Advanced Heat Integration Tool for Simulation-based Optimization Framework

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Simulation-Based Optimization

+ Treats simulation as black box (does not require mathematical details of model)
  → Easy to implement

+ Does not require simplification of the process model
  → High-fidelity models applied

+ Readily adapted for parallel computing
  → Computational time reduced

− Not well suited for problems with many variables such as heat integration, and superstructure optimization
  → Heat integration is a separate module linked to simulation-based optimization algorithm

Goal: Develop a simulation-based optimization framework with heat integration for large-scale high-fidelity process models.
Simulation-Based Optimization with Heat Integration

Optimization Solver

\[
\begin{align*}
\min_{x} & \quad f(x) \\
\text{s.t.} & \quad g(x) \leq 0
\end{align*}
\]

Process Simulator(s)

Optimal values for Decision Variables

DFO

Simultaneous process optimization and heat integration based on rigorous process simulations are achieved in this framework

Heat Integration Tool

Heat Integration Results:

- Minimum utility cost (or consumption)
- Minimum heat exchanger area

Parameters

Initial Inputs

Optimal Outputs

Aspen Plus, ACM, gPROMS

Process Results

Optimal Outputs

Physical Properties

GAMS LP Models

Hot/Cold Stream Information

e.g., Flow rates, Temperatures, Enthalpy, …
Minimum Utility Cost (Consumption)

- **LP Transshipment Model**

\[
\min \quad Z = \sum_{m \in S} c_m Q^S_m + \sum_{n \in W} c_n Q^W_n
\]

\[
\text{s.t.} \quad R_{ik} - R_{i,k-1} + \sum_{j \in C_k} Q_{ijk} + \sum_{n \in W_k} Q_{ink} = Q^H_{ik} \quad i \in H_k'
\]

\[
R_{mk} - R_{m,k-1} + \sum_{j \in C_k} Q_{mjk} - Q^S_m = 0 \quad m \in S_k'
\]

\[
\sum_{i \in H_k} Q_{ijk} + \sum_{m \in S_k} Q_{mjk} = Q^C_{jk} \quad j \in C_k
\]

\[
\sum_{i \in H_k} Q_{ink} - Q^W_n = 0 \quad n \in W_k \quad k = 1, \ldots, K
\]

\[
R_{ik}, R_{mk}, Q_{ijk}, Q_{mjk}, Q_{ink}, Q^S_m, Q^W_n \geq 0 \quad R_{i0} = R_{iK} = 0
\]

- Heat loads of the streams are calculated directly from the total change of enthalpy from the simulation results.

- Assumption: **Constant** heat capacity flowrates (FCps) for streams.

Stream with Variable FCp

- A process stream with phase change

A mixture stream of CO\textsubscript{2} and H\textsubscript{2}O (CO\textsubscript{2}: 40%, H\textsubscript{2}O: 60%; 1kmol/hr; 1 bar)
Problems with Constant FCps

- Overestimate the heat recovery
- Infeasible heat exchanger network design
• More accurate heat integration results
• Assume constant FCps in each small temperature interval
• Build a series of sub-streams with identical temperature change or heat load in process models
Minimum Heat Exchanger Area

- **LP Area Targeting Model** (Modified from LP Transportation Model)

\[
\begin{align*}
\text{min} & \quad \frac{1}{Ft} \sum_{k=1}^{K} \sum_{l=1}^{K} \frac{1}{\text{LMTD}_{k,l}} \sum_{i \in H_k} \sum_{j \in C_l} q_{ik,jl} \\
\text{s.t.} & \quad \sum_{l=k}^{K} \sum_{j \in C_l} q_{ik,jl} = Q^H_{ik} \quad i \in H_k \\ & \quad \sum_{k=1}^{K} \sum_{i \in H_k} q_{ik,jl} = Q^C_{jl} \quad j \in C_l
\end{align*}
\]

- Temperature interval should be smaller than the minimum utility problem for accurate area targets.
- Number of temperature intervals: accurate results vs. CPU times.
- Double-temperature approach: **HRAT & EMAT**.

Implementation - Graphical User Interface

Framework for Optimization and Quantification of Uncertainty and Sensitivity (FOQUS)
Simulation Model (1)

ACM Simulation Model

Input Variables

<table>
<thead>
<tr>
<th></th>
<th>Name</th>
<th>Value</th>
<th>Unit</th>
<th>Category</th>
<th>Default</th>
<th>Min</th>
<th>Max</th>
<th>Description</th>
<th>Tags</th>
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</thead>
<tbody>
<tr>
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<td>Fixed</td>
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<tr>
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<td>m</td>
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<td>0.0</td>
<td>0.0</td>
<td></td>
<td>[]</td>
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Simulation Model (2)

Output Variables

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Unit</th>
<th>Description</th>
<th>Tags</th>
</tr>
</thead>
<tbody>
<tr>
<td>BFB_Comp_F</td>
<td>0.0</td>
<td>kmol/hr</td>
<td>Output stream</td>
<td></td>
</tr>
<tr>
<td>BFB_Comp_P</td>
<td>0.0</td>
<td>bar</td>
<td>Output stream</td>
<td></td>
</tr>
</tbody>
</table>
Heat Integration Tool (1)

Heat Integration Model (GAMS)

EMAT (Exchanger Minimum Approach Temperature)

HRAT (Heat Recovery Approach Temperature)

Heat Integration Inputs
Heat Integration Tool (2)

Utility Consumptions

Minimum Heat Exchanger Area

Minimum Utility Cost

Heat Integration Outputs
Optimization Solver

Solver Selection

Description of Current Solver

Solver Option Settings

<table>
<thead>
<tr>
<th>Option</th>
<th>Setting</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10.0</td>
<td>Upper bound on scaled variables (usually 10.0)</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
<td>Lower bound on scaled variables (usually 0.0)</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>Random number seed (0 uses clock)</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>Maximum number of iterations (0 go until converges)</td>
</tr>
<tr>
<td>5</td>
<td>25</td>
<td>Number of samples per iteration</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>Initial standard deviation about starting point</td>
</tr>
</tbody>
</table>
Optimization Problem Setting

- Run Optimization
- Select Decision Variables
  - Variable Scaling Method (Input variables are scaled to be 0 at min and 10 at max)
  - Min/Max Bounds
  - Current Value (Initial Guess)
- Objective Function (Python expression)
- Inequality Constraint (Python expression enforced with penalty)
Case Study – A Power Plant with CO₂ Capture

Steam Cycle

- Boiler
- High Pressure Turbine
- Intermediate Pressure Turbine
- Low Pressure Turbine
- Condenser

Carbon Capture System

- Adsorber
- Regenerator
- Compressor
- Intermediate Cooler
- CO₂ Stream
- To Storage

Clean Gas
Vent

Cooling Water

CO₂ Stream
Water

Solid Sorbent

Heater
Cooler

Gas Stream
Water/Steam Stream
Solid Stream
Problem Statement

Objective Function: Maximizing Net efficiency
Constraint: CO₂ removal ratio ≥ 90%
Flowsheet evaluation (via process simulators)
Minimum utility and area target (via heat integration tool)
Decision Variables (23): Bed length, diameter, sorbent and steam feed rates, temperatures
Case Study Results (1)

<table>
<thead>
<tr>
<th></th>
<th>Base case w/o CCS: 650 MW&lt;sub&gt;e&lt;/sub&gt;, 42.1 %</th>
<th>Simultaneous optimization and heat integration</th>
<th>Sequential optimization and heat integration approach</th>
<th>Optimization w/o heat integration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Net power efficiency (%)</strong></td>
<td>33.8</td>
<td>32.2</td>
<td>30.5</td>
<td></td>
</tr>
<tr>
<td><strong>Net power output (MW&lt;sub&gt;e&lt;/sub&gt;)</strong></td>
<td>522.2</td>
<td>497.9</td>
<td>471.1</td>
<td></td>
</tr>
<tr>
<td><strong>CO₂ removal ratio (%)</strong></td>
<td>90.2</td>
<td>90.1</td>
<td>90.1</td>
<td></td>
</tr>
<tr>
<td><strong>Electricity consumption (MW&lt;sub&gt;e&lt;/sub&gt;)</strong></td>
<td>85.2</td>
<td>73.8</td>
<td>73.8</td>
<td></td>
</tr>
<tr>
<td><strong>IP steam withdrawn (GJ/hr)</strong></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td><strong>LP steam withdrawn (GJ/hr)</strong></td>
<td>768.5</td>
<td>1113.7</td>
<td>1231.9</td>
<td></td>
</tr>
<tr>
<td><strong>Cooling water consumption (GJ/hr)</strong></td>
<td>1820.3</td>
<td>1594.2</td>
<td>3333.6</td>
<td></td>
</tr>
<tr>
<td><strong>Heat addition to feed water (GJ/hr)</strong></td>
<td>562.9</td>
<td>467.4</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td><strong>Heat exchanger area (million m²)</strong></td>
<td>0.751</td>
<td>1.125</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: Constant FCps are assumed here and piecewise linear approximation is not used.

**Optimization and heat integration significantly increased the net efficiency of the power plant with CCS.**
## Case Study Results (2)

<table>
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<th>Base case w/o CCS: 650 MW&lt;sub&gt;e&lt;/sub&gt;, 42.1 %</th>
<th>Heat integration with constant FCps</th>
<th>Heat integration with variable FCps (5 segments)</th>
<th>w/o heat integration</th>
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<td>0</td>
<td></td>
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<td>0.923</td>
<td></td>
<td></td>
</tr>
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After considering variable FCps and using piecewise linear approximation of the composite curve, the net efficiency is somewhat decreased but the obtained results become much more realistic.
Conclusions

• Simulation-based optimization framework with heat integration is a suitable tool for optimization of large-scale high-fidelity process models.

• This framework can be easily implemented in the software FOQUS.

• Performance of power plant with CCS can be significantly increased by simultaneous optimization and heat integration.

• More accurate heat integration results are obtained by using piecewise linear approximation for the composite curve of process streams.
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