Reflections on Chris Floudas and the Heat Exchanger Network Synthesis Problem

Dr. Amy Ciric
May 6, 2017
Hot Process Streams Release Heat

Hot Utilities Supply Additional Heat

Heat Exchanger Network

Cold Process Streams Absorb Heat

Cold Utilities Absorb Extra Heat

A set of $H$ hot streams with flow rates $m_{hi} (i = 1,\ldots,H)$ have to be cooled from supply temperatures $T_{hsi} (i = 1,\ldots,H)$ to target temperatures $T_{hti} (i = 1,\ldots,H)$. A set of $C$ cold streams with flow rates $m_{cj} (j = 1,\ldots,C)$ have to be cooled from supply temperatures $T_{csj} (j = 1,\ldots,C)$ to target temperatures $T_{ctj} (j = 1,\ldots,C)$. It is required to determine the structure of the heat exchanger network to achieve this objective at minimum total cost.

- Masso and Rudd (1969)
Early Work on Heat Exchanger Network Synthesis

Undergraduate Class of 1970

Row 1: Kostin, Ollis, Johnson, Lapidus, Toner, Weed, Gillham.
Row 2: Klang, Klurfeld, Penna, Weaver, Hallock, Birger, Brighthouse, Jannarone, Schabel.
Second Law Limitations to Heat Integration

Pinch Point

\[ Q_s = 220 \text{ kW} \]
\[ R_1 = 0 \]
\[ R_2 = 160 \text{ kW} \]
\[ R_3 = 350 \text{ kW} \]
\[ R_4 = 350 \text{ kW} \]
\[ Q_W = 350 \text{ kW} \]
Chris’s First Publication:


• Identified pinch point and minimum utility consumption by automating the Papoulias and Grossmann’s (1983) LP transshipment model.

• Identified stream matches and heat duties by automating the Papoulias and Grossmann’s (1983) MILP transshipment model.

• Identified the network structure by solving an NLP based on Chris’s superstructure.

• This was the first automated method for generating optimum heat exchanger networks.
Superstructure Optimization
Construct a superstructure with many possible designs embedded within it..

Floudas, Ciric and Grosssmann, 1986
Construct a superstructure with many possible designs embedded within it..

Floudas, Ciric and Grosssmann, 1986
Construct a superstructure with many possible designs embedded within it..

Parallel

Floudas, Ciric and Grosssmann, 1986
Construct a superstructure with many possible designs embedded within it..

Floudas, Ciric and Grosssmann, 1986
Write a model of the superstructure..

\[ \sum_{j \in R_i} f_{kj}^{l,i} = F^l \quad \text{for } k \in \text{HCT} \]

\[ f_j^{l,i} + \sum_{k \in S_{ij}} f_{kj}^{R,l} - f_{j}^{E,l} = 0 \quad \text{for } j \in R_i, k \in \text{HCT} \]

\[ f_j^{O,l} + \sum_{k \in S_{ij}} f_{kj}^{R,l} - f_{j}^{E,l} = 0 \quad \text{for } j \in R_i, k \in \text{HCT} \]

\[ \tau_i f_j^{E,l} + \sum_{k \in S_{ij}} \tau^{O,l}_{k} f_{kj}^{R,l} - \tau^{l,i} f_{j}^{E,l} = 0 \quad \text{for } j \in R_i, k \in \text{HCT} \]

\[ f_j^{E,l} (t_j^{l,i} - t_j^{O,i}) = Q_{ij} \quad \text{for } i \in M \]

\[ f_i^{E,l} (t_i^{l,i} - t_i^{O,i}) = Q_{ij} \quad \text{for } i \in M \]

\[ \Delta T_{1ij} = t_i^{l,i} - t_i^{O,i} \quad \text{for } i \in M \]

\[ \Delta T_{2ij} = t_j^{O,i} - t_j^{l,i} \quad \text{for } i \in M \]

\[ \Delta T_{1ij} \geq \Delta T_{\text{min}} \quad \text{for } i \in M \]

\[ \Delta T_{2ij} \geq \Delta T_{\text{min}} \quad \text{for } i \in M \]

\[ \text{LMTD}_{ij} = \frac{2}{3} (\Delta T_{1ij} \cdot \Delta T_{2ij})^{1/2} + \frac{\Delta T_{1ij} + \Delta T_{2ij}}{2} \quad \text{for } i \in M \]
..and use that model as constraints in an optimization problem.

\[
\begin{align*}
\text{min} & \quad \sum_{ij \in M} c \left( \frac{Q_{ij}}{U_{ij} LMTD_{ij}} \right)^{0.6} \\
\text{Subject to} & \quad \sum_{j \in R_i} f_{ij}^{l,i} = F^i \\
& \quad f_{ij}^{l,i} + \sum_{j \in S_{ij}} f_{jk}^{B,i} - f_{ij}^{E,i} = 0 \\
& \quad f_{ij}^{O,i} + \sum_{j \in S_{ij}} f_{jk}^{B,i} - f_{ij}^{E,i} = 0 \\
& \quad T_{ij}^{l,i} + \sum_{j \in S_{ij}} t_{ij}^{O,i} f_{ij}^{B,i} - t_{ij}^{l,i} f_{ij}^{E,i} = 0 \\
& \quad f_{ij}^{E,i} (t_{ij}^{l,i} - t_{ij}^{O,i}) = Q_{ij} \\
& \quad f_{ij}^{E,i} (t_{ij}^{l,i} - t_{ij}^{E,i}) = Q_{ij} \\
& \quad \Delta T_{1ij} = t_{ij}^{l,i} - t_{ij}^{O,i} \\
& \quad \Delta T_{2ij} = t_{ij}^{O,i} - t_{ij}^{l,i} \\
& \quad \Delta T_{1ij} \geq \Delta T_{\text{min}} \\
& \quad \Delta T_{2ij} \geq \Delta T_{\text{min}} \\
& \quad LMTD_{ij} = \frac{2}{3} \left( \Delta T_{1ij} \cdot \Delta T_{2ij} \right)^{1/2} + \frac{\Delta T_{1ij} + \Delta T_{2ij}}{2}
\end{align*}
\]
.. Solving this optimization problem extracts the best design from the superstructure.

Cost: $25,163
.. Solving this optimization problem extracts the best design from the superstructure.

Cost: $20,427
.. Solving this optimization problem extracts the best design from the superstructure.

Cost: $19,850
Solving this optimization problem extracts the best design from the superstructure.

Cost: $18,693
Ideally, all good solutions are in the search space

Feasible region / search space

infeasible
But hidden constraints can eliminate some good options.
Heuristics and decomposition approaches artificially limit the search space.

• Constant minimum temperature approach
• No matches across the pinch
• Minimize the number of matches before designing the network
• etc
Strategy to reduce the number of artificial constraints:

Add yes/no decisions to the superstructure model

Mixed Integer Nonlinear Programming Problems (MINLP)
Chris’s early work at Princeton applied this approach to many process synthesis problems:

• Distillation Sequences
• Reactor Networks
• Heat Exchanger Networks
• Power Cycles
Heat Exchanger Network Synthesis and Global Optimization
Energy balances at the mixing points and across the heat exchangers have bilinear \((x \cdot y)\) terms:

\[
T^i f^l_{j,i} + \sum_{k \in S_{ij}} t^o_{k,j} f^b_{j,k} - t^l_{j,i} f^e_{j,i} = 0
\]

\[
f^e_{j,i} (t^l_{j,i} - t^o_{j,i}) = Q_{ij}
\]

\[
f^e_{i,j} (t^o_{i,j} - t^l_{i,j}) = Q_{ij}
\]
..these terms are *nonconvex* and create a *nonconvex search space*:
Which may lead to more than one locally optimal solution.

\[ f(x) = 10 \]
\[ f(x) = 5 \]
\[ f(x) = 8 \]
\[ f(x) = 3 \]
Heat Exchanger Network Synthesis and Global Optimization

But if the temperature or flow rate variables are held constant, the equations become linear:

\[ T^i f^l_{j,i} + \sum_{k \in S_{ij}} t^0_{k,j} f^{B,i}_{j,k} - t^l_{j,i} f^{E,i}_{j} = 0 \]

\[ f^{E,i}_{j} (t^l_{j,i} - t^0_{j,i}) = Q_{ij} \]

\[ f^{E,j}_{i} (t^0_{i,j} - t^l_{i,j}) = Q_{ij} \]
Chris’s first paper on global optimization exploited this structure of the energy balances

Floudas, Aggarwal and Ciric (1989):

- Solve the superstructure optimization problem using Generalized Benders Decomposition
- Choose the flow rate-heat capacity variables ($f$) as the complicating variables

**Convex master problem provides**
- Values of $f$
- Lower bound on the global optimum

**Convex primal problem provides**
- Values of $t$
- Upper bound on the global optimum

Successive iterations between the master and primal problems converge to the global optimum
Personal Reflections
Consider the general optimization problem after stages 1 and 2 of the proposed approach, that is, after the identification of nonconvexities and partitioning of the variable and constraint sets. This is problem \( P \) as shown in the last section. If the first two stages are performed in such a manner that problem \( P \) satisfies the following criteria:

(a) \( f(x, y) \) is convex in \( x \) for any fixed \( y \) and convex in \( y \) for any fixed \( x \);
(b) \( g_i(x, y) \) is convex in \( x \) for any fixed \( y \) and convex in \( y \) for any fixed \( x \);
(c) \( h_i(x, y) \) is linear in \( x \) for any fixed \( y \) and linear in \( y \) for any fixed \( x \);
(d) \( g_2(y) \) is convex in \( y \);
(c) \( h_2(y) \) is linear in \( y \);

then it will be shown that \( (P) \) has the following three properties. Using the proposed decomposition approach and selecting \( y \) as the complicating variables:

**Property 1**—The solution of each primal subproblem is a global solution of that problem.

**Property 2**—The solution of each master subproblem is a global solution of that problem.

**Property 3**—For every value of \( k \in K^{x_{*}} \), and for every element \( y^{*} \) in the set \( y^{M*} \):

\[
1^{*}(y^{*}) \leq f(x^{*}, y^{*})
\]
Thank you!

1959-2016