MINLP model for work and heat exchange networks synthesis considering unclassified streams

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Abstract
The optimal synthesis of work and heat exchange networks (WHENs) is deeply important to achieve simultaneously high energy efficiency and low costs in chemical processes via work and heat integration of process streams. This paper presents an efficient MINLP model for optimal WHENs synthesis derived from a superstructure that considers unclassified streams. The derived model is solved using BARON global optimization solver. The superstructure considers multi-staged heat integration with isothermal mixing, temperature adjustment with hot or cold utility, and work exchange network for streams that are not classified a priori. The leading advantage of the present optimization model is the capability of defining the temperature and pressure route, i.e. heating up, cooling down, expanding, or compressing, of a process stream entirely during optimization while still being eligible for global optimization. The present approach is tested to a small-scale WHEN problem and the result surpassed the ones from the literature.

Keywords: Work and heat exchange networks, Mixed-integer nonlinear programming, Unclassified streams, Process synthesis, Global optimization.

1. Introduction
Recovering work and heat in chemical processes is fundamental for achieving high energy efficiencies, and it can be performed through the optimal synthesis of work and heat exchange networks (WHENs). This synthesis problem can be approached with superstructure-derived mixed-integer nonlinear programming (MINLP). The main challenge of WHENs synthesis is the lack of predefined pressure and temperature change routes of process streams, which hampers a priori stream classification. In other words, differently from heat integration and because of temperature variation in compression and expansion, a stream may change its thermal identity from hot to cold or vice-versa, making it difficult to target energy demands. The resulting MINLP models are intrinsically difficult to solve due to nonconvexity and combinatorial complexity that scales up quickly with the size of the problem, i.e. with the number of streams and superstructure stages (Santos et al., 2020b).
This problem has been addressed via either thermodynamic analysis (pinch variations to account for work and heat) or mathematical programming. The latter approach has shown promising results in the literature. Wechsung et al. (2011) proposed a superstructure with fixed thermodynamic routes for process streams that were classified as hot or cold, and
with fixed or variable pressure. To further simplify the MINLP problem, heuristics were considered for the appropriate placement of pressure manipulators. The optimization problem aimed to minimize the WHEN irreversibility.

Onishi et al. (2014a) proposed a WHEN superstructure based on Wechsung et al. (2011), except that the well-known heat exchanger network (HEN) superstructure from Yee and Grossmann (1990) was introduced for heat integration, and mathematical programming was used for placing the pressure manipulators. The MINLP formulation was developed to minimize the network total annualized cost (TAC). Onishi et al. (2014b) elaborated a multi-stage superstructure considering high-pressure streams as cold streams and low-pressure as hot streams. Huang and Karimi (2016) presented some modifications to the work of Onishi et al. (2014b), like the decision of the final device to adjust stream temperature based on the stream need instead of its identity.

Onishi et al. (2018) developed an innovative WHEN superstructure to deal with streams that are not classified a priori. Generalized disjunctive programming (GDP) was used to deal with the pressure manipulator selection and the classification of the stream. The problem had an MINLP formulation that was a convex hull reformulation of the GDP. It was incorporated with a Pinch-based optimization model for heat integration to minimize the TAC. Nair et al. (2018) added to the model of Onishi et al. (2018) the possibility of phase change, variable heat capacity, as well as compression and expansion of streams with no net pressure change (cycles).

Differently from previous authors that relied on mathematical programming, some interesting results used meta-heuristics to deal with the WHEN synthesis problem. Pavão et al. (2019) proposed a new approach to WHEN synthesis considering non-isothermal mixing and utilities in every HEN stage in parallel with the other heat transfer devices. The solution approach comprised Simulated Annealing (SA) for the combinatorial level and Rocket Fireworks Optimization for the continuous one. Santos et al. (2020a) proposed a new superstructure-derived MINLP model with a reduced number of decision variables. Change of variables and inner-level optimization were considered to diminish the combinatorial size of the optimization problem. The solution approach consisted of a two-level meta-heuristic optimization, using SA in the combinatorial problem and Particle Swarm Optimization in the nonlinear problem. Lin et al. (2021) proposed a two-piece WHEN synthesis framework composed of a targeting phase followed by the detailed HEN synthesis. The former was performed by optimizing a model of thermodynamic paths of process streams using hybridization of genetic algorithm and golden section method. The latter was performed using mathematical programming to minimize TAC.

A major challenge in this synthesis problem is dealing with streams classification. Some authors considered energy targeting or fixed temperature and pressure routes based on thermodynamic insights. Other authors included the classification of the stream as binary decision variables in the optimization problem. The objective of this paper is to present a WHEN superstructure and a derived MINLP model that deals with streams classification without binary decision variables or thermodynamic heuristics. That is achieved by introducing the novel reciprocal heat exchangers in the heat integration superstructure.

2. WHEN model

2.1. Problem definition

The WHEN synthesis problem can be defined as determining a set of electric turbines and compressors, single-shaft turbine-compressors, helper motors, electric generators, heat exchangers, heaters, and coolers that perform the required temperature and pressure
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changes of process streams with minimum operating and capital costs. Therefore, for the set of S streams \((s = 1, \ldots, S)\), it is given their initial and final states \((T_{in}, Pin, Tout, and Pout)\), heat capacity flow rates \((CP)\) and heat exchange coefficients \((h)\). Hot and cold utilities are available with known inlet and outlet temperatures \((TSin, TWin, TSout, and TWout)\), individual heat exchange coefficients \((hs \text{ and } hw)\) and costs \((CHU \text{ and } CCU)\). The prices of purchase and selling electricity \((CE \text{ and } PE)\) are given as well as economic capital cost equations \((capC, capT, \text{ and } capA)\), polytropic coefficient \((\kappa)\); and compression and expansion efficiencies \((\eta_c \text{ and } \eta_e)\).

2.2. Superstructure

The superstructure is based on Santos et al. (2020 a), but without a classification section (Figure 1). The proposed superstructure has three sections: heat integration, temperature adjustment, and work exchange network. The heat integration section is based on Yee and Grossmann (1990), updated to deal with unclassified streams with reciprocal heat exchangers. This superstructure artifice consists of using the notation of \(s, ss, nn, k\) for a heat exchanger between hot stream \((s, n)\) and cold stream \((ss, nn)\) in heat integration stage \(k\) for the hot stream and \(K - k - 1\) for the cold one, where \(s\) is the stream number, \(n\) is the WHEN superstructure stage and \(K\) is the total number of heat integration stages. The temperature adjustment section allows using a hot or cold utility to achieve the desired cooling or heating task. The work exchange network section is based on Onishi et al. (2018), which uses convex hull reformulation of a GDP model to deal with the selection of compressors and turbines.

2.2.1. MINLP Model

In the heat integration section, Eqs. (1) – (6), the binary variable \(y_{s,n,ss,nn,k}\) stands for the existence (1) or inexistence (0) of a heat exchanger between hot stream \((s, n)\) and cold stream \((ss, nn)\) in heat integration stage \(k\) for the hot stream and \(K - k - 1\) for the cold one. In addition, \(Q, T, dTh, dTc, \text{ and } A\) are the heat load, temperature, temperature difference at the hot and cold end, and area of a heat exchanger, respectively, considering their subscript index. \(CP, h, \text{ and the upper and lower limits of temperature } (T^{up} \text{ and } T^{lo})\) are parameters given by the problem statement. Note that to deal with pre-classified streams one might just fix to zero the heat load and binary variable of the heat exchangers that regard streams with opposite thermal identity.

\[
T_{s,n,k+1} = T_{s,n,k} - \sum_{ss,nn\epsilon he} \frac{Q_{s,n,ss,nn,k}}{CP_s} + \sum_{ss,nn\epsilon he} \frac{Q_{ss,nn,s,n,k}Q^{up}}{CP_s} \tag{1}
\]

\[
Q_{s,n,ss,nn,k} \leq y_{s,n,ss,nn,k}Q^{up} \tag{2}
\]
\begin{align*}
dT_h,s,n,ss,nn,k & \leq T_{s,n,k} - T_{ss,nn,k-1} + (T^{up} - T^{lo})(1 - y_{s,n,ss,nn,k}) \\
dT_c,s,n,ss,nn,k & \leq T_{s,n,k+1} - T_{ss,nn,k-1} + (T^{up} - T^{lo})(1 - y_{s,n,ss,nn,k}) \\
y_{s,n,ss,nn,k} + y_{ss,nn,s,n,k-1} & \leq 1 \\
A_{s,n,ss,nn,k} \left( \frac{dT_h,s,n,ss,nn,k + dT_c,s,n,ss,nn,k}{2} \right)^{\frac{1}{3}} & \geq Q_{s,n,ss,nn,k} \frac{h_s + h_{ss}}{h_s h_{ss}}
\end{align*}

In the temperature adjustment section, Eqs. (7) – (16), it is possible to place a heater \( y_{s,n} = 1 \), a cooler \( y_{w,n} = 1 \), or none \( y_{w,n} + y_{s,n} = 0 \) at stream \( s \) in stage \( n \). \( Q_s, Q_w, dT_h, dT_s, dT_sc, dT_wh, dT_wc, A_s, \) and \( A_w \) are the heat load of the heater and cooler, temperature difference at the hot and cold end for the heater and cooler, and heat exchange area of the heater and cooler, respectively, considering the subscript index referred to streams and stages. The upper limit of heat load \( Q^{up} \), \( TS_{out}, TS_{in}, TW_{out}, TW_{in} \), and \( hw \) are parameters given by the problem statement.

\begin{align*}
\forall s, n, k & = K - 2: \\
T_{s,n,k+1} & = T_{s,n,k} + Q_{s,n}/CP_s - Q_{w,n}/CP_s \\
Q_{s,n} & \leq y_{s,n}Q^{up} \\
Q_{w,n} & \leq y_{w,n}Q^{up} \\
y_{w,n} + y_{s,n} & \leq 1 \\
dT_{sh,s,n} & \leq TS_{out} - T_{s,n,k} + (TS_{in} - T^{lo})(1 - y_{s,n}) \\
dT_{sc,s,n} & \leq TS_{in} - T_{s,n,k+1} + (TS_{in} - T^{lo})(1 - y_{s,n}) \\
dT_{wh,s,n} & \leq T_{s,n,k} - TW_{out} + (T^{up} - TW_{in})(1 - y_{w,n}) \\
dT_{wc,s,n} & \leq T_{s,n,k+1} - TW_{in} + (T^{up} - TW_{in})(1 - y_{w,n}) \\
A_{s,n} \left( \frac{dT_{sh,s,n} + dT_{sc,s,n}}{2} \right)^{\frac{1}{3}} & \geq Q_{s,n} \frac{h_s + hs}{h_s} \\
A_{w,n} \left( \frac{dT_{wh,s,n} + dT_{wc,s,n}}{2} \right)^{\frac{1}{3}} & \geq Q_{w,n} \frac{h_s + hw}{h_s hw}
\end{align*}

The work exchange network (WEN) section is based on Onishi et al. (2018). The cost calculation is based on Santos et al. (2020a), in which the TAC is the sum of operating and capital costs of WEN and HEN. The resulting MINLP model is implemented in GAMS 37.1.0 and solved with the global optimization solver BARON 21.1.13 (Tawarmalani & Sahinidis, 2005) to minimize the TAC.

3. Case study

This two-stream problem was proposed by Onishi et al. (2014a) and later approached by Lin et al. (2021). Table 1 and Table 2 present the stream and cost data, in which \( WC, WT, QS, \) and \( QW \) are given in kW, and \( A \) is given in m². Notice that the problem statement contains several considerations to simplify mathematically the synthesis task. Some other parameters from the problem statement include \( T^{lo} \) and \( T^{up} \) of 350 and 750 K, minimum temperature approach \( (dT^{min}) \) of 5 K, polytropic coefficient of 1.352, compressor and turbine efficiencies of 100 %, and annualization factor of 0.18. Notice that \( dT^{min} \) is the lower limit of all \( dT \) variables. For this case study, the authors disregarded the use of single-shaft turbine-compressors. The model size for this small-scale case study was 397 equations, 397 variables (80 discrete ones), and the best solution is found in about 5 s.
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The results of solving this WHEN synthesis problem with the proposed MINLP model are illustrated in Figure 2.

Table 1. Stream data for the case study.

<table>
<thead>
<tr>
<th>Stream</th>
<th>$T_{in}$ [K]</th>
<th>$T_{out}$ [K]</th>
<th>$P_{in}$ [MPa]</th>
<th>$P_{out}$ [MPa]</th>
<th>$CP$ [kW/K]</th>
<th>$h$ [kW/m²K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>s1</td>
<td>650</td>
<td>370</td>
<td>0.1</td>
<td>0.5</td>
<td>3.0</td>
<td>0.1</td>
</tr>
<tr>
<td>s2</td>
<td>410</td>
<td>650</td>
<td>0.5</td>
<td>0.1</td>
<td>2.0</td>
<td>0.1</td>
</tr>
<tr>
<td>HU</td>
<td>680</td>
<td>680</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CU</td>
<td>300</td>
<td>300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Cost data for the case study.

<table>
<thead>
<tr>
<th>Operation</th>
<th>Capital cost</th>
<th>Unit</th>
<th>Operating cost</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressors</td>
<td>$C_a = 30.317 Wc^{0.62}$</td>
<td>(k$)</td>
<td>$CE = 0.45504$</td>
<td>(k$/kW y)$</td>
</tr>
<tr>
<td>Turbines</td>
<td>$C_T = 1.5338 Wt^{0.61}$</td>
<td>(k$)</td>
<td>$PE = 0.0$</td>
<td>(k$/kW y)$</td>
</tr>
<tr>
<td>Heat exchangers</td>
<td>$C_p = 21.778 + 3.4467A$</td>
<td>(k$)</td>
<td>$UT = 0.377Q_s + 0.1Q_w$</td>
<td>(k$/y)$</td>
</tr>
</tbody>
</table>

The TAC of this solution is 834.7 k$/year, a value that surpassed the literature results of 1207 in Onishi et al. (2014a) and 837 k$/year in Lin et al. (2021). This shows that strategies of energy targeting and fixing thermodynamic routes can simplify big-size WHEN problem at the price of potentially disregarding the global optimum.

Figure 2. WHEN result for the case study.

Compared to the result of Lin et al. (2021), the proposed solution for this small-scale WHEN synthesis problem has one less heat exchanger recovers 2.2 kW more heat, consumes 2.1 kW less net work, and consumes 2.2 kW less cold utility. The main advantages of the present WHEN are achieving a higher inlet temperature to the second turbine, producing more work, and the increased heat integration, which saved utility.

For future work, one might consider using the idea of reciprocal heat exchangers and the present MINLP model for medium or big-sized WHEN problems. For solving such problems efficiently with global optimization solver, such as BARON, improving the model to provide tighter bounds might be required.
4. Conclusions
An efficient MINLP model for optimal WHENs synthesis was proposed from a superstructure that considers unclassified streams via reciprocal heat exchangers. A small-scale WHEN case study from the literature was used to test the developed model. It was solved using the BARON global optimization solver in GAMS. The leading advantage of the present optimization model is the capability of defining the temperature and pressure route of a process stream entirely during optimization, instead of relying on energy targeting or fixed thermodynamic routes. Results surpassed the ones from the literature from 837.0 to 834.7 k$/year of total annualized cost. For future work, the present MINLP model should be tested to medium or big-sized WHEN problems and be modified to tighten the bounds for global optimization.

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