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Highly efficient heat integration of a power-to-liquid process using MILP

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Abstract:

Synthetic fuels are needed to decarbonize the non-electrifiable parts of the transportation sector, such as shipping and aviation. The synthesis of fuels using power-to-liquid (PtL) processes has already been investigated and tested. However, economic implementation has failed to gain traction due to high plant and product costs and insufficient PtL-efficiencies. In this paper, we will use heat exchanger network synthesis (HENS) to optimize the heat integration of a novel 1 MW PtL-process. A unique feature of this case study is that the internal heat is supplied by oxidizing a Fischer-Tropsch tail gas within a combustion system (CS). The inlet and outlet temperatures of the exhaust gas flow of the three serially connected CS can be adjusted by the mass flow of excess air and the tail gas. Using HENS implies specifying inlet and outlet temperatures. We apply an adaptation of the HENS that allows for variable stream temperatures and flow capacities. This allows the CS, an internal hot utility, to be optimally tailored to the specific process. Linearization of the non-linear relations, such as stream- and stage-wise energy balance, is done with simplices. The linear approximation is transferred to MILP using highly efficient logarithmic coding. We show that implementing the CS in HENS significantly improves the total annual costs and PtL-efficiency. With the developed method, the design engineering of highly efficient PtL-processes can be successfully supported and the technology can be brought closer to an economically viable market maturity.

Keywords:

synthetic fuels, power-to-liquid, heat exchanger network synthesis, mixed-integer linear programming.

1. Introduction

In 2019, about 16.6 % of the global CO_2 emissions were caused by the transport sector. About three quarters of that are caused by road traffic [1]. The electrification of road traffic will lead to long-term emission reduction. However, replacing vehicles before they reach their lifetime will lead to higher emissions in the medium term. Climate-neutral transportation, using emission-free synthetic fuels (also known as eFuels), offers the possibility to continue using existing vehicles. Furthermore, due to the high energy density of liquid fuels, shipping and aviation will presumably continue to rely on them in the long term.

Despite a technology readiness level (TRL) greater than 7, large-scale industrial production of eFuels has yet not taken off [2]. The first commercial integrated PtL-plant Haru Oni was built by the lead developing company HIF and its partner network in Punta Arenas, Chile. In December 2022, the first tank was filled with eFuel, which was produced with one 3.4 MW wind turbine in the pilot phase. From March 2023, the goal is to produce 130 000 L liters of synthetic fuel per year.

A key inhibitor of this technology are the costs. A significant share of the costs arises from the energy required to heat and cool process streams. Efficient heat integration is a crucial element for cost-effectiveness. With heat exchanger network synthesis (HENS), cost-optimal heat integration can be realized using mathematical programming. Using the non-linear superstructure formulation from Yee & Grossmann [3], all stream and utility temperatures and flow capacities must be defined a priori. Furthermore, the utility heat transfer is only possible in one stage and without stream splits. Huber et al. [4] presented an extension of the superstructure formulation from Yee & Grossmann, which allows the implementation of utilities as streams with variable temperatures and flow capacities. It has been shown that significant cost savings result from variable temperatures and multi-stage heat exchanges with stream splits of utilities [4]. Utilizing only the sensible heat of a fluid such as thermal oil, water or flue gas, allow flexibility in selecting temperatures. As long as technical limitations are considered, both the outlet and inlet temperatures can be varied within a certain range. When designing new plants, integrating the design of the utilities into the HENS formulation offers significant advantages in terms of efficiency and total annual costs (TAC).

In this paper, we adapt the method presented by Huber et al. [4] to simultaneously optimize the internal heat supply and the heat exchanger network (HEN). As a use case, the design of a novel 1 MW PtL-plant is opti-

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mized. The PtL-plant combines solid co-electrolysis (co-SOEC) with efficient CO_2 processing and a Fischer-Tropsch (FT) reactor. The internal heat supply is provided by three combustion systems (CS) where a process tail gas from the FT-reactor is oxidized. The hot exhaust gas streams from the CS are used as an internal hot utility. In this paper, we compare the design case with the results applying classical HENS. We additionally demonstrate that previously untapped potential for optimization can be activated by optimizing the CS stream temperatures and heat capacity flows. The results show that the TAC can be reduced, and the efficiency can be increased simultaneously. Thus, production costs of synthetic fuels can be lowered, and large-scale industrial deployment can be strengthened.

2. Methods

2.1. HENS superstructure formulation

The objective of the optimization is to minimize the total annual costs (TAC) of the heat exchanger network according to Equation (1).

$$\begin{aligned}
\min TAC = & \underbrace{\sum_i c_{\mathrm{uc}}\, q_{\mathrm{uc},i}}_{\text{cold utility costs}} + \underbrace{\sum_j c_{\mathrm{uh}}\, q_{\mathrm{uh},j}}_{\text{hot utility costs}} \\
& + \underbrace{\sum_i \sum_j \sum_k c_{\mathrm{f}}\, z_{ijk} + \sum_i c_{\mathrm{f}}\, z_{\mathrm{uc},i} + \sum_j c_{\mathrm{f}}\, z_{\mathrm{uh},j}}_{\text{step-fixed investment costs}} \\
& + \underbrace{\sum_i \sum_j \sum_k c_{\mathrm{v}} \left(\frac{q_{ijk}}{U_{ij}\, LMTD_{ijk}} \right)^{\beta}}_{\text{variable HEX stream costs}} + \underbrace{\sum_i c_{\mathrm{v}} \left(\frac{q_{\mathrm{uc},i}}{U_{\mathrm{uc},i}\, LMTD_{\mathrm{uc},i}} \right)^{\beta}}_{\text{variable HEX cold utility costs}} + \underbrace{\sum_j c_{\mathrm{v}} \left(\frac{q_{\mathrm{uh},j}}{U_{\mathrm{uh},j}\, LMTD_{\mathrm{uh},j}} \right)^{\beta}}_{\text{variable HEX hot utility costs}}
\end{aligned} \tag{1}$$

The mathematical formulation of the optimization problem is based on the superstructure formulation of Yee & Grossmann [3]. Huber et al. [4] extended this HENS formulation to implement utilities as streams with variable temperatures and flow capacities. Consequently, the utility heat exchange is possible in multiple stages with stream splits. In this context, utilities implemented as multi-stage streams are referred to as utility streams. Different sets of constraints were added to the Yee & Grossmann formulation, which are activated depending on the utility stream definition. This ensures that no utilities can be placed at the stream ends. Further constraints have been added to limit the heat capacity flows, inlet and outlet temperature to pre-defined ranges. The modifications to the superstructure formulation as well as all necessary constraints can be found in [4].

2.2. Piecewise-linear approximation

To apply fast MILP solvers and to prevent the solver from getting stuck in local optima, all non-linear terms such as reduced HEX areas for streams and utilities, LMTD and energy balances are piecewise-linear approximated and transferred to MILP. To increase the accuracy of the linearization and to decrease the number of binaries, the functions of the reduced HEX areas are trimmed to the feasible domain according to Beck et al. [5]. The three-dimensional function of the stream's reduced HEX area is piecewise-linear approximated with superpositioned planes, see Figure 3 (left) in Appendix A. The two-dimensional function of the reduced utility HEX area is approximated piecewise-linear with straight lines and transferred to MILP with an SOS2 approach, see Figure 3 (right) in Appendix A. The piecewise-linear approximation of the three-dimensional function for the LMTD, stage- and stream-wise energy balances is done with plane triangles, see Figure 4 in Appendix A. The plane equations are transferred to MILP with a highly efficient logarithmic coding according to Vielma & Nemhauser [6]. In all piecewise linear approximations, lines, planes, or triangles are added until a root-mean-square error (RMSE) of less than 1 % is reached.

2.3. PtL-efficiency

The performance of the PtL-process is evaluated from an economic point of view by TAC and from a technical point of view with the PTL-efficiency. The PtL-efficiency η_{PtL} is calculated with the ratio of the electrical energy input to the sum of the lower heating values, see Equation (2).

Since the output of synthetic fuels is independent of the heat integration, the PtL-efficiency is only affected by the additional required electrical energy. Depending on the heat integration, P_{base} is increased by the electrical energy demand for hot P_{uh} and cold utilities P_{uc}. For the cooling of hot streams, energy is dissipated to the environment, while the energy for hot utilities is provided by an electric steam generator. For both processes, it is assumed that an additional 5 % of electric energy must be supplied to operate the circulation pumps and to cover losses. With these assumptions, the PtL-efficiency is calculated according to Equation (2).

$$\eta_{\text{PtL}} = \frac{\sum LHV}{P_{\text{base}} + P_{\text{uh}} + P_{\text{uc}}} = \frac{\sum LHV}{P_{\text{base}} + 1.05 \cdot \sum q_{\text{uh}} + 0.05 \cdot \sum q_{\text{uc}}} \tag{2}$$

3. PtL-process

Within the research project *IFE* (Innovation Flüssige Energie, engl.: innovation liquid energy), a two-stage PtL-process with a H_2O + CO_2 high-temperature solid oxide co-electrolysis (co-SOEC) and Fischer-Tropsch (FT) synthesis is being fully conceptualized and basically engineered. The plant, powered by renewable electricity, has a total electric load of approximately 1 MW. A schematic diagram of the six major components is shown in Figure 1. In the stationary process, an industrial offgas from a cement production plant containing about 15 wt% CO_2 and N is conditioned and reformed together with steam in the co-SOEC to a gas of H_2 and CO. In the downstream FT-reactor, a syngas is reformed. The subsequent strippers separate the syngas into the components, naphtha, diesel and FT-wax. Annually, about 160 000 L of naphtha, 100 000 L of diesel and 360 000 L of Fischer-Tropsch wax are produced climate-neutrally. The sum of the lower heating values $\sum LHV$ is 650.31 kW. The electrical energy requirement of the system without utilities P_{base} is 1135.90 kW. A significant part of this, viz. 992.32 kW, is used by the co-SOEC. 143.59 kW are required for compressors, pumps and to cover losses.

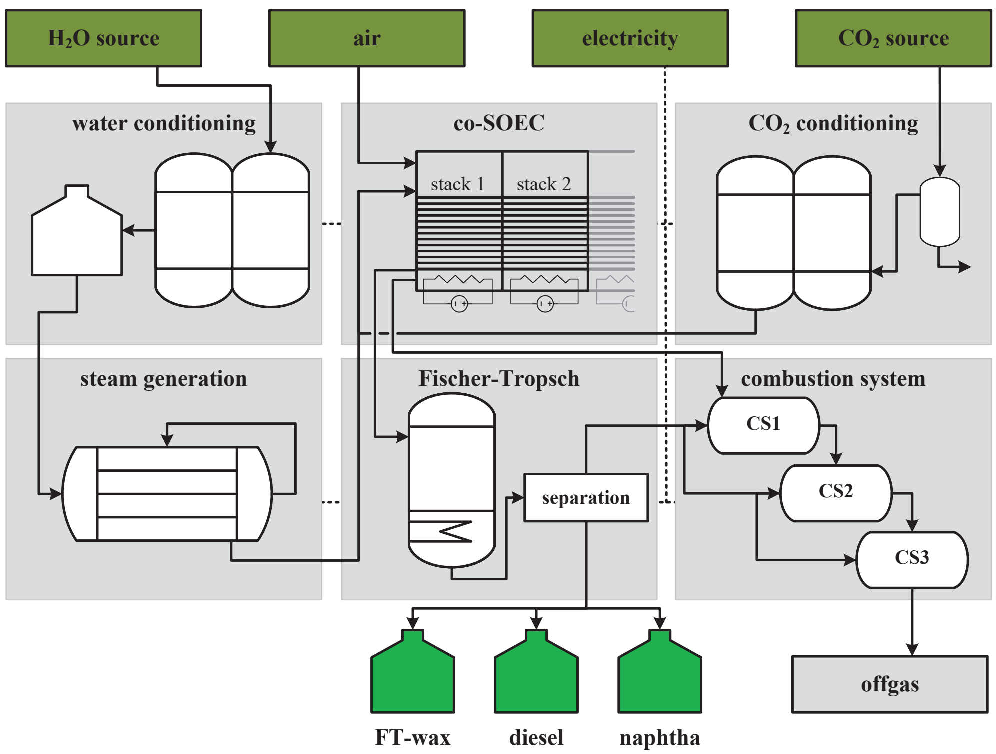

Figure 1: Schematic representation of the 1 MW PtL-process with the main components: water conditioning, CO_2 conditioning, steam generation, co-SOEC, Fischer-Tropsch reactor and combustion systems.

As a starting point for basic engineering, the entire PtL-process was modeled and simulated using Aspen HYSYS. The crucial process streams for heat integration can be reduced to 15 hot and 7 cold process streams. The stream data can be found in Table 1. The necessary energy for heating the cold process streams is provided by oxidizing a tail gas from the FT-reactor. The tail gas cannot be further circulated and must otherwise be flared. Together with the exhaust air from the co-SOEC, the tail gas is oxidized in three combustion systems (CS). The exhaust air of the co-SOEC has a temperature of almost 900 °C. Due to the high amount of sensible heat, the entire exhaust air is used for oxidation. The three CS are connected in series, with new tail gas being added at each stage. Regarding HENS, the CS's exhaust gas streams CS1 to CS3 are used as hot utilities to provide heating energy. The inlet temperatures of the CS streams of 848.90 °C, 893.16 °C and 492.60 °C result from the empirical definition of the fuel quantity at each stage. Additionally, a high-temperature electric steam generator serves as a hot utility. The energy needed to cool the hot process streams is provided by

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Table 1: Stream and cost data for the PtL-process

stream	T^{in} / °C	T^{out} / °C	F / kW/K	h / kW/(m^2 K)
H1	40.00	35.00	2.1558	1.0
H2	131.09	35.00	0.1174	1.0
H3	174.05	35.00	0.1190	1.0
H4	209.98	190.00	0.2801	1.0
H5	190.00	120.00	0.5767	1.0
H6	120.00	30.00	0.4978	1.0
H7	56.96	31.00	2.9471	1.0
H8	139.86	138.86	188.7246	1.0
H9	825.45	35.00	0.1297	1.0
H10	50.72	35.00	0.8830	1.0
H11	101.80	30.00	0.6404	1.0
H12	190.00	189.00	153.7523	1.0
CS1	848.90	786.71	0.4203	1.0
CS2	893.16	278.50	0.4122	1.0
CS3	492.60	132.88	0.4025	1.0
CS1^v	900.00	[890.00, 150.00]	[0.0349, 2.6138]	1.0
CS2^v	900.00	[890.00, 150.00]	[0.3377, 25.3284]	1.0
CS3^v	900.00	[890.00, 150.00]	[0.1930, 14.4781]	1.0
C1	319.18	824.96	0.1816	1.0
C2	116.90	124.40	25.1158	1.0
C3	58.79	825.00	0.3306	1.0
C4	138.86	139.86	285.2732	1.0
C5	138.86	426.62	0.1039	1.0
C6	35.00	145.42	0.0566	1.0
C7	20.27	189.47	0.2110	1.0
uh	600.00	598.00	-	1.0
uc	15.00	20.00	-	1.0

HEX costs: c_f = 1013 €/y, c_v = 62 €/(m$^{2\beta}$ y), β = 0.8
utility costs: c_{uh} = 200 €/(kW y), c_{uc} = 10 €/(kW y)
min. approach temperature: ΔT_{min} = 1 °C

cooling water. The cost parameters for utilities and HEX are shown at the bottom of Table 1. Parameterization of the degressive HEX cost function was performed using cost information from the DACE Price Booklet [7] and multiple feedback rounds with the project partners.

3.1. Case study

With this paper, we show that HENS is a highly efficient tool for determining cost-optimal heat integration. Applied to the actual design problem of a novel PtL-plant, basic engineering can be actively supported and the potential of HENS can be quantified. Implementing the CS's exhaust gas stream as utilities with variable outlet temperatures and heat capacity flows, the utility design problem can be optimized holistically using mathematical optimization. The following cases are investigated to quantify the method's potential in terms of cost reduction and efficiency increase.

base This case represents the plant design from basic engineering. The HEN and the temperatures of the CS streams were determined empirically. This case serves as a reference to evaluate the achievable improvements.

baseHENS Only the HEN configuration is optimized. The stream temperatures resulting from the process simulation remain unchanged. With these assumptions, we demonstrate the potential of classical HENS and provide a cost-optimal heat integration.

advancedHENS Both the HEN and the CS are optimized. The outlet temperatures and the flow capacities of the CS streams are included as variables in the optimization problem. In Table 1, the CS streams are shown with the allowed ranges for temperature and flow. The inlet temperatures of the streams CS1^v to CS3^v are set to the material-specific limit of 900 °C. The outlet temperature can range from 150 °C to 890 °C. The permissible range of the flow capacity F was determined to ensure that no energy balances were violated.

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4. Results

The optimization problem in this paper was modeled in MATLAB R2022a [8] using Yalmip R20210331 [9]. Gurobi 9.5.2 [10] was used as the MILP solver on a 128-core system (AMD EPYC 7702P) with 256 GB RAM. As a termination criterion, a relative gap of less than 0.01 % was set. The relative gap is defined as the gap between the best feasible solution objective and the best bound.

4.1. Optimization

The results of the case study are summarized in Table 2. The corresponding stream plots are shown in Appendix B. Remarkably, no hot utility is needed in all three cases.

Table 2: Comparison of costs, PtL-efficiency, heat loads and HEX area.

case	*TAC* / €/y	η_{PtL} / %	q_{UC} / kW	q_{UH} / kW	A_{HEX} / m^2
base	29 394.70	56.04	244.60	0	60.15
baseHENS	27 213.00	56.04	244.30	0	55.68
advancedHENS	23 576.13	56.16	219.78	0	49.35

The base case with TAC of 29 394.70 €/y and a PtL-efficiency of 56.04 % is the most expensive case. With identical PtL-efficiency, the TAC for the baseHENS case are 27 213.00 €/y. Using HENS, a reduction of the TAC by 8.01 % can already be achieved. In both cases, the capacity of the cold utilities are almost identical at 244.60 kW and 244.30 kW, respectively. The base case requires 21 HEX and the baseHENS case requires 22 HEX. Despite the larger number of HEX in the baseHENS case, less HEX area is required, 60.15 m^2 compared to 55.68 m^2. It can be concluded that the savings from a smaller HEX area outweigh the increased fixed costs due to one additional stream match. Counter-intuitively, a HEN with more HEX can still lead to lower TAC.

The advancedHENS case is based on different stream data. As shown in Figure 7, the solution of the optimization problem results in outlet temperatures of 877.4 °C, 878.3 °C and 887.5 °C at the streams CS1^v to CS3^v, respectively. The high temperatures close to the inlet temperature of 900 °C ensure a large LMTD at the HEX. A large LMTD reduces the HEX area required for the same amount of heat to be transferred. Compared to the base case, the HEX area is reduced from 60.15 m^2 to 49.35 m^2. Also, instead of 21 or 22 HEX, only 19 HEX are required. The smaller HEX area and number of HEX are the main reasons for the significant cost savings. With TAC of 23 576.13 €/y, 24.68 % of the costs can be saved compared to the base case. Approx. 4.27 % of the cost savings, i.e. 248.20 €/y, result from the lower cold utility load. 95.73 % of the cost savings, i.e. 5570.37 €/y, results from the fewer HEX and the decreased HEX area.

4.2. Composite curves & PtL-efficiency

According to Equation (2), the highest possible PtL-efficiency would be 57.25 % if no utilities are required. Evaluation of the composite curves (CC) at different minimum temperature differences shows that the theoretically achievable PtL-efficiency can not be achieved and must be lowered. Figure 2 on the left shows the CC of the process for a fictive minimum temperature difference of 0 K. It should be noted that the cases base, respectively baseHENS (solid lines) and advancedHENS (dashed line), show different composite and PtL-efficiency curves due to the different stream data. The results show that in the advancedHENS case, considerably more heat is transferred in the upper-temperature range due to the higher temperatures of the CS streams. The higher temperature difference between the streams generally results in higher LMTD at the HEX. Therefore, less HEX area is needed and costs can be saved.

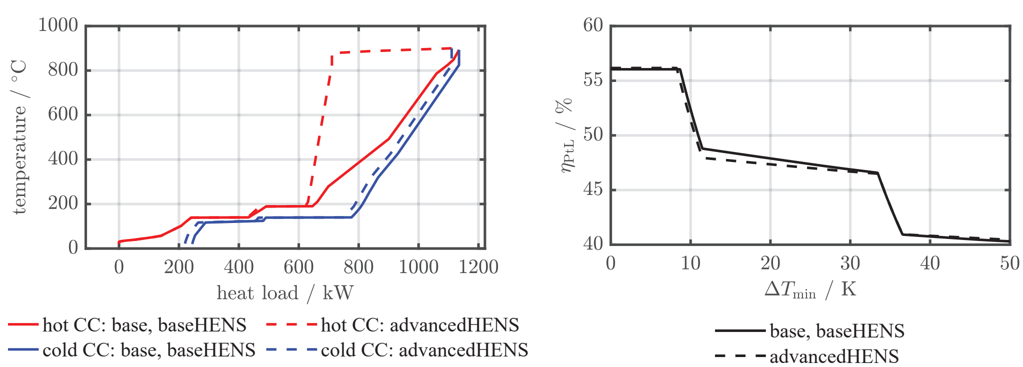

Figure 2: Left: Composite curve at a minimum temperature difference of ΔT_{min} = 0 K. Right: Maximum achievable efficiency as a function of the minimum temperature difference.

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Figure 2 on the right shows the maximum achievable efficiency as a function of the minimum temperature difference. Up to a minimum temperature difference of 9 K, the pinch point is located at the upper right end of the CC. Consequently, no hot utilities are needed for the threshold problem. Up to ΔT_{min} of less than 9 K, a maximum efficiency of 56.04 % can be achieved for the base and baseHENS case. Due to optimized temperatures and flow capacities of the CS streams, the maximum achievable efficiency for the advancedHENS case can be increased to 56.16 %. Additional hot utilities are needed for ΔT_{min} higher than 9 K and the efficiency drops below 50.00 % for all cases. In all cases of the case study, the theoretical upper limit of the PtL-efficiency is reached.

5. Conclusion

Synthetic fuels are necessary to decarbonize the non-electrifiable transport sectors such as aviation and shipping. They also serve as a transitional solution for existing vehicles. High fuel production costs inhibit large-scale synthetic fuel production because of high total annual costs (TAC) and low PtL-efficiency. In this paper, we used an adapted HENS formulation and implemented the combustion systems (CS) of a novel 1 MW PtL-plant as internal hot utilities in the heat exchanger network design problem. The outlet temperatures and flow capacities of the internal hot utilities are implemented as optimization variables, unlike conventional HENS, and optimized simultaneously with the HEN. By coupling the optimization, a holistic examination is made possible, which opens up new potential for cost reduction and efficiency increase.

In the base case, the design case from the process simulation with Aspen HYSYS, as well as the baseHENS case, a PtL-efficiency of 56.04 % could be achieved. Using HENS in the baseHENS case, it was possible to find a HEN that is 8.01 % less expensive with TAC of 27 213.00 €/y. In the advancedHENS case, the inlet temperature of the CS streams has been set to the upper technical limit of 900 °C. The outlet temperatures resulting from the optimization problem are above 850 °C, compared to the base and baseHENS case. The high temperatures and the small temperature differences between the feed and return ensure a large LMTD at the heat exchangers. This allows smaller and also less expensive HEX to be used. TAC can be reduced by 24.68 % to 23 576.13 €/y. It can be concluded that the temperature of hot utilities should always be set as high as possible as long as the utility costs are not affected. Optimizing the temperature and flow capacity of the CS streams, allows the CS streams' heat flow to be reduced. The resulting shift in composite curves subsequently reduces the need for cold utilities. Therefore, the PtL-efficiency can be increased to 56.16 % and cold utility costs can be lowered.

In this paper, we showed that for given stream parameters, TAC can be significantly reduced using classical HENS. A key finding is that the coupled optimization of stream parameters and HEN lead to significant cost reductions and efficiency improvements simultaneously. From the results, it can be concluded that the main cost reduction stems from the higher temperatures of the hot utilities and the simultaneously optimized lower-cost HEN. With this paper, we show that the coupled optimization of utility parameters and HEN enables the activation of previously untapped potential for optimization. Applied to the use case of a PtL-plant, we can accelerate the economically viable production of synthetic fuels. Therefore, decarbonization of the transport sector can be achieved more quickly and emissions can be reduced in the long term.

Acknowledgments

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Appendix A Piecewise-linear approximation

Figure 3 (left) shows the piecewise linear approximated reduced heat exchanger area for a stream HEX with the following stream data:

- Hot stream: T^{in} = 270 °C, T^{out} = 160 °C, F = 18 kW/K, h = 1 kW/(m^2 K)
- Cold stream: T^{in} = 50 °C, T^{out} = 210 °C, F = 20 kW/K, h = 1 kW/(m^2 K)
- $\beta = 0.8$

Figure 3 (right) shows the piecewise linear approximated reduced heat exchanger area for a utility HEX with the following stream data:

- Hot stream: T^{in} = 270 °C, T^{out} = 160 °C, F = 18 kW/K, h = 1 kW/(m^2 K)
- Cold utility: T^{in} = 10 °C, T^{out} = 30 °C, h = 1 kW/(m^2 K)
- $\beta = 0.8$

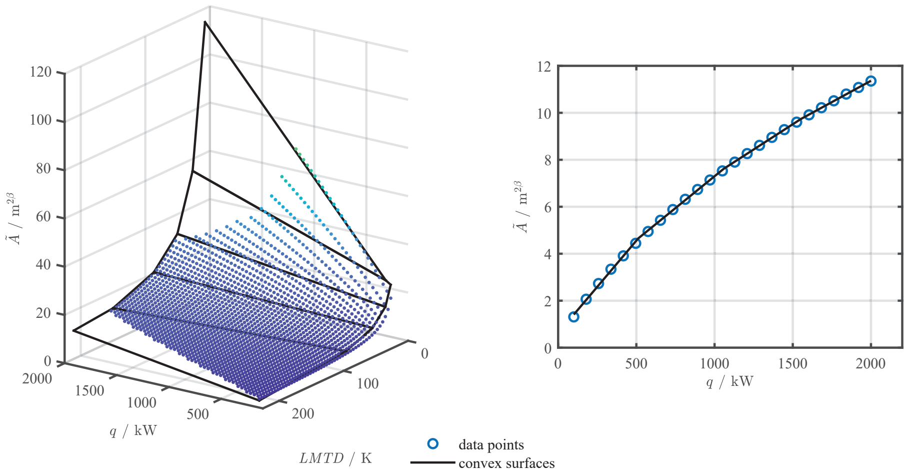

Figure 3: Piecewise linear approximation of the reduced stream HEX area $\tilde{A}$ as a function of the heat flow q and $LMTD$ with five hyperplanes ($RMSE$ = 1.26 %). Right: Piecewise linear approximation of the reduced utility HEX area $\tilde{A}$ as a function of the heat flow q with four lines ($RMSE$ = 0.38 %).

Figure 4 (left) shows the piecewise linear approximated function of the $LMTD$ within a temperature range of 10 K to 200 K. Figure 4 (right) shows the piecewise linear approximated function of the stream-wise energy balance within the following stream data:

- Hot stream: T^{in} = 270 °C, T^{out} = [50, 160] °C, F = [2, 20] kW/K.

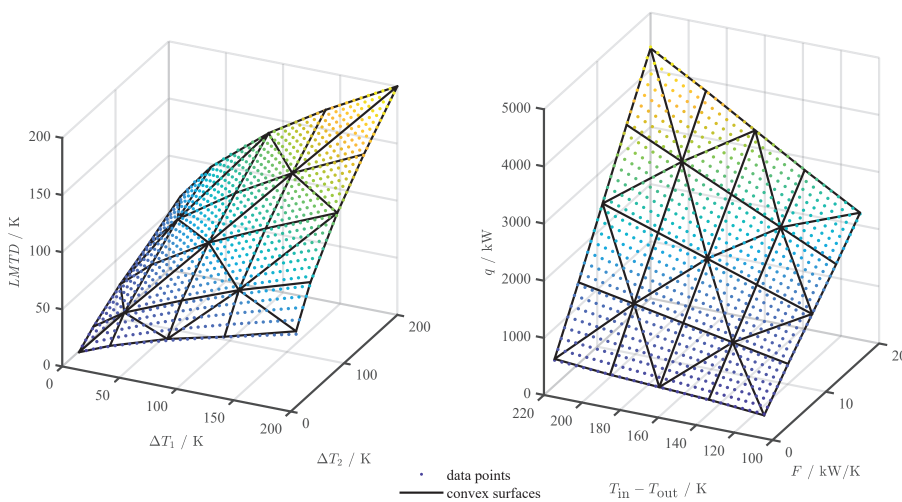

Figure 4: Left: Piecewise linear approximation of the $LMTD$ as a function of the two temperature differences ΔT_1 and ΔT_2 ($RMSE$ = 0.34 %). Right: Piecewise linear approximation of the stream-wise energy balance as a function of the flow capacity F and the temperature difference $T_{\text{in}} - T_{\text{out}}$ with 32 simplices ($RMSE$ = 0.28 %).

Appendix B Stream plots

Figure 5 to 7 shows the stream plots. Red arrows represent hot process streams that need to be cooled down. Blue arrows represent cold process streams that need to be heated. Utilities are characterized by dark gray circles at the stream ends. Light gray circles and black lines represent connected heat exchangers between hot and cold streams.

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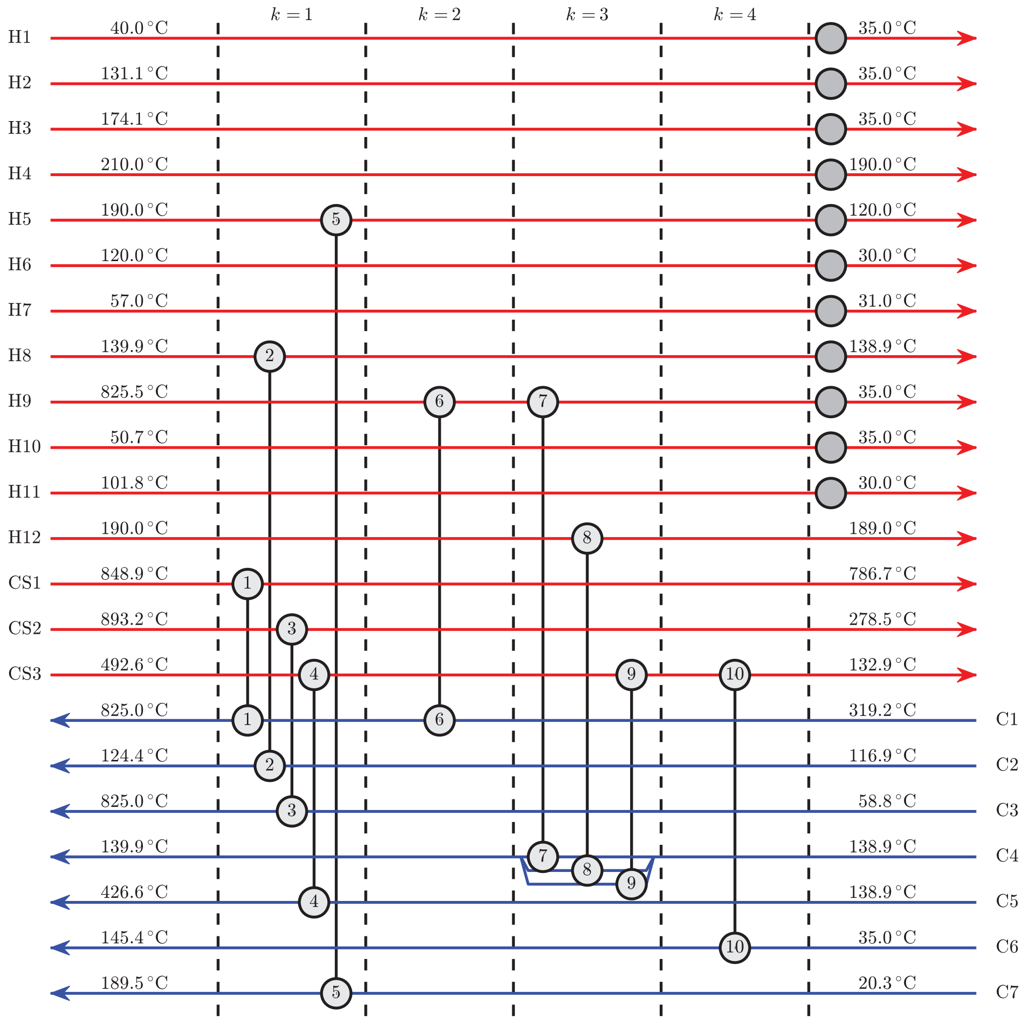

Figure 5: Stream plot of the case *base*. *TAC* = 29 394.70 €/y. η_{PtL} = 56.04 %.

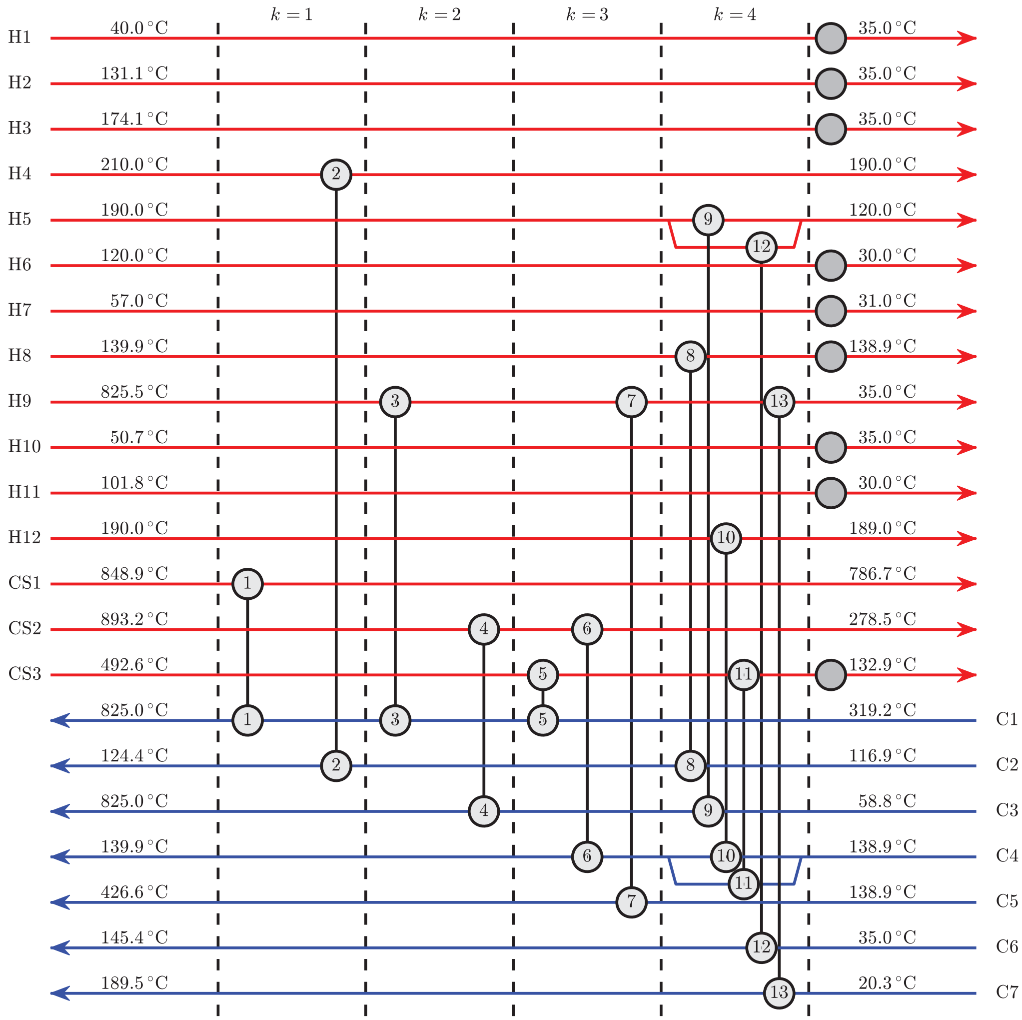

Figure 6: Stream plot of the case *baseHENS*. *TAC* = 27 213.00 €/y. η_{PtL} = 56.04 %.

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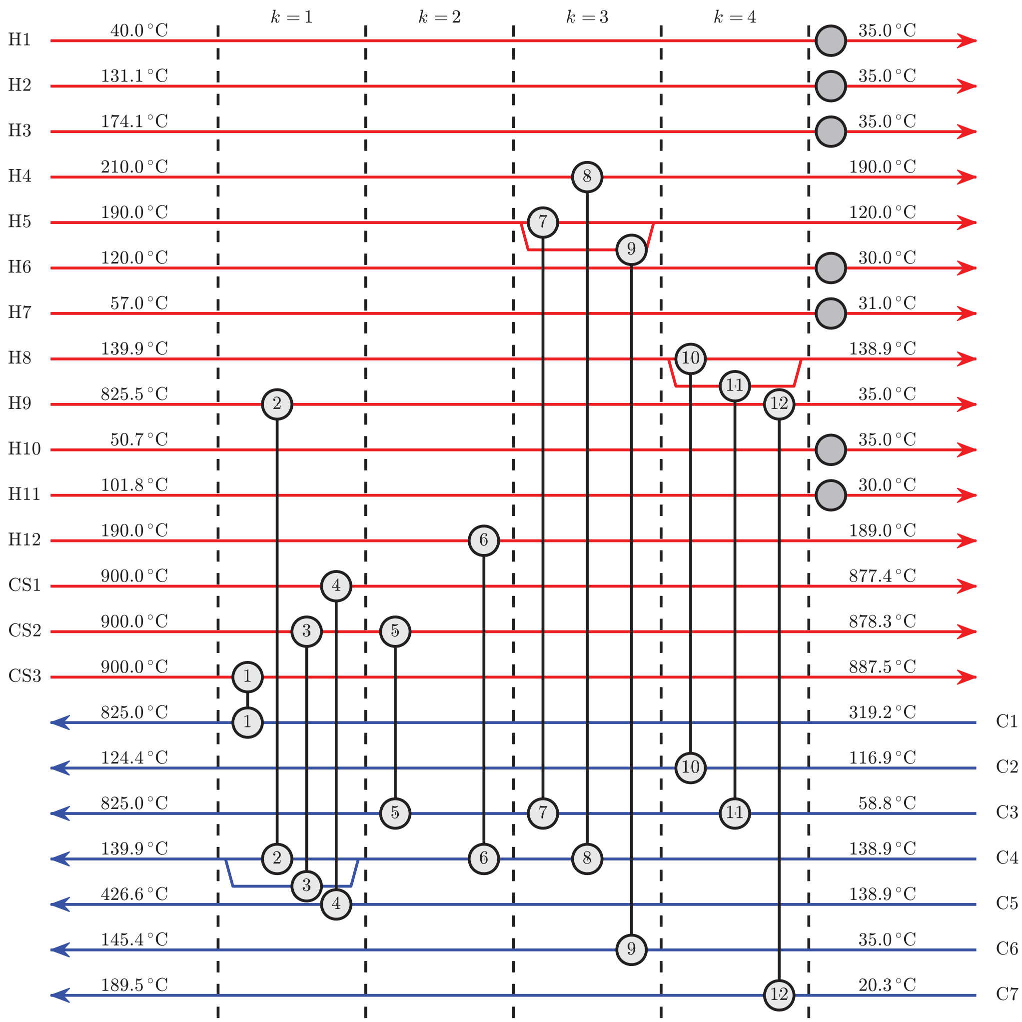

Figure 7: Stream plot of the case *advancedHENS*. *TAC* = 23 576.13 €/y. η_{PtL} = 56.16 %.

Nomenclature

Letter symbols

$\tilde{A}$ reduced HEX area, m^2

F flow capacity, kW/K

h heat transfer coefficient, kW/m^2K

k stage, –

$LMTD$ logarithmic mean temperature difference, K

n number of plane triangles, –

q heat flow, kW

P load, kW

$RMSE$ root mean square error, %

T temperature, °C

U heat transfer coefficient for stream matches, $kW/m^2/K$

Greek symbols

β cost exponent, $-$

ΔT temperature difference, K

η efficiency, %

Subscripts and superscripts

base electric consumption of the PtL plant without utilities

f fixed

i hot stream

j cold streams

k stage

uc cold utility

uh hot utility

v streams with variable outlet temperature and flow capacity, variable

in inlet

out outlet

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