Superstructure-based Simultaneous Optimization of Heat and Water Integration

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Motivation

Water and energy are important resources in the process industries

<table>
<thead>
<tr>
<th>Water issues</th>
<th>Energy issues</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rapidly growing demand for freshwater</td>
<td>Steadily growing demand for energy</td>
</tr>
</tbody>
</table>
Goal

To determine the flowsheet configuration and operating conditions that achieve optimal water and energy use to minimize cost

Two essential steps:

1. **Determine the minimum freshwater flowrate (target) required for a given set of water-using units**
   - **Challenges:**
     1. Multi-contaminant water stream integration
     2. Realistic wastewater system

2. **Perform simultaneous optimization on heat and water integration of a process flowsheet**
   - **Note:** only process flowsheet and HENS optimization has been performed (*Duran and Grossmann, 1986*)
Advantage

- Captures tradeoffs among raw material, investment cost and operating cost

Why simultaneous optimization?

<table>
<thead>
<tr>
<th>Cost</th>
<th>Overall conversion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total cost (sequential)</td>
<td></td>
</tr>
<tr>
<td>Total cost (simultaneous)</td>
<td></td>
</tr>
<tr>
<td>Energy &amp; water cost (sequential)</td>
<td></td>
</tr>
<tr>
<td>Energy &amp; water cost (simultaneous)</td>
<td></td>
</tr>
<tr>
<td>raw material cost</td>
<td></td>
</tr>
</tbody>
</table>
Targeting approach

Determine a performance index ahead of detailed design of system configuration

Examples:
- Heat-exchanger network: heating and cooling utilities
- Water network: freshwater flowrate
- Distillation sequencing: recovery ratio

Advantages:
- Avoiding combinatorial problems
- Reduces problem dimensionality to a manageable size
- Offers insights into the system performance and characteristics
Levels of model complexity

Aggregated model (LP/NLP/MILP)
- e.g. Utility level
  - Transshipment model HENS/MENS (Papoulias, Grossmann, 1983; El-Halwagi, Maniousouthakis, 1989)
  - Distillation Sequences (Papalexandri, Pistikopoulos, 1996; Caballero, Grossmann, 1999)
  - Reactor networks (Balakrishna, Biegler, 1992; Kravanja, Bedenik, Pahor, 2003)

Short-cut model (NLP/MINLP)
- e.g. Cost optimization
  - HENS: (Yee et al., 1990; Ciric and Floudas, 1991)
  - Distillation sequences: (Aggrawal, and Floudas, 1990; Yeomans and Grossmann, 1998)
  - Process flowsheets: (Kocis and Grossmann, 1989; Türkay and Grossmann, 1996; Lee et al, 2003)

Rigorous model (NLP/MINLP)
- e.g. Unit performance

Minimum utility requirement

Not all models require a great amount of details!
Simultaneous flowsheet, heat, and water integration

Path 0: Unrealistic

Path 1: Optimal solution (simultaneous optimization; MINLP)

Path 2: Can we avoid solving that MINLP but still get to the same optimal solution?
Proposed strategy – simultaneous integration

**PROCESS STRUCTURE**

**PROCESS FLOWSHEET**

**WATER TARGETING**
- Water streams
- Fresh water
- Wastewater

**HEAT TARGETING**
- Cold streams
- Hot streams
- MUC*

**WN STRUCTURE**
- Utility networks

**HEN STRUCTURE**
- Cold utility
- Hot utility

*MUC – minimum utility consumption

**PROCESS FLOWSHEET WITH HEN AND WN**
Heat Integration – Targeting strategy

- Linear formulation
- Determines the minimum heating and cooling requirement (targets)
- Difficult to solve (MINLP)
- Determines the network structure
Conventional Water Network

- Raw Water
- Freshwater
- Water-using unit 1
- Water-using unit 2
- Water-using unit 3
- Process uses
- Storm Water
- Wastewater

- Boiler Feedwater treatment
- Boiler
- Steam System
- Steam
- Boiler Blowdown
- Wastewater
- Water Loss by Evaporation
- Cooling Tower
- Cooling Tower Blowdown
- Condensate Losses

- Utility uses
- Water Loss by Evaporation

- Other Uses (Housekeeping)
- Wastewater
- Discharge

- No reuse
- No regeneration reuse

Ahmetović and Grossmann (2009)
Water Integration – Targeting strategy

Pinch

Limiting composite curve
Water supply line without water gain

C (ppm)

Δm (kg/h)

Freshwater

Process

Treatment

Discharge

Nonlinear network formulation
Valid for multiple contaminants

Linear formulation
Valid only for single-contaminant system

Carnegie Mellon
Proposed work - freshwater targeting

Relax nonlinear WN formulation into linear formulation

- **Necessary condition of optimality** (Savelski and Bagajewicz, 2003)
  
  “If a system is optimum, freshwater user processes have at least one component reaching its maximum concentration.”

- The proposed LP model predicts the EXACT target for minimum freshwater consumption of a set of water-using processes
  - Does not provide the network structure
  - Accounts for process units that have water loss / gain
  - No treatment unit included
Simultaneous optimization - example

methanol synthesis from syngas

Duran & Grossmann (1986); Turkay & Grossmann (1998)
Preliminary results – sequential vs. simultaneous comparison

<table>
<thead>
<tr>
<th></th>
<th>SEQUENTIAL</th>
<th>SIMULTANEOUS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Profit</strong> (1000 $/yr)</td>
<td>62,695</td>
<td>73,416</td>
</tr>
<tr>
<td><strong>Investment cost</strong> (1000 $)</td>
<td>1,891</td>
<td>1,174</td>
</tr>
<tr>
<td><strong>Operating costs and parameters</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>electricity (KW)</td>
<td>6.59</td>
<td>1.84</td>
</tr>
<tr>
<td>freshwater (kmol/s)</td>
<td>202.4</td>
<td>162.5</td>
</tr>
<tr>
<td>heating utility (10^9 KJ/yr)</td>
<td>0.29</td>
<td>0</td>
</tr>
<tr>
<td>cooling utility (10^9 KJ/yr)</td>
<td>67.3</td>
<td>72.7</td>
</tr>
<tr>
<td>Steam generated (10^9 KJ/yr)</td>
<td>2448</td>
<td>1965</td>
</tr>
<tr>
<td>overall conversion</td>
<td>0.23</td>
<td>0.29</td>
</tr>
<tr>
<td><strong>Material flowrate (10^6 kmol/yr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>feedstock</td>
<td>48.04</td>
<td>37.13</td>
</tr>
<tr>
<td>product</td>
<td>10.89</td>
<td>10.89</td>
</tr>
<tr>
<td>byproduct</td>
<td>9.95</td>
<td>4.41</td>
</tr>
</tbody>
</table>

Solved with BARON

17% improvement
Conclusions:

- Developed water targeting formulation for water using units excluding treatment units
- Developed targeting strategy for solving simultaneous flowsheet, heat and water integration
  - Captures tradeoffs between capital and operating costs

Future work:

- Water network
  - Non-isothermal water network
  - Include wastewater treatment units

Thank you!
Heat Integration for PC Power Plant with CO$_2$ Capture

Question: how to integrate the system to minimize power loss due to CO$_2$ capture?

NETL CCSI project
Heat Integration for PC Power Plant with CO$_2$ Capture

Steam cycle

Sorbent cycle

CO$_2$ compression
T-Q Curve (original design)

HRAT = 18°F
T-Q Curve (optimized design)

HRAT = 18°F
H1 - CO2 compression streams
H2 - stripper to absorber
H3 – condensed steam extract IP-02
H4 - stripper condenser
H5 – condensing steam extract IP-02

C1 - absorber to stripper
C2 – boiler feed water
C3 - stripper reboiler
Heat integration:

Water integration:
Ahmetović, E.; Grossmann, I. E. Global superstructure optimization for the design of integrated process water networks. AIChE Journal. 2010

Others:
Figure 3-3. Water flow schematic for a greenfield supercritical pulverized coal power plant utilizing a wet cooling tower and a wet FGD
Water network – problem statement

Given
- A set of freshwater sources with/without contaminants
- A set of water-using operations units and their inlet/outlet maximum concentration level for contaminants
- A set of wastewater treatment units
- Maximum discharge contaminant concentrations

Determine
- Optimal water network

Minimize
- Freshwater consumption
- Annual cost of water network
Water targeting – pinch method for single contaminant system

Past works
- El-Halwagi and Manousiouthakis (1989)
- Wang and Smith (1994)

Comparison with heat pinch analysis

Similarities:
- Heat pinch: heat load
  Water pinch: mass load
- Heat pinch: Heating/cooling utilities
  Water pinch: freshwater/wastewater flowrates

Differences:
- Heat pinch: transfers heat only
- Water pinch: transfers MULTIPLE contaminants
  - Solution not rigorous

Need to find other method for freshwater targeting

- Integrated water network with reuse, recycle, and regeneration schemes
- Constraints and objective functions are nonconvex
- Can determine global optimal solution with branch and bound algorithm
Given

- A set of hot process streams to be cooled
- A set of cold process streams to be heated
- Available utilities and their costs
- Heat recovery approach temperature (HRAT)

Determine

- Network configuration

Minimize

- Heating utility required
- Cooling utility required
- Investment cost of heat exchanger units
Yee and Grossmann (1990)

Objective Function
- Min capital and utility costs

Constraints
- Overall energy balance for each stream
- Energy balance for each stage
- Heating and cooling duties
- Logical constraints
- Temperatures differences
Heating and cooling target – pinch analysis

T-Q curve:
Hohmann (1971); Linnhoff and Flower (1978)

LP transshipment: Fixed F, T
Papoulias and Grossmann (1983)

Pinch location method: Variable F, T
Duran & Grossmann (1986)

$$g^{HEN} (u, Q_H, Q_C) \leq 0$$