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# A Data-Driven Conceptual Approach to Heat Pump Sizing in Chemical Processes with Fluctuating Heat Supply and Demand

**Thorben Hochhaus[a#*], Johannes Wloch[a#], Marcus Grünewald[a], and Julia Riese[b]**

[a] Ruhr University Bochum, Laboratory of Fluid Separations, Bochum, Germany
[b] Paderborn University, Fluid Process Engineering, Paderborn, Germany
[#] Thorben Hochhaus and Johannes Wloch contributed equally to this work.
[*] Corresponding Author: thorben.hochhaus@fluidvt.rub.de.

## ABSTRACT

Heat pumps play a crucial role in decarbonizing the chemical industry. The integration and sizing of heat pumps in chemical processes is a challenging task in multi-product chemical processes due to the fluctuating waste heat supply and heat demand. Integrating heat pumps may require a retrofit of the utility system. Mathematical optimization is a useful tool to tackle this challenge by enabling the analysis of correlation between relevant system parameters and equipment sizing. This study demonstrates the utilization of mathematical optimization and parameter studies for utility system equipment sizing addressing fluctuating heat supply and demand profiles.

**Keywords**: Energy Systems, Batch Systems, Optimization, Renewable and Sustainable Energy, Energy Storage

## INTRODUCTION

To achieve the goal of climate neutrality by 2045, Europe must cut down $CO_2$ emissions significantly [1]. This initiative directly impacts the chemical and pharmaceutical industries, which account for a substantial share of energy usage and related $CO_2$ emissions [2]. One potential approach to lower these emissions is the electrification of chemical and pharmaceutical processes, ideally powered by renewable electricity with a smaller carbon footprint, for instance, through the integration of heat pumps [3]. Pharmaceutical processes are often multi-product plants where heat is supplied using heating and cooling circuits. In these cases, heat is supplied centrally to the utility system. When integrating heat pumps, not only the correct sizing of the heat pump must be determined but also a possible retrofit of the utility system, additional components such as heat storages and backup systems and optimal operation must be considered. This results in a complex integration problem. Mathematical optimization is a method that can solve complex problems like the aforementioned. Different problem types have been solved in the context of utility system optimization for chemical processes. The scope of this paper is to give a brief overview of mathematical optimizations in different applications of utility systems. We further analyse optimal equipment sizing for a utility system in a multi-product plant with fluctuating waste heat supply and heat demand. By using mathematical optimization and parameter studies, we analyse the correlation between system parameters such as specific investment cost or heat profile characteristics and equipment sizing.

## LITERATURE REVIEW

The optimization of utility systems without the integration of heat pumps is a topic that has been extensively studied. A utility system should deliver mostly electricity and heat. Papoulias and Grossmann developed a MILP to minimize costs of a utility system that provides electricity and steam in the context of a chemical plant and to derive the optimal structure of equipment and operation [4]. Other work included nonlinear equations of cost functions and operational constraints, resulting in a MINLP for optimizing the utility system [5]. Mitra et al. optimized operation of an existing utility system under fluctuating electricity prices. Solving the resulting MILP requires precise knowledge of the flexibility parameters of the components. [6]

Several studies also optimize the design and

operation of utility systems including heat pumps with respect to minimizing costs. Bischi et al. linearized non-linear performance curves of equipment to minimize costs using a MILP [7]. Baumgärtner et al. developed a model for a low-carbon utility system incorporating heat pumps. By accounting for time-dependent emission factors, a MILP was employed to analyze the trade-off between economic and environmental impacts. [8] Prendl et al. examined the sizing and operation of a heat pump and heat storage within heat exchanger networks, aiming to minimize total annual costs using a MILP [9].

As previously mentioned, integrating heat pumps into chemical processes poses significant challenges. It may be worthwhile looking at different sectors which also implement heat pumps in their utility system to find possible analogies. One such sector is the residential sector where various methods for heat pump integration and equipment sizing are studied, including mathematical optimization. Molyneaux et al. solved the problem of choosing between centralized and decentralized heat pump integration for district heating in residential buildings using a multi-objective optimization. They compared different systems using multi-objective optimization regarding economic and ecological parameters. [10] Rinaldi et al. determined the optimal size of a system which includes photovoltaic, battery storage and a heat pump for residential buildings by minimizing the total cost. The heat pump enables the system to increase the utilization of electricity generated by the photovoltaic system. Furthermore, the heat pump can be operated flexibly to reduce operating costs, leveraging the building's thermal inertia, as heat only needs to be provided over the course of the day rather than at specific times. [11] Renaldi et al. also analyzed a residential heating system including a heat pump and a thermal storage, by minimising the total costs using a MILP. They considered flexible heat pump operation with upper and lower operating bounds for the heat pump. [12]

A few optimisation approaches compare the solution of mathematical optimization with rules of thumb. Alay et al. use a mathematical approach to optimize the design of a hybrid ground source heat pump for different case studies. The results of the optimization have been compared afterwards with an existing rule of thumb regarding the percentage of the total heat demand covered directly by the heat pump. It became evident that results of the optimisation could not confirm the rule of thumb but rather also vary in a range for different case studies. Furthermore, they highlighted that rules of thumb are often restricted to a specific sector, as general conditions, such as the ratio of cooling to heating, can vary significantly depending on the sector. [13] Fischer et al. examined existing heuristic sizing methods of thermal energy system components like heat pumps and heating storage depending on the operation mode of the heat pump (monovalent, monoenergetic and bivalent). They applied mathematical optimization to minimize total cost for different case studies in the residential sector, taking variable electricity prices into account and compared the results with the heuristic rules. They found sufficient agreement between the heuristic-based design and mathematical optimization approach. Moreover, they underline that the heat demand profile has the greatest impact on sizing. [14]

This further motivates investigating the impact of heat profiles on component sizing within other sectors, such as the chemical industry. In non-continuous chemical processes in particular, the heat demand profiles are not as characteristic as in the building sector and can therefore present an additional challenge for deriving sizing methods for heat pumps. In order for heat pumps to be integrated in chemical processes such as non-continuous processes, their flexibility parameters must be available. Sadjjadi et al. underline the importance of developing methods for sizing and operational strategies of large-scale heat pumps for industrial applications [15]. Part-load efficiencies are relevant to model the flexibility of heat pumps. However, Xu et al. point out that there is no uniform standard for part-load efficiency calculations of heat pumps [16]. Walden et al. used an approach to determine heat pump part-load efficiency by taking the individual component part-load efficiencies into account. They compared this approach to a standard approach which calculates the part-load efficiency by means of a degradation coefficient. [17]

This brief literature review illustrates that equipment sizing for processes requiring flexible operation, such as non-continuous chemical processes, presents a significant challenge. Mathematical optimization proves to be a valuable method to address this complexity, and to analyze the impact of fluctuating heat supply and demand profiles on equipment sizing and operation while incorporating the flexibility characteristics of components.

## PROBLEM STATEMENT

Using mathematical optimization in combination with robust parameter studies allows for the sizing equipment of a utility system and is applied to an application in a multi-product chemical process with resulting fluctuating waste heat supply and heat demand in this work.

To analyze the impact of fluctuating waste heat supply and heat demand, an exemplary scenario has been analyzed as depicted in Figure 1. This can be a typical energy supply system to multiple batch processes with fluctuating heat and cooling demand. Batch operated processes often require heating and cooling intervals following fixed patterns to produce the desired product. These patterns can vary for different products considering heating and cooling duties as well as their duration.

Additionally, batch plants can be multi-product plants without fixed production schedules which can lead to further fluctuations in heat supply and demand.

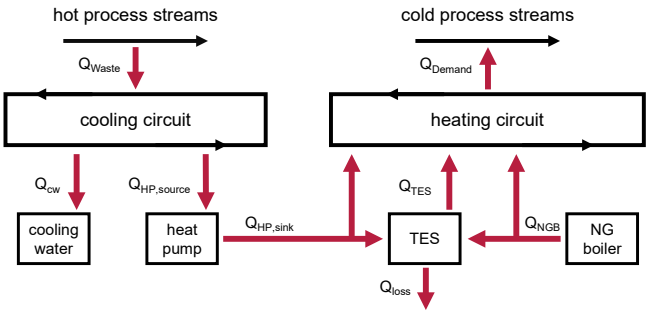


**Figure 1.** Schematic of the examplary utility system.

We assume a brownfield scenario for the chemical process side where heat is supplied to cold process streams using a heating circuit at a supply temperature of maximum 105 °C e.g. through thermal oil or steam. A cooling circuit is used to collect waste heat from the processes at a return temperature of minimum 25 °C e.g. through thermal oil or cooling water. We assume the holdup in the system to be in the range of 15 minutes. To ensure normal operation, the energy demand of the process system must be met by the energy supply for every 15-minute period. The necessary heating and cooling duties are supplied centrally to the heating and cooling circuits.

For the utility side, three technologies are available for a new investment. Firstly, a natural gas boiler which can be used to supply heat to the heating circuit by burning natural gas. Secondly, a vapor compression heat pump which can be used to upgrade waste heat from the cooling circuit to the heating circuit by using electricity to drive the compressor. Lastly, a thermal energy storage can be used to store thermal energy supplied by the natural gas boiler or heat pump and supply it to the heating circuit.

We use a synthetic profile with fluctuations around a mean to emulate a fluctuating heat demand and waste heat profile. The fluctuations are evoked by normally distributed random noise and small and large spikes with normally distributed random amplitude and time between spikes. These fluctuations are assumed to result from fluctuating heating and cooling demand from process streams which must be met by the different utility components. Although we assume a multi-product batch system on the process side, we assume the heating and cooling demand to follow similar patterns. Thus, the cooling duty profile differs from the heating duty profile only by assuming a lag of 15 minutes, as shown in the supplementary material.

## MODEL FORMULATION

The impact of fluctuating demand profiles on equipment sizing was examined using a MINLP to determine the minimum total annual cost. For this purpose, we used simple energy balance models that incorporate efficiency correlations and operational constraints for all components of the utility system. This reduces computational effort and allows for a general system comparison without technology specific characteristics. Including operational expenditure and investment cost allows for minimization of total annual costs. The equations used to model the utility system as well as underlying operational constraints are described in more detail in the following sections and in the supplementary material.

### MINLP

The MINLP formulation minimizes the objective function $c$ subject to sets of linear and nonlinear equality and inequality constraints, represented by $g$ and $f$, respectively. The decision variables include binary variables $x$ and continuous variables $y$.

$$\min_{x,y} c(x,y) \tag{1}$$
$$\text{s.t. } g(x,y) = 0$$
$$f(x,y) \leq 0$$
$$x \in \{0,1\}^m,\ y \in \mathbb{R}^n$$

The component and system constraints must be satisfied for each time interval $t$. Since energy supply and demand must be balanced in 15-minute intervals, this condition applies to every 15-minute timestep within the optimization time horizon of 48 hours.

### Heat Pump

We consider the heat pump (HP) to be a closed-cycle mechanical vapor compression HP. It can be operated with load flexibility concerning its sink duty $\dot{Q}_{HP,sink}(t)$ in a range of 40-100% of the nominal sink duty $\dot{Q}_{HP,sink,nom}$. A constant part-load efficiency is assumed by using a constant coefficient of performance (COP).

To account for operational constraints, we used minimum uptime and downtime constraints. We used binary variables to indicate startups and shutdown and summation constraints to ensure minimum uptime and downtime of the HP. Additionally, we added constraints on the time between load shifts of the HP to account for real world operational challenges during load shifts.

### Natural gas boiler

For the natural gas boiler (NGB), we used a simple model consisting of boiler efficiency ($\eta_{NGB}$) as well as the same operational constraints as for the HP. The duty of the NGB $\dot{Q}_{NGB}(t)$ is allowed to range from 20-100% of the

nominal duty $\dot{Q}_{NGB,nom}$. Again, we assume no decrease in efficiency during partial load.

The same operational constraints were applied for the NGB as for the HP. Binary variables indicate startup and shutdown of the NGB as well as load changes. Limitations for minimum uptime, minimum downtime and time between load changes were implemented analogically. This was done due to a lack of experimental data as well as the motivation to compare different heat supply system configurations instead of a detailed technological comparison. This also ensures that no unbiased preference is given to one component over the other. It follows that the primary distinction between the heat pump and natural gas boiler is the heat pumps supply of cooling duty and different efficiencies for heat supply.

### Thermal energy storage

The simple energy model for the thermal energy storage (TES) includes charging ($\eta_{TES,ch}$) and discharging efficiencies ($\eta_{TES,dis}$) to account for non idealities during charging and discharging. The energy level at the beginning and at the end of the time horizon of optimization is assumed to be 50% of the maximum storage capacity. Moreover, we assume an operating range of 0-100% of the nominal capacity of the TES ($C_{TES,nom}$). The charging and discharging rates of the TES are limited in correlation to the nominal TES capacity. Heat loss $\dot{Q}_{TES,loss}(t)$ to the environment was modeled as a linear efficiency of the actual storage level $C_{TES}(t)$ and efficiency factor $\eta_{TES,loss}$.

### System

The heat demand $\dot{Q}_{heating}(t)$ given by the fluctuating demand profile must be provided to the heating circuit by a combination of the three possible components HP, NGB and TES. Similarly, the waste heat $\dot{Q}_{cooling}(t)$ must be removed from the cooling circuit either by the HP or through cooling water $\dot{Q}_{cw}(t)$. It follows that the HP is limited by the waste heat supply.

### $CO_2$ emissions

As costs for $CO_2$-emission certificates are rising significantly and are expected to still rise in the future, we considered $CO_2$-emissions during operation of the HP and NGB, $e_{HP}(t)$ and $e_{NGB}(t)$ respectively. For the heat pump we used emission factors for electricity $EF_{CO_2,el}$ assuming the compressor is driven by electricity. Likewise, the emission factor of natural gas $EF_{CO_2,NG}$ was used for calculating the emissions of the NGB.

### Cost functions

The minimization of total annual costs (TAC) requires the consideration of operating expenditure (OPEX) as well as investment cost (CAPEX). We are assuming that all components are greenfield and use specific cost factors $f_{inv,i}$ for the HP, NGB and TES. We do not consider operating costs for the TES and only consider costs for $CO_2$-emissions, the required electricity of the heat pump, natural gas as well as costs for cooling water.

## CASE STUDIES

The MINLP has been solved in Python using Gurobi [18]. In the first case study (CS 1), current cost factors for equipment and operation have been used to find the optimal equipment sizing. The profile and cost parameters as well as operating limitations are shown in the supplementary material. Equipment sizing is significantly impacted by the economic parameters as well as the parameters affecting component flexibility. In the case of CS 1, the operational cost of the natural gas boiler combined with costs for cooling water are lower than the operational costs of a heat pump.

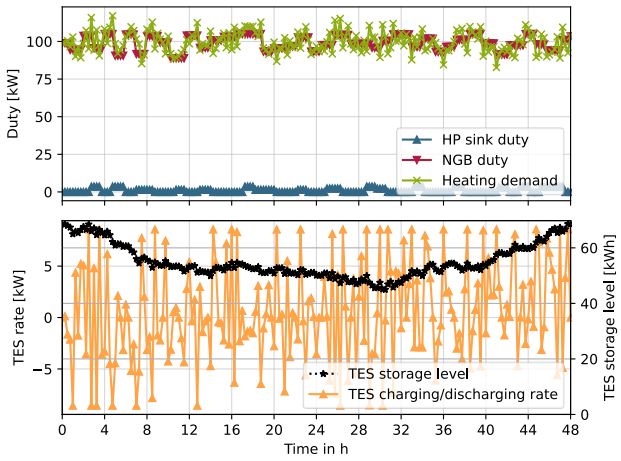


**Figure 2.** Operation and sizing results for CS 1.

Nevertheless, a small heat pump is used to improve the flexibility of the system as shown in Figure 2. NGB and HP are both constraint to a maximum of one load change per hour. With a fluctuating heat demand changing every 15 minutes, this results in heat surplus or heat deficit supplied by the NGB and HP. This mismatch of heat supply and demand can be reduced by shifting the load changes of the HP to time periods where no load shift is allowed for the NGB and vice versa. The remaining mismatch is met by charging and discharging the TES. This subsequently leads to the required storage size. The maximum allowable charging and discharging rates are a function of the nominal storage capacity. Thus, the required storage capacity is directly influenced by the fluctuating heat demand and the flexibility of the other components. In case of no restrictions on load changes of HP and NGB, no TES might be required. On the other hand, with fewer load changes allowed, the required storage capacity increases. Moreover, it is evident that the TES is operated such that the storage level is lower than the

starting and ending level. This is likely because the thermal energy loss is a function of the current energy stored in the energy storage. By reducing the energy stored in the storage, the energy loss is reduced.

In case study 2 (CS 2), we conducted a parameter study to determine the effect of varying specific HP investment cost on equipment sizing. As shown in Figure 3, for low specific investment costs, the heat pump is preferred over the natural gas boiler. The TES is used to buffer the supply and demand mismatch which result from load change restrictions of the HP. High specific investment cost led to a small HP design. This requires higher TES capacity to buffer the mismatch between heat supply and demand, because load changes of the HP only have a small contribution. In cases where the operational and investment costs of the HP exceed those of a NGB, the HP may nonetheless be favored due to its ability to provide cooling services. This characteristic contributes to a reduction in costs associated with cooling water consumption.

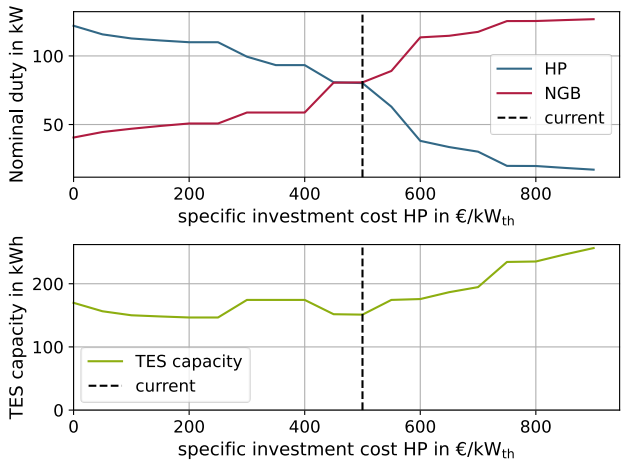


**Figure 3.** Impact of specific HP investment cost on equipment sizing.

To further examine the impact of different economic and profile parameters on equipment sizing, we conducted a parameter study in case study 3 (CS 3). The sensitivity parameter ranges are shown in the supplementary material. As depicted in Figure 4, there is a strong correlation between the standard deviation of the demand profile and the required capacity of the TES. For cases with restrictions on load shifts for the HP and NGB, the TES is required to buffer the resulting mismatch between heat supply and demand. For current price ratios of electricity to natural gas and lower investment cost of the NGB favor the NGB over the HP. The TES is required to buffer the mismatch between heat supply and demand resulting from load shift limitations of the NGB. As shown in Figure 4, for a price ratio of 1.5, the HP has lower operational costs and is therefore preferred over the NGB. With increasing standard deviations, the NGB and TES are utilized to buffer profile fluctuations. At a standard deviation of around 33, a new trend can be identified. The nominal heat duty of the NGB increases significantly and the required TES capacity is reduced. In profiles with standard deviations greater than 33, low waste heat supply and peaks in heat demand appear at the same time. In these cases, the HP can not be used to supply heat which requires the NGB and TES to buffer the mismatch. The NGB requires lower investment costs for the same output heat duty than the TES and is therefore preferred over the TES.

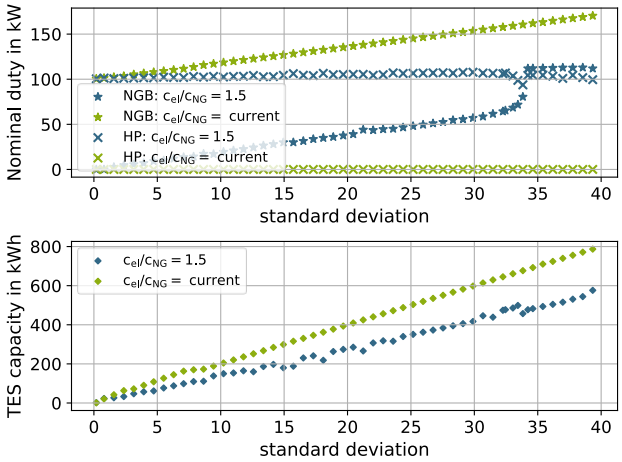


**Figure 4.** Correlation between the standard deviation of the demand profile and nominal TES capacity for different ratios of operating costs.

## CONCLUSION

In the present study, we analyzed the impact of fluctuating waste heat supply and heating demand in the context of chemical processes on utility equipment sizing. It is evident that equipment sizing is a complex task which is affected by many different aspects such as profile and cost parameters as well es equipment constraints. Parameter studies may support understanding the dependencies in a utility system and identifying economically feasible conditions. They can also help in identifying change points in optimal solutions e.g. for different degrees of fluctuations in the demand profile.

From our view, it is important to conduct further research on equipment flexibility parameters, since equipment sizing for fluctuating profiles is significantly dependent on equipment flexibility. Moreover, different types of profile fluctuations can be studied such as step profiles and seasonal profiles. Comparing statistical parameters of real-world profiles and synthetic profiles or combinations of synthetic profiles may help in qualitatively identifying the best combination and sizing of equipment.

## DIGITAL SUPPLEMENTARY MATERIAL

Detailed description of the model, parameters for the different case studies and figure of exemplary waste heat supply and heat demand. LAPSE:2025.0011

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