}{M(x_k) - M(x_k + s_k)} \)

\( \Delta_{k+1} \leq \Delta_{min} \)?

\( x_{k+1} = x_k \)

Shrink \( \Delta_k \)

Is \( \rho_k \geq \eta_1 \) ?

Yes

\( x_{k+1} = x_k + s_k \)

Update \( \Delta_k \)

No

Stop

Case study: Post-combustion capture

2-bed 4-step PSA process
Zeolite 13X adsorbent
Feed: N\textsubscript{2} (85%) and CO\textsubscript{2} (15%)
Pressure: 101.32 kPa
Temperature: 310 K

Optimization problem
max CO\textsubscript{2} recovery
s.t. Bed Model
CO\textsubscript{2} purity ≥ 50%
101.32 kPa ≤ P\textsubscript{h} ≤ 300 kPa
40 kPa ≤ P\textsubscript{t} ≤ 101.32 kPa
35 sec ≤ t\textsubscript{p} ≤ 150 sec
50 sec ≤ t\textsubscript{a} ≤ 400 sec
10 cm/sec ≤ u\textsubscript{a} ≤ 25 cm/sec

Bed Model – Isothermal PSA process

Component mass balance
\[ \varepsilon_b \frac{\partial C_i}{\partial t} + (1 - \varepsilon_b) \rho_s \frac{\partial q_i}{\partial t} + \frac{\partial (vC_i)}{\partial z} = 0 \quad \forall i \]

Overall mass balance
\[ \frac{\partial v}{\partial z} + (1 - \varepsilon_b) \rho_s \frac{RT}{P} \sum_i \frac{\partial q_i}{\partial t} = 0 \]

LDF equation
\[ \frac{\partial q_i}{\partial t} = k_i (q_i^* - q_i) \]

Dual-site Langmuir Isotherm
\[ q_i^* = \frac{q_{1i}^* b_{1i} y_i}{1 + \sum_{j=1}^{nc} b_{1j} y_j} + \frac{q_{2i}^* b_{2i} y_i}{1 + \sum_{j=1}^{nc} b_{2j} y_j} \]
## ROM accuracy

<table>
<thead>
<tr>
<th>Decision variable</th>
<th>Base value</th>
<th>ROM</th>
<th>True model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adsorption pressure ($P_h$)</td>
<td>150 kPa</td>
<td>93.68%</td>
<td>93.67%</td>
</tr>
<tr>
<td>Desorption pressure ($P_l$)</td>
<td>50 kPa</td>
<td>80.32%</td>
<td>80.11%</td>
</tr>
<tr>
<td>Pressurization step time ($t_p$)</td>
<td>50 s</td>
<td>38.28%</td>
<td>37.71%</td>
</tr>
<tr>
<td>Adsorption step time ($t_a$)</td>
<td>150 s</td>
<td>67.65%</td>
<td>68.76%</td>
</tr>
<tr>
<td>Adsorption feed flow ($u_a$)</td>
<td>20 cm/s</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Gas-phase CO₂ mole fraction profiles

#### Adsorption

- **True model**
- **ROM**

#### Desorption

- **True model**
- **ROM**
Optimization results (penalty, zero-order)

- ROM completely discretized in TR subproblem
- Box trust-region used in TR subproblem
- TR subproblem solved using IPOPT in AMPL

Computational results
No. of variables: 52247
Degrees of freedom: 5
TR iterations: 13
Optimization CPU time: 35.7 min.

Optimal parameters
- Adsorption pressure ($P_h$): 203 kPa
- Desorption pressure ($P_l$): 40 kPa
- Pressurization step time ($t_p$): 55.4 s
- Adsorption step time ($t_a$): 161.1 s
- Adsorption feed flow ($u_a$): 20.8 cm/s

<table>
<thead>
<tr>
<th></th>
<th>ROM</th>
<th>True model</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$ purity</td>
<td>51.41%</td>
<td>50.01%</td>
</tr>
<tr>
<td>CO$_2$ recovery</td>
<td>85.11%</td>
<td>81.74%</td>
</tr>
</tbody>
</table>

Solution not optimal !!
Computational results
No. of variables: 52247
Degrees of freedom: 5
TR iterations: 92
Optimization CPU time: 1.88 hrs.

Optimal parameters
Adsorption pressure \((P_h)\): 300 kPa
Desorption pressure \((P_l)\): 40 kPa
Pressurization step time \((t_p)\): 35 s
Adsorption step time \((t_a)\): 160.9 s
Adsorption feed flow \((u_a)\): 14.9 cm/s

<table>
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</tr>
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<tbody>
<tr>
<td>CO₂ purity</td>
<td>50.54%</td>
<td>50.01%</td>
</tr>
<tr>
<td>CO₂ recovery</td>
<td>99.04%</td>
<td>97.19%</td>
</tr>
</tbody>
</table>
**Optimization results (filter, hybrid)**

### Computational results
- No. of variables: 52247
- Degrees of freedom: 5
- TR iterations: 51
- Optimization CPU time: 1.36 hrs.

### Optimal parameters
- Adsorption pressure ($P_h$): 300 kPa
- Desorption pressure ($P_l$): 40 kPa
- Pressurization step time ($t_p$): 35 s
- Adsorption step time ($t_a$): 187.9 s
- Adsorption feed flow ($u_a$): 12.8 cm/s

### Table: Optimization results (filter, hybrid)

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<th>ROM</th>
<th>True model</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ purity</td>
<td>50.29%</td>
<td>50.01%</td>
</tr>
<tr>
<td>CO₂ recovery</td>
<td>98.43%</td>
<td>97.26%</td>
</tr>
</tbody>
</table>

- Fewer trust-region iterations
- Less optimization CPU time

**Optimal solution found**
Conclusions and Future work

Conclusions

- POD-based ROMs are reasonably accurate and can be used for efficient PSA optimization
- Trust-region based algorithm successfully applied for ROM-based PSA optimization
- Filter method better than exact penalty formulation

Future Work

- Large-scale PSA processes and other applications
- Approaches to construct more accurate ROMs
Thank You