"Water is the fastest growing market at the moment, with a size of $500 billion globally."
"If nothing is done, there will be a 40 percent gap between supply and demand by 2030."

Projected Global Water Scarcity, 2025

<table>
<thead>
<tr>
<th>Scarcity Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical water scarcity</td>
<td>More than 75% of river flows are allocated to agriculture, industries, or domestic purposes. This definition of scarcity — relating water availability to water demand — implies that dry areas are not necessarily water-scarce.</td>
</tr>
<tr>
<td>Economic water scarcity</td>
<td>Water resources are abundant relative to water use, with less than 25% of water from rivers withdrawn for human purposes, but malnutrition exists.</td>
</tr>
<tr>
<td>Little or no water scarcity</td>
<td>Abundant water resources relative to use. Less than 25% of water from rivers is withdrawn for human purposes.</td>
</tr>
<tr>
<td>Not estimated</td>
<td></td>
</tr>
</tbody>
</table>

Source: International Water Management Institute.
Conventional water network

Raw Water

Raw Water Treatment

Freshwater

Water-using unit 1

Water-using unit 2

Water-using unit 3

Process uses

Storm Water

Wastewater

No reuse

Boiler Feedwater treatment

Boiler

Steam System

Boiler Blowdown

Water Loss by Evaporation

Cooling Tower

Cooling Tower Blowdown

Water Loss by Evaporation

Other Uses (Housekeeping)

No regeneration reuse

Wastewater Treatment

Discharge
» Integrated water network with reuse, recycle, and regeneration schemes
» superstructure is formulated using a nonconvex NLP model

Karuppiah & Grossmann (2006); Ahmetovic & Grossmann (2010)
**Goal:** determine minimum freshwater consumption

\[
\begin{align*}
\text{min} \quad & Z = F_{\text{fw}} \\
\text{s.t.} \quad & F^k = \sum_{i \in \text{in}} F^i \quad \forall m \in MU, k \in m_{\text{out}} \\
& F^k C^k_{j,\text{max}} \geq \sum_{i \in \text{in}} (F^i C^i_{j,\text{max}} + F_{\text{fw}} C_{\text{fw}}) \quad \forall j, \quad \forall m \in MU, k \in m_{\text{out}} \\
& F^k = \sum_{i \in \text{out}} F^i \quad \forall s \in SU, k \in s_{\text{in}} \\
& C^k_{j} = C^i_{j} \quad \forall j, \quad \forall s \in SU, \quad \forall i \in s_{\text{out}}, k \in s_{\text{in}} \\
& F^k = P^p_{\text{in}} \quad \forall p \in PU, k \in p_{\text{out}} \\
& F^i = P^p_{\text{out}} \quad \forall p \in PU, i \in p_{\text{in}} \\
& F^i C^i_{j} + L^p_{j} = F^k C^k_{j} \quad \forall j, \forall p \in PU, i \in p_{\text{in}}, k \in p_{\text{out}} \\
\end{align*}
\]

**(LP)**

**Mixer mass balances**

**Splitters mass balances**

**Process unit mass balances**

**This formulation provides target for a network consists of a set of water-using process units using linear constraints**

Assumption: for some contaminant \(j\) that reaches its concentration upper bound at a given unit, it also reaches the upper bound at all other process units from which reuse streams have non-zero flowrate.
Heat-integrated WN reported in the literature

Use heat and water network formulation (MINLP model) to obtain network structure

749 continuous variables
115 binary variables

Bogataj & Bagajewicz (2007)
Extension: heat-integrated water network

Objective fcn

\[ \min \phi = c_H Q_H + c_C Q_C + c_{fw} F_{fw} \]

Water targeting (LP)

\[ F^k = \sum_{i=m_{\text{in}}}^{i=m_{\text{out}}} F^i \quad \forall m \in MU, k \in m_{\text{out}} \]

\[ F^k C_{j,\text{max}}^{k,\text{max}} \geq \sum_{i=m_{\text{in}}}^{i=m_{\text{out}}} (F^i C_{j,\text{max}}^{i,\text{max}} + F^i_{fw} C_{fw}) \quad \forall j, \forall m \in MU, k \in m_{\text{out}} \]

\[ F^k = \sum_{i=s_{\text{out}}}^{i=s_{\text{in}}} F^i \quad \forall s \in SU, k \in s_{\text{in}} \]

\[ C_{j}^{\text{in}} \quad \forall j, \forall s \in SU, \forall i \in s_{\text{out}}, k \in s_{\text{in}} \]

\[ F^k = P_{in}^p \quad \forall p \in PU, k \in p_{\text{out}} \]

\[ F^i = P_{out}^p \quad \forall p \in PU, i \in p_{\text{in}} \]

\[ F^i C_{j}^i + L^p_j = F^k C_{j}^k \quad \forall j, \forall p \in PU, i \in p_{\text{in}}, k \in p_{\text{out}} \]

Heat targeting (LP)

\[ Q_H \geq \sum_{js \in \cup s_{\text{out}}} f_{js} c_{js} \max \{0, t_{js}^{\text{out}} - (T^p - \Delta T_m)\} \]

\[ - \max \{0, t_{js}^{\text{in}} - (T^p - \Delta T_m)\} \]

\[ - \sum_{is \in H \cup s_{\text{out}}} F_{is} C_{is} \max \{0, T_{is}^{\text{in}} - T^p\} \]

\[ Q_C = Q_H + \sum_{is \in H \cup s_{\text{out}}} F_{is} C_{is} (T_{is}^{\text{in}} - T_{is}^{\text{out}}) \]

\[ - \sum_{js \in \cup s_{\text{out}}} f_{js} c_{js} (T_{js}^{\text{out}} - t_{js}^{\text{in}}) \]

\[ T^p = T_{is}^{\text{in}} \quad \forall p = is \in H \cup s_{\text{out}} \quad \forall s \in SU \]

\[ T^p = (t_{js}^{\text{in}} + \Delta T_m) \quad \forall p = is \in C \cup s_{\text{out}} \quad \forall s \in SU \]

All black streams can participate in heat integration.
Revisit: heat-integrated water network utility targeting

Use heat and water targeting formulation:

Minimum heating utility: 3767 kW
Minimum cooling utility: No cooling utility required
Minimum freshwater consumption: 324 ton/h

Same result as network approach
Simultaneous optimization strategy

\[
\min. \quad \phi = F(x,u,v) + \sum_{i \in H U} c_H^i Q_H^i + \sum_{j \in C U} c_C^j Q_C^j + c_{fw} F_{fw}
\]

s.t. \quad h(x,u,v) = 0
\quad g^P(x,u,v) \leq 0
\quad g^{HEN}(u,Q_H,Q_C) \leq 0
\quad g^{WN}(v,F_{fw}) \leq 0
\quad x \in X, \quad u \in U, \quad v \in V
Simultaneous optimization: methanol synthesis from syngas

Duran & Grossmann (1987)
Sequential vs. simultaneous result comparison

<table>
<thead>
<tr>
<th></th>
<th>SEQUENTIAL</th>
<th>SIMULTANEOUS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Profit (1000 $/yr)</td>
<td>62,695</td>
<td>73,416</td>
</tr>
<tr>
<td>Investment cost (1000 $)</td>
<td>1,891</td>
<td>1,174</td>
</tr>
<tr>
<td>Operating parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>electricity (KW)</td>
<td>6.59</td>
<td>1.84</td>
</tr>
<tr>
<td>freshwater (kg/s)</td>
<td>36.43</td>
<td>29.25</td>
</tr>
<tr>
<td>heating utility (10^9 KJ/yr)</td>
<td>0.293</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>0.68</td>
<td>0.88</td>
</tr>
<tr>
<td>Material flowrate (10^6 kmol/yr)</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>
</tbody>
</table>

Solved with BARON 9

17% improvement
Example 2: Bioethanol production

Water network superstructure

### Components
- **PU 1**, **PU 2**, **PU 3**
- **Boiler loop**
- **Cooling cycle**
- **Reverse osmosis**
- **Anaerobic tank**
- **Screens**

### Flowchart
- **Freshwater**
- **Warmwater inlet**
- **Coldwater outlet**
- **Cooling Tower**
- **Condensate**
- **Steam**
- **Steam loss**
- **Feedwater**
- **boiler**
- **blowdown**

### Table

<table>
<thead>
<tr>
<th>$C_{j_{in,\text{max}}}^{\text{ppm}}$</th>
<th>TSS</th>
<th>TDS</th>
<th>ORG</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boiler loop</td>
<td>2</td>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td>Cooling cycle</td>
<td>10</td>
<td>500</td>
<td>10</td>
</tr>
<tr>
<td>$1-\beta_j^t$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Screens</td>
<td>95%</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Reverse osmosis</td>
<td>0</td>
<td>90%</td>
<td>0</td>
</tr>
<tr>
<td>Anaerobic tank</td>
<td>0</td>
<td>0</td>
<td>99%</td>
</tr>
</tbody>
</table>
**Multieffect columns**

**Formulation**
- Dew point equation - condenser temperature
- Bubble point equation - feed and reboiler temperature
- Fenske equation - # of trays
- Watson's equation – heat of vaporization
- Mass balance
- Energy balance

**Assumptions**
- Constant relative volatility
- Ideal solution
- Water is the only component contributing to heat of vaporization
- Temperature change due to pumps is negligible
## Result

<table>
<thead>
<tr>
<th></th>
<th>No integration</th>
<th>Sequential single column</th>
<th>Sequential w/ multieffect</th>
<th>Simultaneous w/ Multieffect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost (MM$/yr)</td>
<td>14.91</td>
<td>11.77</td>
<td>8.57</td>
<td>8.57</td>
</tr>
<tr>
<td>Cooling water use (kg/s)</td>
<td>2895.6</td>
<td>1998.3</td>
<td>1127.3</td>
<td>1124.8</td>
</tr>
<tr>
<td>Freshwater use (kg/s)</td>
<td>40.8</td>
<td>127.6</td>
<td>90.0</td>
<td>90.0</td>
</tr>
<tr>
<td>Steam use (kg/s)</td>
<td>35.1</td>
<td>28.3</td>
<td>21.2</td>
<td>21.3</td>
</tr>
<tr>
<td>CPU(s)</td>
<td>387</td>
<td>387</td>
<td>470</td>
<td>563</td>
</tr>
<tr>
<td># eqns</td>
<td>2,232</td>
<td>2,232</td>
<td>3,213</td>
<td>5,221</td>
</tr>
<tr>
<td># cont var</td>
<td>2,921</td>
<td>2,921</td>
<td>3,914</td>
<td>5,392</td>
</tr>
</tbody>
</table>

NLP solver: CONOPT 3  
MINLP solver: BARON 9  
GAMS 23.7  

Even though the objective function did not improve using simultaneous method, we can see that the solution time did not increase drastically.

Reboiler duty reduced by ~36% by with multieffect column
Utility integration – power, water, & heat
**Problem statement**

**Objective function**

\[
\phi = \sum_{st} c_b^{fix} Y_b^{st} + \sum_{st} c_b^{var} F_b^{st} + \sum_{st} \sum_{d} c_{tur}^{fix} Y_d^{st} + \sum_{d} c_{ext}^{fix} Y_d^{ext} + \sum_{st} \sum_{d} c_{tur}^{var} W_d^{st} + \sum_{s} c_s F_s + c_{fw} F_{fw}
\]

- Boiler cost
- Turbine cost
- Flowsheet stream cost
- Freshwater cost

**HEN**
- 2 hot streams/2 cold streams
- Inlet and outlet temperature can vary within +/- 10 K
- Heat capacity flowrate can vary within 20%
- Two streams have assigned costs
- Hot utility - HP, MP, and LP steam
- Cold utility - cooling water

**Utility system**
- Existence of boiler
- Existence of turbine
- Back pressure turbine
- Extraction turbine (additional cost $20,000)
- Flowsheet power demand (7500kW)
- 70% condensate return

**Multiple hot utility targeting**
(Duran & Grossmann)
- Heating utilities targets
- Cooling utility target

**Utility system**
- Logical constraints
- Demand constraints
- Power balances
- Mass balances

**Water network**
- Mass balances
- Power demand constraint

- HP boiler has more stringent feedwater requirement
- HP boiler/MP boiler have different blowdown rates
- RO consumes electricity
- Raw water needs treatment
- TSS, TDS, GAS present in freshwater
- Discharge limit imposed
## Result

<table>
<thead>
<tr>
<th></th>
<th>Sequential</th>
<th>Simultaneous</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cost (1000 $ / yr)</strong></td>
<td>884.2</td>
<td>641.5</td>
</tr>
<tr>
<td><strong>Utility</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP boiler flowrate (kg/s)</td>
<td>Yes</td>
<td>17.66</td>
</tr>
<tr>
<td>MP boiler flowrate (kg/s)</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Power demand external (kW)</td>
<td>HP → LP</td>
<td>7500</td>
</tr>
<tr>
<td>Reverse osmosis power demand (kW)</td>
<td>MP → LP</td>
<td>62.0</td>
</tr>
<tr>
<td><strong>HEN Utility (kW)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cooling</td>
<td>1463.8</td>
<td>751.1</td>
</tr>
<tr>
<td>HP steam</td>
<td>3820.2</td>
<td>5727.2</td>
</tr>
<tr>
<td>MP steam</td>
<td>13628.2</td>
<td>21065.7</td>
</tr>
<tr>
<td>LP steam</td>
<td>4743.4</td>
<td>19110.2</td>
</tr>
<tr>
<td>Fcp,H1 (kW/K)</td>
<td>48</td>
<td>32</td>
</tr>
<tr>
<td>Fcp,C2 (kW/K)</td>
<td>144</td>
<td>216</td>
</tr>
<tr>
<td><strong>WN flowrate (kg/s)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Freshwater</td>
<td>7.26</td>
<td>6.47</td>
</tr>
<tr>
<td>Sand filter</td>
<td>7.2</td>
<td>6.4</td>
</tr>
<tr>
<td>Reverse osmosis</td>
<td>5.6</td>
<td>5.8</td>
</tr>
<tr>
<td>Scrubber</td>
<td>2.4</td>
<td>1.2</td>
</tr>
</tbody>
</table>
Conclusion

» Developed LP formulations for targeting minimum freshwater consumption for a set of water-using process units under a specific condition
» Extended the water targeting formulation to nonisothermal water network
» Targeting method can be used to improve objective function and computational effort under the simultaneous approach for flowsheet optimization
» The interaction among power use, heat use, and water use can be exploited to achieve better flowsheet design

Thank you!