

Optimization of Site-wide Heat-Integrated Utility Systems with Heat Pumps using MILP

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ABSTRACT

The reduction of CO₂-emissions in the chemical industry is essential to meet European climate targets. Particularly, the reliance on fossil fuels for process heat supply is a key factor for CO₂-emissions. Electrically driven compression heat pumps are a promising option to reduce fossil fuel consumption by upgrading low-temperature waste heat to a higher temperature level, provided that low-carbon electricity is available. However, the integration of heat pumps into chemical utility systems remains a challenge due to economic constraints and the high complexity associated with site-wide heat integration and retrofit of existing structures. This work presents a mixed-integer linear programming (MILP) approach for the optimization of utility systems with integrated heat pumps. To address computational complexity, candidate utility temperature levels are pre-selected, and feasible heat pump coefficients of performance (COP) are precomputed. The framework is applied to both greenfield and retrofit scenarios for a synthetic case study consisting of 400 process streams. In the greenfield scenario, optimal utility temperature levels and heat pump integration configurations are identified. For the retrofit scenario, temperature levels of an existing utility system are modified to reduce total annual costs (TAC). Additionally, sensitivity analysis is conducted to assess the influence of key economic and environmental parameters. The presented case studies demonstrate short solution times, highlighting the suitability of the proposed framework for screening studies and systematic sensitivity analyses in early-stage design and retrofit applications.

Keywords: Energy Systems, Optimization, Renewable and Sustainable Energy

INTRODUCTION

The CO₂-emissions of the chemical industry must be reduced significantly to meet Europe's climate goals of zero net-emissions by 2050 [1]. A large proportion of the process heat demand is still met by burning fossil fuels such as natural gas which results in the emission of CO₂ [2]. Therefore, an effort should be made to reduce the share of process heat supplied from fossil fuels. This can be achieved by improving the efficiency of chemical processes or using alternative, low-carbon sources of heat supply. Compression heat pumps offer a possibility of providing heat with low CO₂-emissions when powered by electricity with a low CO₂-emission factor [3]. The use of formerly unused waste heat which is lifted to a higher temperature level by the heat pump can substitute process heat provided by fossil fuels.

Despite the advantages of heat pumps for providing process heat with low CO₂-emissions, heat pump integration into chemical processes is still limited by major challenges. Among these are economic feasibility and the inherent complexity of the systems involved. [4] In the context of chemical sites, complexity arises, on the one hand, from the large number of potential heat sources and sinks that must be considered for heat integration. On the other hand, both heat integration and the integration of heat pumps increase system complexity by introducing intra- and inter-process dependencies. The integration task then includes the appropriate sizing of heat pumps and identifying optimal integration points that allow independent operation of different considered processes.

In chemical sites, heat is usually provided to the processes via different utility levels such as steam and hot

water at different temperatures. Waste heat from the processes is either used to supply heat to the heating utilities or collected via cooling utilities such as cooling water. The temperature levels of these utilities are often based on historical design decisions. Over time, the design may have become suboptimal due to changes in process conditions or configurations as well as evolving energy trends such as energy price developments and alternative sources of heat supply.

The scope of this contribution is heat pump integration between different temperature levels of the site-wide utility system. This allows the utilization of surplus heat from the lower level and electricity to supply heat to the higher temperature utility level to substitute fossil-based heat. While the integration of heat pumps between different utility levels is limited in efficiency compared to the integration in selected process heat sources and sinks with lower temperature lifts, it offers several advantages. Centralized heat pump integration requires only one power line, it mitigates space limitations associated with integration close to the processes and the utility system may act as a buffer in case of operational fluctuations. Increasing the efficiency of centrally integrated heat pumps may require changing the temperature levels of the existing utility system to optimize waste heat usage and resulting temperature lifts for heat pumps which will be discussed in this work.

LITERATURE REVIEW

The concept of pinch analysis, introduced by Linnhoff and Hindmarsh in 1983, represents a foundational approach to process heat integration and enables the identification of minimum external energy requirements [5]. Using the problem table algorithm, feasible heat transfer from higher to lower temperature levels is ensured through heat cascading [6]. The methodology was later extended to chemical sites by the concept of total site heat integration which allows targeting and optimization of utility levels as well as cogeneration potentials [7].

Building on these concepts, mathematical optimization approaches have since been developed to address increasingly complex heat integration and utility design problems in process plants and chemical sites. Papoulias and Grossmann proposed MILP optimization based on the transshipment model to minimize utility consumption in a heat recovery network by splitting the temperature range into temperature intervals and solving interval energy balances [8]. Bagajewicz and Barbaro introduced a non-linear targeting approach that optimizes heat pump integration in total sites with continuous decision variables for heat pump temperature levels [9]. Oluleye et al. incorporated heat pump integration in the optimization of existing site cogeneration systems by means of MILP

modeling [10]. They focused on different heat upgrading technologies and optimal operational parameters to minimize emissions and total annual costs. Wallerand et al. presented a superstructure-based MINLP optimization of heat pumps into industrial processes [11]. They used a decomposition strategy to solve the complex non-convex optimization task by iteratively solving non-linearities in a master level and technology selection by means of integer variables in a slave level.

The combinatorial complexity of heat transfer between process streams, utility levels and technologies such as cogeneration and heat pumps poses significant challenges for large-scale optimization problems. This may lead to convergence issues for large scale problems which is why many studies employ several simplifications to reduce the solution space. Simplifying utility system optimization is often done by applying simplified equipment models [9, 10, 12], discretizing or using fixed utility candidate temperature levels often from heuristic preselection [13, 14, 15] or linearization of non-linear constraints such as cost functions [16]. While this might exclude the global optimum from the solution space, applying simplified models allow faster solution times which can be valuable for gaining an understanding of the system, optimization under uncertainty or scenario and parameter studies [17].

Heat pump integration into utility systems of chemical sites has been subject to several studies as it provides a valuable option for waste heat utilization and reduction of external heating services [4, 9, 10]. Liew and Walmsley propose a total site targeting method that incorporates open cycle vapor recompression heat pumps with the goal of decreasing boiler energy demand to supply high quality steam [18]. Miah et al. proposed a framework for identifying possible heat integration at different scales incorporating heat pumps to upgrade waste heat and substitute external heating [19].

While previous optimization-based approaches address heat pump integration in utility systems, they often rely on fixed or finely discretized or continuous candidate temperature levels, which can be computationally expensive for large-scale systems. This limits their applicability for extensive parameter studies such as future price scenarios. Based on these limitations, this contribution proposes a mixed-integer linear programming framework for integrating heat pumps into utility systems of chemical plants. Computational complexity is reduced by a structured precomputation of candidate utility temperature levels and corresponding heat pump coefficients of performance, enabling short solution times. The approach is applicable to large-scale systems with several hundred heat sources and sinks and is well suited for screening studies under varying economic and operational conditions.

METHODOLOGY

Problem formulation

In chemical sites, heating and cooling services for cold and hot process streams are commonly supplied by site-wide utility systems with different temperature levels, often realized by steam at different pressure levels or water at different temperatures. This allows providing heat to cold streams with a temperature level higher than the cold stream target temperature plus the required minimum temperature difference in heat exchangers. The same principle applies to hot streams which can be cooled down by supplying heat to a utility level with a lower temperature than the process target temperature minus the required minimum temperature difference in heat exchangers. This way, heat surplus from hot process streams can substitute external heat supply to the utility level to supply the cold stream heat demand. The degree of heat integration in existing plants can often be improved by optimizing the utilisation of surplus heat to possibly maintain high quality heat in terms of exergy. While this might increase required heat exchanger area, it may further decrease external heat demand. The same principle applies to heat sinks, where the optimal temperature level for supplying heat to the process stream is not always selected. This aspect becomes particularly relevant when heat pumps are used to supply heat to utility systems. The COP of heat pumps decreases with higher temperature differences between heat source and heat sink and they are limited to sink temperatures of around 200°C [20, 21]. Therefore, process heat sources and heat sinks should be connected to optimal temperature levels to increase the potential for heat pump integration in utility systems of chemical sites.

This can become a challenging task in chemical sites as often several hundred hot and cold streams are connected to the utility system as they cannot be integrated in the processes themselves. The MILP formulation proposed in this work considers the optimization of utility systems. Simple constraint modifications in the MILP allow the analysis of retrofit scenarios as well as the design of new utility systems. The user must supply duties and target temperatures of hot and cold process streams. The approach considers central closed cycle heat pump integration between different temperature levels of the utility system and connections between process streams and utility levels. Optimal utility level temperatures, external heating or cooling requirements for every utility level, optimal connections between streams and utility levels as well as heat pump design and integration are selected during the optimization.

Candidate temperature level reduction

To enable fast MILP solution times, the number of candidate utility temperature levels must be reduced to

reduce combinatorial complexity. In this approach, candidate temperature levels are selected by identifying the highest and lowest feasible temperature levels for hot and cold streams, respectively, that still allow reaching the target temperatures. These levels correspond to the temperatures at which kinks occur in the hot and cold composite curves. While this enables fast calculation, solutions requiring intermediate utility levels for cascaded heat pump configurations are excluded, which is discussed later as a model limitation.

Heat pump modeling and COP precomputation

As the presented approach should serve as a screening support in decision-making, a simple heat pump model that incorporates thermodynamic principles is applied. The COP is modeled as a function of the Carnot COP by including source (T_{source}) and sink (T_{sink}) temperatures, required temperature differences in heat exchangers ($\Delta T_{min,source}$ and $\Delta T_{min,sink}$ for source and sink respectively) and compressor efficiency (η_C) as shown in equation (1).

$$COP = \eta_C \cdot \frac{T_{sink} + \Delta T_{min,sink}}{T_{sink} + \Delta T_{min,sink} - (T_{source} - \Delta T_{min,source})} \quad (1)$$

The maximum temperature lift was assumed to be 60 K for single stage heat pumps with a maximum sink temperature of 200°C [20]. As the candidate temperature levels are predefined, COP values for all feasible combinations of source and sink utility level were also calculated to avoid nonlinearities in the optimization model. The heat pump must further follow the energy balance shown in equation (2) with electricity power demand P_{el} , heat demand at the source temperature \dot{Q}_{source} and heat supply at the sink temperature \dot{Q}_{sink} and the COP relation between heat supply and electricity power demand as shown in equation (3).

$$\dot{Q}_{sink} = \dot{Q}_{source} + P_{el} \quad (2)$$

$$COP = \frac{\dot{Q}_{sink}}{P_{el}} \quad (3)$$

Another reduction of model complexity was achieved by eliminating thermodynamically infeasible matches between process streams and utility levels and only keeping feasible matches as sets to be considered during optimization.

Objective function and constraints

The optimization model is set up as a MILP which minimizes the objective function c subject to sets of linear equality and inequality constraints, represented by g and f , respectively. The decision variables include binary variables x and continuous variables y .

$$\min_{x,y} c(x,y) \quad (4)$$

$$\begin{aligned} \text{s.t. } & g(x, y) = 0 \\ & f(x, y) \leq 0 \\ & x \in \{0, 1\}^m, y \in \mathbb{R}^n \end{aligned}$$

The MILP was solved in Python using Gurobi Optimizer [22] on a desktop computer equipped with an Intel® Core™ i7-12700 CPU @ 2.10 GHz (12 cores, 20 threads). The objective function can be chosen to be TAC, operational expenditure (OPEX), capital expenditure (CAPEX) or CO₂-emissions. In this work, only heat pump investment costs were considered as we focused on retrofit scenarios. We assume electricity driven heat pump compressors and natural gas boilers as existing external heating equipment. Detailed cost calculations and all assumed cost parameters are given in the supplementary material.

Binary variables control the existence of components such as heat pumps and utility temperature levels and the connection between process streams and utility levels. We further define that every process stream must be connected to exactly one utility level.

To accurately model the utility system, energy balances were set up for every utility level. As depicted in Figure 1 of the supplementary material, each utility level can supply heat to cold process streams and receive heat from hot process streams. If that results in a heat deficit, heat must be supplied to this utility level either by an external heat source (e.g. natural gas boiler), a heat pump or through heat cascading from a higher temperature level. If it results in a heat surplus, the utility level must reject heat either via external cooling, to a heat pump or through heat cascading to a lower utility level.

Model limitations

As this modeling approach is designed for screening purposes in utility system optimization, it focuses on fast solution times. In the following, we briefly discuss several simplifications that must be considered when interpreting the results. The first simplification arises from the candidate temperature level reduction. By only allowing temperature levels based on process stream data, heat pump integration might be limited e.g. in cases with gaps between candidate utility levels that exceed the maximum allowable temperature lift of a heat pump. Another limitation comes from the shortcut heat pump model which neglects detailed design of heat pump components as well as working fluid selection.

Moreover, no investment cost for new utility levels is considered as this would require tracking the length of required piping which introduces nonlinearities. While this might be sufficient in retrofit scenarios, where only temperature levels of the existing utility system are adjusted slightly, this becomes important in scenarios where new utility levels are added. For screening purposes, fixed investment costs can be assumed for each

candidate levels to address this simplification. The same applies to heat exchangers, where no additional costs were considered, as heat exchangers were assumed to exist in retrofit scenarios. It should be checked whether the existing heat exchanger area is sufficient for the proposed utility level and process stream connection. Fixed cost parameters for additional heat exchanger area requirements could be provided as input values for every process stream with predefined utility levels. For heat pumps, fixed specific investment costs were considered (see supplementary material). As effects of scale exist for heat pumps [20], this could be accounted for by including linear estimations of cost correlations from the literature. We further assume no temperature glide in heat exchangers on the utility side. While this is accurate for utility levels with latent heat supply and demand via condensation and evaporation, it neglects sensible heat transfer e.g. in cooling water. Finally, no stream splitting is allowed, which neglects potentials for higher energy efficiency especially with process streams with a high temperature difference between starting and target temperature.

CASE STUDY

The synthetic case study discussed in this work consists of 200 hot streams that require cooling and 200 hot streams that require heating. Inlet and outlet temperatures and required heat duties are given as input data, and the respective distributions as well as grand composite curve are presented in the supplementary material. The minimum temperature difference for heat exchangers for every stream of 10 K is provided for every stream. Heat cascading between utility levels is allowed for all scenarios in this work. Sensitivity analysis and parameter studies conducted on the case study are presented in the results and discussion section. The scenarios include analysis of optimal temperature levels for a new utility system as well as retrofit scenarios on an existing utility system.

RESULTS AND DISCUSSION

In the following, the results for several application scenarios for the proposed utility system optimization approach are presented and discussed.

Greenfield scenario

The first scenario is the design of a new utility system for the synthetic case study. This includes the selection of optimal temperature levels and the design of heat pumps. The maximum number of utility levels was increased stepwise from 2 to 15, and the resulting impact on TAC and the number of required heat pumps was evaluated for each configuration. All other parameters were

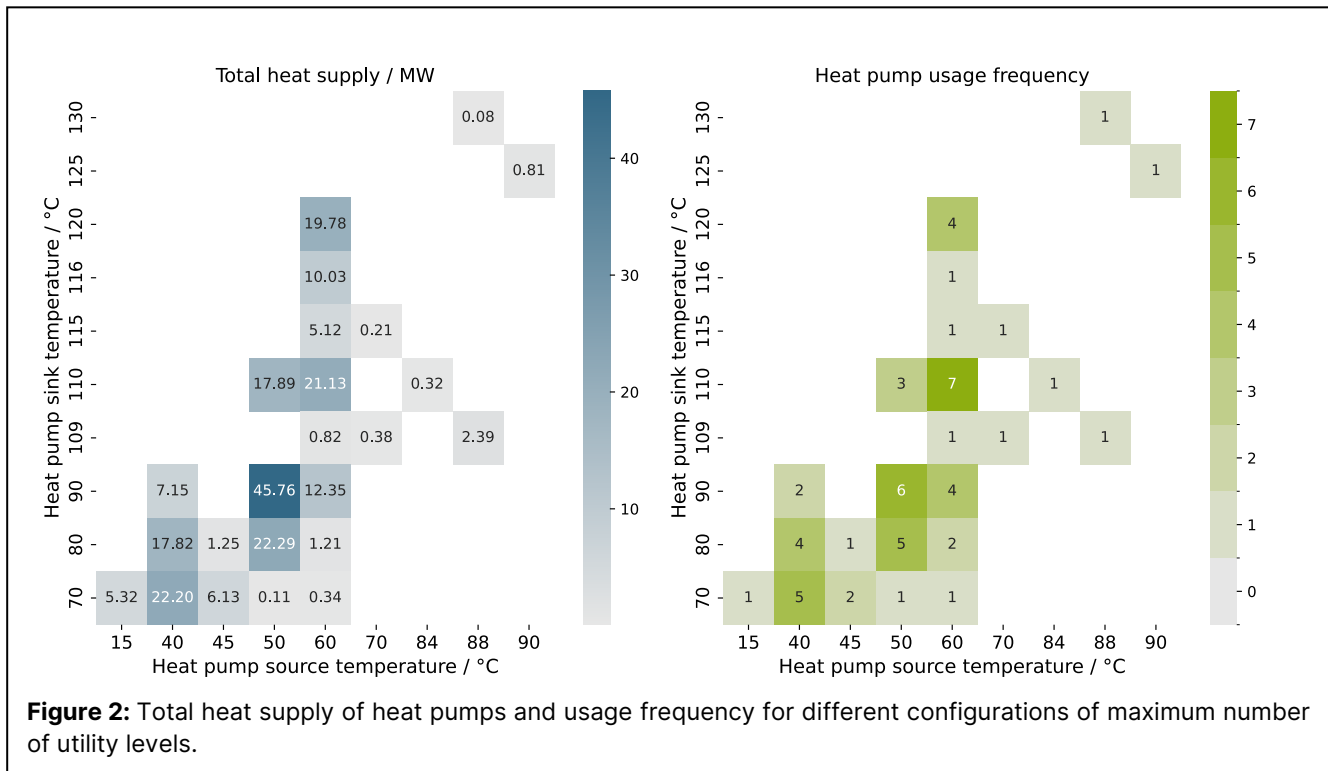


Figure 2: Total heat supply of heat pumps and usage frequency for different configurations of maximum number of utility levels.

kept constant. Candidate temperature level reduction resulted in 156 possible utility temperature which results in an average solver time of 8.5 seconds per configuration. As shown in Figure 1, an increasing number of utility levels results in lower TAC as this allows heat integration and heat pump integration becomes more feasible.

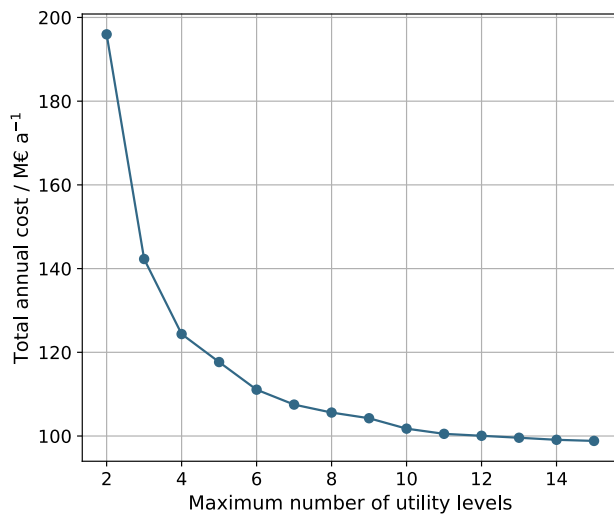


Figure 1. Total annual costs for different allowable utility level configurations.

In Figure 2, selected heat pump configurations for different maximum number of utility levels are shown. In the utility level configurations studied, heat pumps with a source and sink temperature of 60 °C and 110 °C were

selected most frequently. The analysis further reveals the total heat supply provided by every configuration. Comparison with the selection frequency reveal configurations with a high individual substitution potential. Although the heat pump configuration with a source and sink temperature of 60 °C and 116 °C is only selected in one utility configuration it provides a high substitution potential of over 10 MW. Through this analysis, relevant heat pump configurations can be assessed quickly. It further supports decision-making in selecting an appropriate number of utility levels by clearly illustrating the trade-off between TAC and system complexity.

Moreover, the moderate computation times enable the evaluation of multiple cost assumptions, facilitating informed decisions and serving as a solid basis for subsequent detailed analysis.

Retrofit scenario 1

In the following, a retrofit scenario for the synthetic case study is discussed. The assumed utility system has temperature levels at 13 °C, 25 °C, 80 °C, 143 °C, 214 °C, 285 °C and 1600 °C. In a first analysis, the potential for changing the temperature of a single utility level is analyzed. The temperature may be adjusted by 10 K. Resulting TAC savings including heat pump investment costs are compared to the existing utility system structure without heat pump integration.

The lowest original temperature level at 13 °C is modified to 15 °C as this is sufficient to supply cooling to the stream with the lowest outlet temperature but it does not affect the potential for heat pump integration. No

modification could be identified for the levels 80 °C, 214 °C, 285 °C and 1600 °C to improve heat pump integration. TAC savings of 0.28 % can be achieved for the levels 13 °C, 80 °C, 214 °C, 285 °C and 1600 °C by integrating the same heat pump between the levels 25 °C and 80 °C. Only the modification of the utility level at 25 °C and 143 °C improve the potential for heat pump integration and therefore results in TAC savings of 0.36 % and 1.08 % respectively. To achieve this reduction in TAC, the level at 25 °C must be increased to 35 °C and the level at 143 °C must be decreased to 136 °C.

Retrofit scenario 2

In a second retrofit scenario, the same existing utility levels were assumed but two temperature levels could be modified simultaneously. Again, TAC compared to the existing utility system structure without heat pump integration were assessed and included annualized heat pump investment cost and operational cost such as cost for natural gas, electricity and emission certificates as described in the supplementary material. The TAC savings achieved by integrating heat pumps and modifying combinations of utility levels are shown in Figure 3.

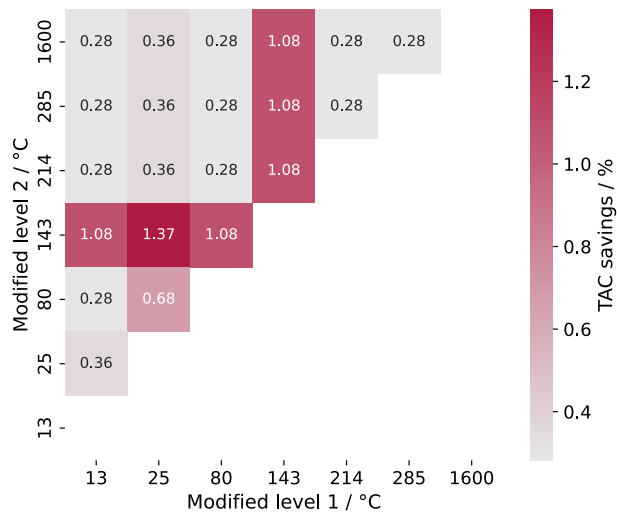


Figure 3. Effect of modifying two utility level temperatures on TAC savings.

While for some combinations, the same savings as in the first retrofit scenario can be seen as no additional heat pump integration is feasible, the combined modification of temperature levels 25 °C and 80 °C leads to TAC savings of 0.68 %. For this, the levels must be adjusted to 35 °C and 90 °C. By modifying level temperatures of 25 °C to 35 °C and 143 °C to 134 °C, higher TAC savings compared to the existing utility structure without heat pumps of 1.37 % can be achieved. Notably, when modifying the 25 °C and 143 °C levels simultaneously, the 143 °C level is adjusted to 134 °C instead of 136 °C, as

observed in retrofit scenario 1 where only a single level was modified at a time.

As both retrofit scenarios only allow temperature adjustments in a range, the number of integer variables for candidate utility levels decreases significantly, resulting in average solver times of 0.2 seconds per configuration which underlines the potential for heat pump integration screening studies of this approach.

Retrofit scenario 3

In cases, where temperature levels of the utility system should not be modified, the complexity of the optimization problem is greatly reduced to only integrating and sizing of heat pumps as well as optimizing connections of process streams to the utility system to increase heat integration. One possible application for this is discussed in the last retrofit scenario. In this scenario, the synthetic case study is used with an existing utility system with the modified temperatures that led to the highest TAC savings in the second retrofit scenario (15 °C, 35 °C, 80 °C, 134 °C, 214 °C, 285 °C, 1600 °C). Sensitivity analysis is used to analyze the effect of different parameters on TAC. The results for varying electricity cost, emission certificate cost, specific heat pump investment cost as well as electricity emission factor are shown in Figure 4 where 0 % variation represents the base value.

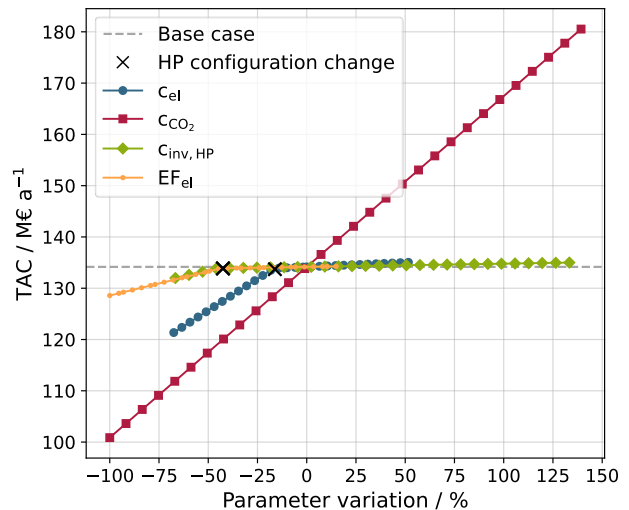


Figure 4. Sensitivity of total annual cost (TAC) to selected model parameters.

Due to the significant reduction of model complexity, the required computational time was around 0.1 seconds per parameter variation.

It is evident that CO₂ certificate costs for emissions associated with heat supplied by burning natural gas and electricity consumption in heat pumps have the highest impact on TAC. At high temperature levels, technical limitations prevent heat pumps from fully replacing external

heat demand, leading to residual emissions. With increasing emission certificate costs in the future, this underlines the importance of defossilization to stay economically competitive. For increases relative to the base value, the remaining parameters lead to only minor rises in TAC. For negative variations, a tipping point, marked as a change in heat pump configuration in Figure 4, can be observed for electricity cost, specific heat pump investment cost and the electricity emission factor. In the base configuration, a single heat pump is used to upgrade heat from the 35 °C utility level to 80 °C. For all cases located to the left of the markers, a second heat pump becomes feasible, enabling a further upgrade from 80 °C to 134 °C. Compared to the base values, a reduction of approximately 45 % in both the specific heat pump investment cost and the electricity emission factor is required for the second heat pump to become feasible, while a reduction of about 16 % in the electricity price is sufficient. In cases with two heat pumps, the total heat supplied by the heat pumps increases significantly, which explains the steeper gradient observed in the sensitivity analysis compared to cases where only one heat pump is feasible. Conducting sensitivity analysis can thus be an important decision support in combination with the utility system optimization in identifying critical model parameters or evaluating future cost and emission scenarios.

CONCLUSION AND OUTLOOK

In this work, a MILP framework for utility system optimization including heat pump integration was proposed. Model complexity was reduced by preselecting relevant utility level candidates, precomputation of feasible heat pump COP as well as elimination of thermodynamically infeasible matches between process streams and utility levels. While the proposed simplifications may exclude certain intermediate optima, they lead to a substantial reduction in computational effort. The resulting short solution times, as demonstrated in the presented case studies, make the approach well suited for screening studies and sensitivity analyses. The optimization framework can be applied to various optimization tasks, including greenfield design and the retrofit of existing utility systems. This was demonstrated with a greenfield design of a utility system, analyzing the impact of allowed utility levels on TAC and heat pump integration. Three retrofit scenarios were analyzed in which selected temperature levels of an existing utility system were modified, and promising adjustments were identified. In addition, the effects of different model parameters on TAC and heat pump integration were identified. Overall, the demonstrated computational performance supports the use of the model in early-stage design and retrofit studies, where multiple design alternatives and parameter variations must be evaluated efficiently. Future studies should further

address the simplifications discussed in the model limitations section, for example by incorporating utility investment costs or additional heat exchanger costs, particularly for applications requiring a more detailed economic assessment. In addition, the influence of the candidate temperature level reduction on solution quality should be systematically assessed and compared to alternative discretization strategies, to quantify the trade-off between computational efficiency and optimality. Overall, the proposed framework provides a robust and computationally efficient basis for the systematic evaluation of heat pump integration options in complex utility system optimization problems.

DIGITAL SUPPLEMENTARY MATERIAL

Detailed description of the model, parameters for different case studies and additional figures. LAPSE:2026.0015

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