• Application of Mathematical programming in process integration applications

– Goals
  • Show how optimization can help in solving the combinatorial nature of the decision space

• Utility system integration
• Heat exchanger network design
  – Heat load distribution
  – Heat exchanger network design
  – Water networks

Integration of the energy conversion system

Energy conversion units with unknown flowrates

Technology w with nominal flow

<table>
<thead>
<tr>
<th>Hot/cold streams</th>
<th>Mechanical power/electricity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{in\ w,i}$, $P_{in\ w,i}$, $m_{w,i}$, $x_{w,i}$</td>
<td>$e_w$</td>
</tr>
<tr>
<td>$q_w = m_{w,i}(h_{w,i}^{in} - h_{w,i}^{out})$</td>
<td>Costs</td>
</tr>
<tr>
<td>$T_{out\ w,i}$, $P_{out\ w,i}$, $m_{w,i}$, $x_{w,i}$</td>
<td>$C1_w$, $C2_w$, $C11_w$, $C12_w$</td>
</tr>
</tbody>
</table>

Decision variables

Level of usage of w

$\bar{f}_w$

Buy/use technology w ?

$y_w$
Mixed Integer Linear Programming (MILP) formulation

Objective function
\[
\min_{R_r, y_w, f_w, E^+, E^-} \left( \sum_{w=1}^{n_w} C^2 w f_w + C_{el^+} E^+ - C_{el^-} E^- \right) * t
\]

Decision variables
\[
+ \sum_{w=1}^{n_w} C^1 w y_w + \frac{1}{\tau} \left( \sum_{w=1}^{n_w} (C^1 I_w y_w + C^2 f_w) \right)
\]

Constraints
Subject to: Heat cascade constraints

Equality
\[
\sum_{w=1}^{n_w} f_w q_{w,r} + \sum_{s=1}^{n_s} Q_{s,r} + R_{r+1} - R_r = 0 \quad \forall r = 1, \ldots, n_r
\]

Feasibility
\[
R_r \geq 0 \quad \forall r = 1, \ldots, n_r; \quad R_{n_r+1} = 0; \quad R_1 = 0 \quad E^+ \geq 0; \quad E^- \geq 0
\]

Inequality
Electricity consumption
\[
\sum_{w=1}^{n_w} f_w e_w + E^+ - E_c \geq 0
\]

Electricity production
\[
\sum_{w=1}^{n_w} f_w e_w + E^+ - E_c - E^- = 0
\]

Energy conversion Technology selection
\[
\text{Integer (yes/no) decision variables } \quad y_w \in \{0, 1\}
\]

Solution

- Balanced composite curve
- all the flows are known => design the heat exchanger network

Multiple pinch points (utility pinch points) 
optimal use of the cheapest utility

T (K)

Q (kW)
Application of mathematical programming

- Calculating heat exchanger network design
  - given a list of all the hot and cold streams
  - given the DTmin and the pinch(s) location
  - Calculate:
    - the heat exchanger network structure
    - The heat loads, temperature and flows in the network
    - The heat exchange area of the heat exchangers
    - The total cost of the heat exchanger network
    - The optimal value of DTmin for each HEN

HEN synthesis

Draw backs of the Pinch Design Method
- multiple solutions
- combinatorial problem
- sequential

Use of mathematical programming:

Heat load distribution:
- which streams exchange heat
- How much
- minimize the number of connections
- satisfies DTmin and MER
Heat load distribution

**Hot stream i**

Hot stream i in temperature interval k

\[ \sum_{j=1}^{nc} Q_{ikj} = Q_{ik} \quad \forall i = 1,...,nh; \forall k = k_1,...,k_2 \]

**Cold streams j in and above temperature interval k**

\[ \sum_{j=1}^{nc} \sum_{r=k}^{k_2} Q_{rj} - \sum_{r=k}^{k_2} Q_{jr} \leq 0 \quad \forall j = 1,...,nc; \forall k = k_1,...,k_2 \]

**Connection between i and j (integer variable)**

\[ \sum_{r=k}^{k_2} Q_{ij} - y_{ij} Q_{\text{max}ij} \leq 0 \quad \forall j = 1,...,nc; \forall i = 1,...,nh \]

---

**MILP formulation**

Minimize the number of connections

\[ \min \sum_{j=1}^{nc} \sum_{f=1}^{nh} y_{ij} \quad y_{ij} \in \{0,1\} \]

\[ \sum_{j=1}^{nc} Q_{ij} = Q_{ik} \quad \forall i = 1,...,nh; \forall k = k_1,...,k_2 \]

\[ \sum_{j=1}^{nc} \sum_{r=k}^{k_2} Q_{rj} - \sum_{r=k}^{k_2} Q_{jr} \leq 0 \quad \forall j = 1,...,nc; \forall k = k_1,...,k_2 \]

\[ \sum_{r=k}^{k_2} Q_{ij} - y_{ij} Q_{\text{max}ij} \leq 0 \quad \forall j = 1,...,nc; \forall i = 1,...,nh \]
Multiple solutions

- Add heuristic rules
  - favor the connexion with utility streams
  - favor close connexion
  - favor connexion in closer sub-systems
- A heuristic rule is applied only if it does not penalize the minimum number of solution target

Introduce heuristic rules in MILP programs

- The weight of priority rule $k$ is given by:
  - the number of possible connexion satisfying rule $k$
    \[
    P_k = \sum_{j=1}^{n_c} \sum_{i=1}^{n_h} (p_{kij})
    \]
  - an improved objective function:
    \[
    \min_{y_{ij}, Q_{ikj}} \quad NT = \sum_{j=1}^{n_c} \sum_{i=1}^{n_h} \left( \prod_{k=1}^{p_{ij}-1} (P_k + 1) y_{ij} \right)
    \]
    \[
    \prod_{k=1}^{r} (P_k + 1) > \sum_{i=1}^{n_h} \sum_{j=1}^{n_c} P_{rij}
    \]
Improving the speed of convergence

Generating multiple solutions

• Integer cut constraint
  – assuming that we know k solutions
  – problem k + 1 is defined by adding to the previous MILP problem the integer cut constraint

\[
\text{Problem}^{k+1} = \text{Problem}^k + \\
\sum_{p=1}^{n_p} \sum_{c=1}^{n_c} (2 \cdot y_{p,c}^k - 1) \cdot y_{p,c}^k \leq \sum_{p=1}^{n_p} \sum_{c=1}^{n_c} y_{p,c}^k
\]
The synthesis method

Calculate the heat load distribution for each section

Multiple solutions using integer cuts
Heuristic rules or user

\[ \sum_{p=1}^{n_p} \sum_{c=1}^{n_c} (2 \cdot y_{p,c}^k - 1) \cdot y_{p,c} \leq \sum_{p=1}^{n_p} \sum_{c=1}^{n_c} y_{p,c}^k \]

-> screening and choice of the appropriate solution

Define the HEN structure
Apply feasibility rules and heuristics
Splits and serial exchanges
Optimize the HEN
Total cost criteria
no DTmin nor MER fixed

Calculation of the optimal HEX area

NLP (Non Linear Programming) optimisation problem

\[ \text{Minimise} = \left( \sum_{u=1}^{N_u} c_u^{+} \cdot \dot{M}_u \right) \cdot \text{time}_{\text{year}} + \frac{1}{T} \sum_{e:x=1}^{N_{ex}} \left( a_{ex} (A_{ex})^{b_{ex}} \right) \]

Constraints
Heat and mass balances
Rating equations
Specifications:

\[ F(X) = 0 \]

Bounds and limits
\[ G(X) \leq 0 \]

\[ X : \text{State variables: pressure, temperature, area, heat exchanged, ...} \]
Heat exchanger network superstructure

- Superstructure embedding different solution

Mixed Integer Non Linear Programming (MINLP) problem

\[
\begin{align*}
\min_{A_h, y_h, \dot{M}_i, y_j} & \sum_{u=1}^{n_u} (y_u C_{1u} + \dot{M}_u C_{u}) + \frac{1}{\tau} \sum_{h=1}^{n_{hx}} (a_h y_h + b_h (A_h)^{c_h}) \\
st. & F(A, y, \dot{M}, T) = 0 \\
& G(A, y, \dot{M}, T) = 0 \\
& A_h^{\min} y_h \leq A_h \leq A_h^{\max} y_h \quad \forall h = 1 \ldots n_{hx} \\
& \dot{M}_i^{\min} y_i \leq \dot{M}_i \leq \dot{M}_i^{\max} y_i \quad \forall i = 1 \ldots n_s
\end{align*}
\]
MINLP formulation extended

\[ \text{Minimise} = \left( \sum_{i=1}^{N_{\text{c}}} c_i^e M_i \right) \text{time}_{\text{year}} + \left( \frac{(i+1)^{\alpha_{\text{c}}} - 1}{\alpha_{\text{c}}} \right) \sum_{i=1}^{N_{\text{c}}} (a_{i,e} A_{i,e})^{\beta_{\text{c}}} \]  

Subject to heat exchanger models (\( \forall e = 1, \ldots, N_{\text{ex}} \))

\[ Q_{\text{ex}} = M_{\text{hot}} \rho_{\text{hot}} (T_{\text{hot,in}} - T_{\text{hot,ex}}) = M_{\text{cold}} \rho_{\text{cold}} (T_{\text{cold,in}} - T_{\text{cold,ex}}) \]
\[ Q_{\text{ex}} = U_{\text{ex}} A_{\text{ex}} \left( \frac{(T_{\text{hot,in}} - T_{\text{cold,ex}})}{(T_{\text{hot,ex}} - T_{\text{cold,in}})} \right) \]

\[ \frac{1}{U_{\text{ex}}} = \frac{1}{\alpha_{\text{cold}}} + \frac{1}{h_{\text{hot}}} \]  

Mixers and splitters models

\[ H(T_i, M_i) = 0 \]  

Heat exchanger network specifications

\[ T_i = T_{i,\text{spec}} \quad M_i = M_{i,\text{spec}} \]  

Inequality constraints

\[ \Delta T_{\text{min}} \geq 0 \]
\[ G(T_i, M_i) \geq 0 \]
\[ y_i M_{\text{min}} \leq M_i \leq y_i M_{\text{max}} \quad i = 1, \ldots, N_{\text{streams}} \]
\[ y_{\text{ex}} A_{\text{min}} \leq A_{\text{ex}} \leq y_{\text{ex}} A_{\text{max}} \quad ex = 1, \ldots, N_{\text{ex}} \]
\[ y_i, y_{\text{ex}} \in \{0, 1\} \]

\( y_i \) an integer representing the existence of stream \( i \)
\( y_{\text{ex}} \) an integer variable representing the existence of exchanger \( ex \).
with
\( N_{\text{ex}} \) the number of utility streams
\( N_{\text{ex}} \) the total number of streams including the utility streams

MINLP : outer approximation

- **Decomposition theorem**
  - Partition variables in 2 sets
    - complicating set (integer)
    - continuous variables
  - Solve 2 problems
    - NLP with fixed integer (lower bound)
    - MILP : outer-approximate the objective function (upper bound)
  - Lower = upper => convergence
    - integer cut to avoid looping
  - **Problems :**
    - NLP converge ?
    - Calculation time ?
    - Initial set feasible ?
    - Derivatives for MILP
      - outer approximation
MINLP sub-problem

- **HRAT**: Heat recovery approach temperature
  - target
- **EMAT**: exchanger Minimum Approach Temperature

\[
\begin{align*}
\min_{A_h, y_h, \dot{M}_i, y_j} & \quad \sum_{u=1}^{n_u} (y_u C_{1u} + \dot{M}_u c_u) + \frac{1}{\tau} \sum_{h=1}^{n_{hx}} (a_h y_h + b_h (A_h)^{c_h}) \\
\text{st.} & \quad F(A, y, \dot{M}, T) = 0 \\
& \quad G(A, y, \dot{M}, T) = 0 \\
& \quad \Delta T_{i,hx} \geq EMAT \quad \forall i = 1, 2 \quad hx = 1, \ldots, n_{hx} \\
& \quad \dot{M}_u = \dot{M}_{u, \text{target}} \quad \forall u = 1 \ldots n_u \\
& \quad A_{h}^{\text{min}} y_h \leq A_h \leq A_{h}^{\text{max}} y_h \quad \forall h = 1 \ldots n_{hx} \\
& \quad \dot{M}_{i}^{\text{min}} y_i \leq \dot{M}_i \leq \dot{M}_{i}^{\text{max}} y_i \quad \forall i = 1 \ldots n_s
\end{align*}
\]

Heat exchanger reuse

If required $A \leq A$ available

=> use a by-pass

=> or accept lower DTmin

\[
A_i \leq \sum_{e=1}^{n_e} y_{e,i} A_e
\]

\[
\sum_{i=1}^{n_i} y_{e,i} \leq 1 \quad \forall e \in \{1..n_e\}
\]
**MINLP problem**

\[
\min C_{\text{Obj}} = \sum_{u=1}^{u} (y_{ui} \cdot C_{ui} + d_{i} \cdot C_{2ui}) \\
+ \sum_{i=1}^{n_{\text{en}}} (y_{ei} \cdot a_{el} + b_{ej} \cdot \Theta_{el} \cdot C_{ej}) \\
+ \sum_{i=1}^{n_{\text{eq}}} (y_{ej} \cdot a_{el} + b_{ej} \cdot (d_{ej} \cdot d_{ej}) \cdot C_{ej})
\]

subject to

- \( F_1(x,y) = 0 \) balance and rating equations
- \( F_2(x,y) = 0 \) Specification equations
- \( G(x,y) = 0 \) the qualities equations

\( y \in (0,1) \) Integer variables representing the YES/NO decisions

where

- \( y_{ui} \) Integer variable associated to the use of the utility;
- \( a_{ul}, C_{2ul} \) Flowrate of the utility;
- \( C_{ui} \) cost coefficients of the utility;
- \( \phi \) rate of return of the investment;
- \( n_{\text{en}} \) number of new heat exchangers in the network;
- \( n_{\text{eq}} \) Actual number of heat exchangers in the network;
- \( A_{i} \) Area of the new heat exchanger;
- \( a_{el}, b_{ej} \) cost coefficients of the new heat exchanger;
- \( d_{ej} \) Integer variable associated to the area added to the existing heat exchanger;
- \( d_{ej} \) area added to the existing heat exchanger;
- \( a_{ej} \) cost coefficients for the area added to the heat exchanger.

The new constraints added for each the existing heat exchangers in the retrofit problem formulation are:

\[
A_{ej} = A_{e0} + d_{ej} \cdot a_{ej} \quad (45.1)
\]

\[
y_{ej} \cdot a_{ej} + b_{ej} \cdot d_{ej} \cdot C_{ej} \quad (45.2)
\]

\[
0 \leq y_{ej} \leq 1 \quad (45.3)
\]

where

- \( A_{ej} \) Area fraction used from the existing exchanger;
- \( A_{e0} \) Actual area of the existing exchanger;
- \( A_{ej} \) New area of the existing heat exchanger;
- \( d_{ej} \) Area added to the heat exchanger;
- \( a_{ej} \) Effective area of the exchanger, calculated by the rating equation (46).

\[
a_{ej} = \frac{a_{el}}{\eta_{ej}} \quad (46)
\]

**Conclusions**

- **Mathematical programming formulation**
  - allows to add constraints
  - allows to handle the combinatorial nature of the problem
  - allows to help in decision
  - allows to systematically generate multiple solutions
  - algorithm to help adding heuristics and improve convergence properties
  - Non linear programming are more difficult to solve.