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

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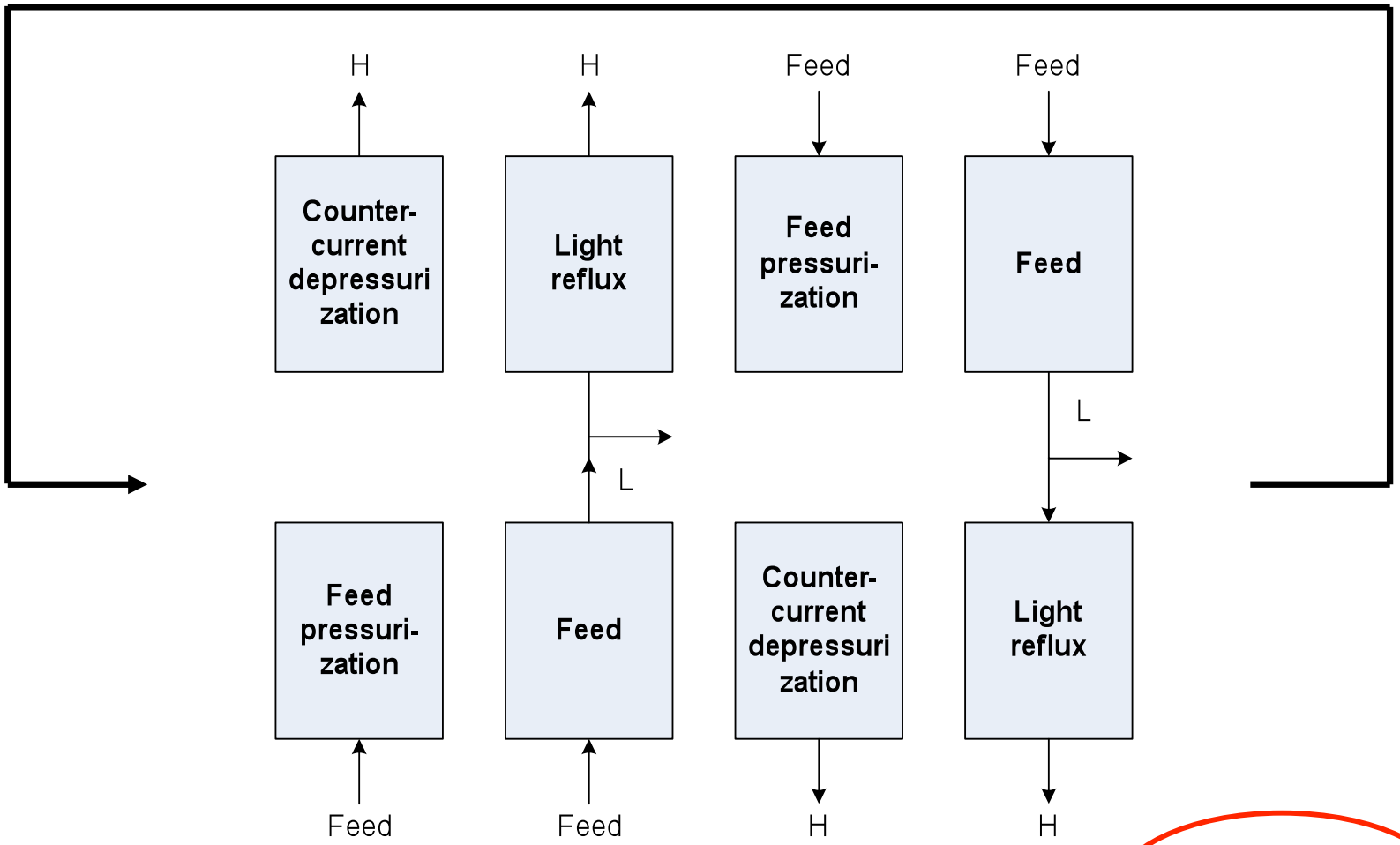
Pressure Swing Adsorption Process

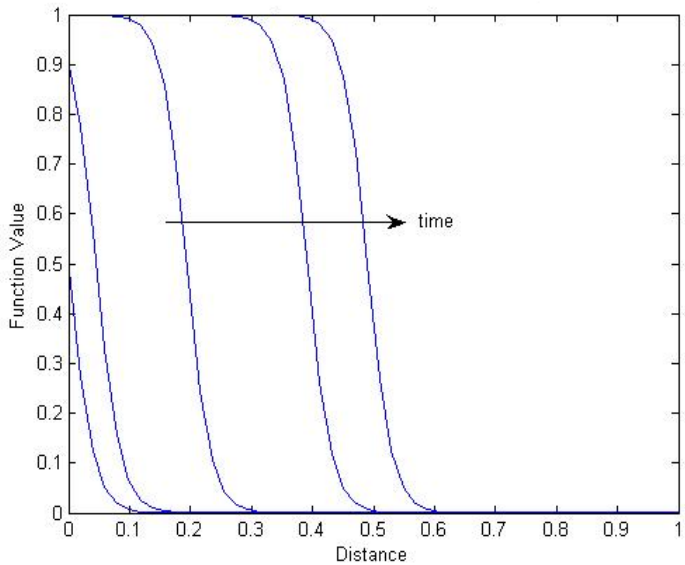
Pressure Swing Adsorption is an adsorption based gas separation technique



A two-bed four-step PSA process

PSA Cycle

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)

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

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

* Jiang, L., Fox, V. G., and Biegler, L. T., AIChE J., 50(11), 2904 (2004).

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)

$$\underset{\varphi^1,\varphi^2,\ldots,\varphi^n}{Min}\ \varepsilon^{POD}(m) = \sum_{i=1}^{p} \| y^i - \sum_{j=1}^{m} (y^i,\varphi^j)\varphi^j \|^2$$

$$s.t. \qquad \|\varphi^i\| = 1 \qquad (\varphi^i,\varphi^i) = 1 \qquad i = 1,2,\ldots n$$

$$(\varphi^i,\varphi^j) = 0 \qquad i = 1,2,\ldots n \quad i \neq j$$

Original Rigorous Model

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

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

Galerkin-type projection

n ~ O(1000s)

m ~ O(10s or 100s)

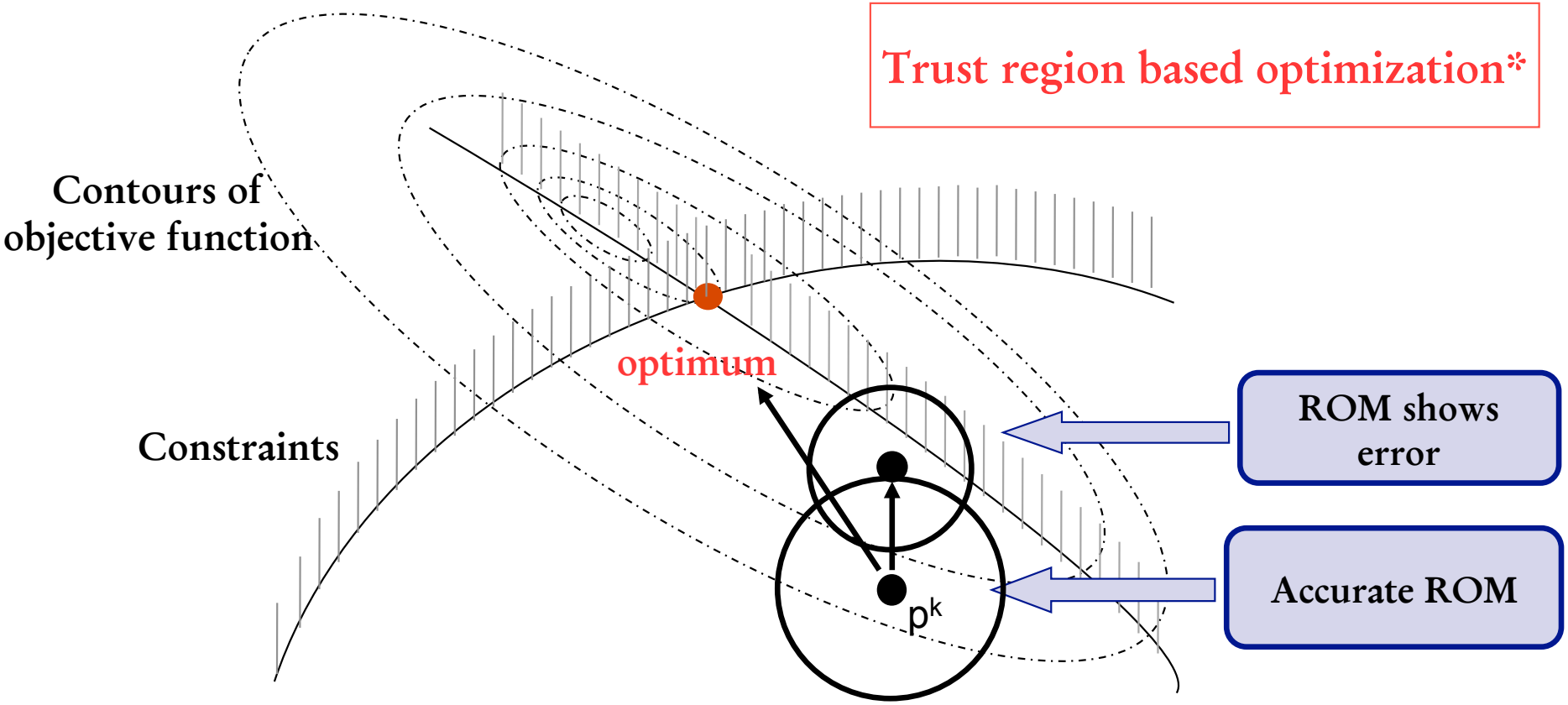
Reduced Order Model

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

$$\frac{da_i}{dt} = f(a,t) \quad i = 1\ldots m$$

ROM-based Optimization

ROM depends on snapshots taken at current value of parameters



*Toint, P.L., "Global convergence of a class of trust-region methods for nonconvex minimization in Hilbert space", IMA J. Numer. Anal., 8(2), 231 (1988)
*Fahl, M., "Trust-region methods for flow control based on reduced-order modeling", Doctoral dissertation, Trier University (2000)

Trust-region subproblem

Original optimization problem

$$\min_{x} \quad f(x)$$
$$\text{s.t.} \quad c(x) \leq 0$$

Corresponding TR subproblem with ROM

$$\min_{s} \quad f_k^R(x_k + s)$$
$$\text{s.t.} \quad c_k^R(x_k + s) \leq 0$$
$$\|s\| \leq \Delta_k$$

For convergence to first order critical point

$$f(x_k) = f_k^R(x_k) \qquad \nabla f(x_k) = \nabla f_k^R(x_k)$$
$$c(x_k) = c_k^R(x_k) \qquad \nabla c(x_k) = \nabla c_k^R(x_k)$$

Zero-order correction*

$$\widetilde{f}_k(x) = f_k^R(x) + (f(x_k) - f_k^R(x_k))$$
$$\widetilde{c}_k(x) = c_k^R(x) + (c(x_k) - c_k^R(x_k))$$

Ensures

$$f(x_k) = \widetilde{f}_k(x_k)$$
$$c(x_k) = \widetilde{c}_k(x_k)$$

First-order correction*

$$\widetilde{f}_k(x) = f_k^R(x) + (f(x_k) - f_k^R(x_k)) + (\nabla f(x_k) - \nabla f_k^R(x_k))^T (x - x_k)$$
$$\widetilde{c}_k(x) = c_k^R(x) + (c(x_k) - c_k^R(x_k)) + (\nabla c(x_k) - \nabla c_k^R(x_k))^T (x - x_k)$$

Ensures

$$f(x_k) = \widetilde{f}_k(x_k)$$
$$c(x_k) = \widetilde{c}_k(x_k)$$
$$\nabla f(x_k) = \nabla \widetilde{f}_k(x_k)$$
$$\nabla c(x_k) = \nabla \widetilde{c}_k(x_k)$$

*Alexandrov, N. M., Dennis, J. E., Jr., Lewis, R. M., and Torczon, V., "A trust-region framework for managing the use of approximate models in optimization," *Struct. Multidisc. Optim.*, 15, 16 (1998).

Inequalities

Exact penalty function

Original optimization problem

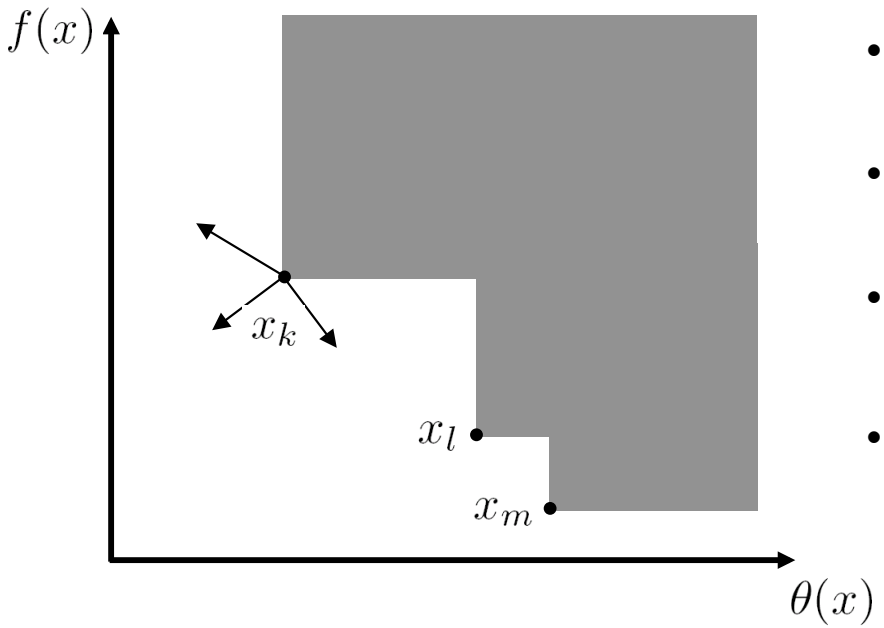
$$\min_{x} \quad F(x) = f(x) + p \sum_{j} \max(0, c_j(x))$$

Corresponding TR subproblem with ROM

$$\min_{s} \quad M(x_k + s) = \widetilde{f}_k(x_k + s) + p \sum_{j} \max(0, \widetilde{c}_{k,j}(x_k + s))$$

$$\text{s.t.} \quad \|s\| \leq \Delta_k$$

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)

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

$$\min_{s} \quad M(x_k+s) = \tilde{f}_k(x_k+s) + p\sum_{j}\max(0, \tilde{c}_{k,j}(x_k+s))$$
$$\text{s.t.} \quad \|s\| \le \Delta_k$$

TR Algorithm*

Choose Δ_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

$$M(x_k) - M(x_k+s_k) \ge \kappa \|g(x_k)\| \min(\delta, \Delta_k)$$

or a weaker condition

$$M(x_k) - M(x_k+s_k) \ge \kappa \min(v_1, v_2\Delta_k)$$

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

Is $\rho_k \ge \eta_1$?

Yes: $x_{k+1}=x_k+s_k$, Update Δ_k

No: $x_{k+1}=x_k$, Shrink Δ_k

$\Delta_{k+1} \le \Delta_{min}$?

No: Return to "Compute step s_k"

Yes: Stop

* Conn, A. R., Gould, N. I. M., and Toint, P. L., Trust Region Methods; SIAM: Philadelphia (2000)

Case study: Post-combustion capture

2-bed 4-step PSA process
Zeolite 13X adsorbent
Feed: N_2 (85%) and CO_2 (15%)
Pressure: 101.32 kPa
Temperature: 310 K

Optimization problem

$$
\begin{aligned}
\max \quad & CO_2 \text{ recovery} \\
\text{s.t.} \quad & \text{Bed Model} \\
& CO_2 \text{ purity} \geq 50\% \\
& 101.32 \text{ kPa} \leq P_h \leq 300 \text{ kPa} \\
& 40 \text{ kPa} \leq P_l \leq 101.32 \text{ kPa} \\
& 35 \text{ sec} \leq t_p \leq 150 \text{ sec} \\
& 50 \text{ sec} \leq t_a \leq 400 \text{ sec} \\
& 10 \text{ cm/sec} \leq u_a \leq 25 \text{ cm/sec}
\end{aligned}
$$

Bed Model – Isothermal PSA process

Component mass balance

$$\varepsilon_b \frac{\partial C_i}{\partial t} + (1-\varepsilon_b)\rho_s \frac{\partial q_i}{\partial t} + \frac{\partial (vC_i)}{\partial z} = 0 \qquad \forall i$$

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

$$q_i^* = \frac{q_{1i}^s b_{1i} P y_i}{1 + \sum_{j=1}^{nc} b_{1j} P y_j} + \frac{q_{2i}^s b_{2i} P y_i}{1 + \sum_{j=1}^{nc} b_{2j} P y_j}$$

ROM accuracy

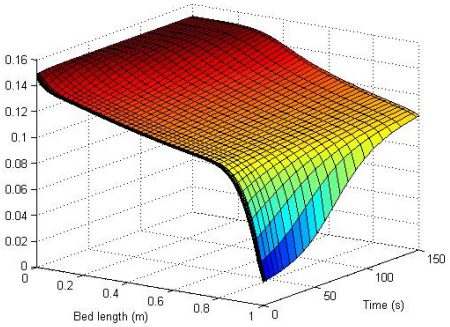
Decision variable	Base value
Adsorption pressure (P_h)	150 kPa
Desorption pressure (P_l)	50 kPa
Pressurization step time (t_p)	50 s
Adsorption step time (t_a)	150 s
Adsorption feed flow (u_a)	20 cm/s

	ROM	True model
N_2 purity	93.68%	93.67%
N_2 recovery	80.32%	80.11%
CO_2 purity	38.28%	37.71%
CO_2 recovery	67.65%	68.76%

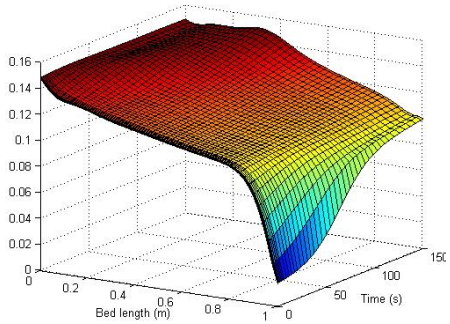
Gas-phase CO_2 mole fraction profiles

Adsorption

True model

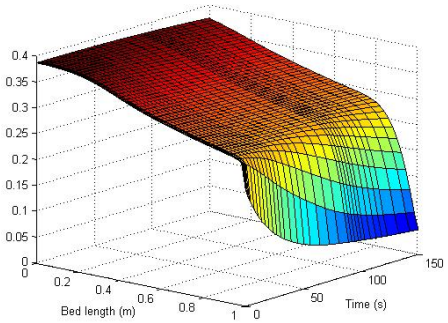


ROM

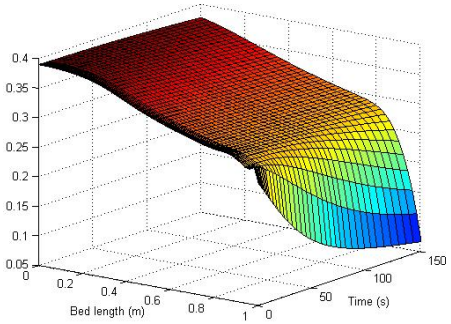


Desorption

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

	ROM	True model
CO_2 purity	51.41%	50.01%
CO_2 recovery	85.11%	81.74%

Solution not optimal !!

Optimization results (penalty, first-order)

- **Same starting guess**
- **TR subproblem solved using IPOPT in AMPL**

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

	ROM	True model
CO_2 purity	50.54%	50.01%
CO_2 recovery	99.04%	97.19%

Optimal solution found

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

	ROM	True model
CO_2 purity	50.29%	50.01%
CO_2 recovery	98.43%	97.26%

Optimal solution found

- **Fewer trust-region iterations**
- **Less optimization CPU time**

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