

**ENERGY RESOURCE EFFICIENT INDUSTRIAL ENERGY SUPPLY SYSTEMS
FOR DECARBONIZATION – ADAPTION OF MIXED-INTEGER DESIGN AND
OPERATION OPTIMIZATION MODELS FOR DISCRETIZED HEAT RECOVERY**Matthias Traninger^{1*}, Anton Beck¹, Sophie Knöttner¹¹AIT Austrian Institute of Technology, Center for Energy, Vienna, Austria*Corresponding Author: matthias.traninger@ait.ac.at**ABSTRACT**

Climate change calls for immediate action in all sectors. Industrial energy supply causes roughly one third of global primary energy consumption and greenhouse gas emissions in the same order of magnitude. Addressing decarbonization goals without taking measures to increase energy efficiency beforehand e.g., through using available excess heat potentials, leads to increased operational expenditures and keeps end energy usage at an unnecessarily high level.

Optimization of heat integration via methods of heat exchanger network synthesis (HENS) as well as design and operation optimization (DOO) based on mixed-integer linear programming (MILP) formulations proved to support energy managers, plant operators and decision makers when evaluating new and adapted concepts for increased energy efficiency in industrial production and energy supply systems.

HENS addresses the question of optimal heat integration within energy supply systems for known heating and cooling requirements. It thereby proved to be a valuable method for identification of exergetically optimal utilization of excess heat potentials in energy supply systems. In contrast, DOO seeks to optimize the structure and the energy flows in energy supply and distribution systems to satisfy predefined process demands, such as heat at given temperature levels, power, or fuel demands.

Simultaneous optimization of heat exchanger network design and supply system design and operation proved to be a demanding task, due to highly non-linear models. This paper introduces a simple MILP component model, that combines some of the advantages of commonly used HENS formulations, with those of state-of-the-art DOO formulations. It allows for utilization and provision of available heat flows in predefined temperature stages within a superstructure of an industrial energy supply system. By considering different cooling and heating requirements, as well as excess heat potentials, the optimal heat flow in the energy supply system can be determined. In future work, this approach can easily be extended for commonly used features in HENS-formulations, such as forbidden or restricted matches of streams and calculation of necessary heat exchanger areas.

To showcase the capabilities of the proposed formulation a case study based on a generalized energy supply model of a pharmaceutical production facility was conducted. It shows that applying cascaded usage of thermal energy, as modeled with this new formulation, the primary energy consumption of a commonly used process in pharmaceutical production can be reduced by 5.7 to 15.5%, compared to the traditional modeling approach used in the reference scenarios.

1 INTRODUCTION

The decarbonization of all major contributing sectors has become increasingly urgent in recent years. Thus, requirements on a regulatory and legislative level are currently defined and rolled out. This results in new challenges for industrial energy supply systems which cause approximately one third of the primary energy consumption worldwide and emissions in the same order of magnitude (Bashmakov *et al.* 2023). In production processes with high temperature requirements, such as the production of different metals, ceramic, cement or various chemicals, fuel switch and electrification are promising measures for future energy supply options. However, the available quantities of green gases for simple fuel switch will remain limited and their exergetically sensible utilization should be treated as a priority. Therefore, energy efficiency measures should be used as means to effectively reduce primary energy consumption in the first place.

Measures such as adaption of existing processes in terms of lowered heat transfer medium temperatures pose a significant improvement potential for sustainable energy supply. Advantages of intermediate temperature heat distribution networks are (1) reduced transport/radiation losses, (2) more efficient energy provision with heat pumps and (3) a higher potential for integration of existing excess heat potentials (e.g., flue gas condensation, heat recovery from compressed air generation, etc.).

In the past, different modeling approaches proved to support energy managers, plant operators and decision makers when evaluating new and adapted concepts for industrial production and energy supply systems. Beside physical simulation models also mathematical programming and especially the class of MILP gained interest in the last two decades. Some examples of optimization applications are DOO, scheduling, and HENS. Especially, for combined techno-economic-ecologic assessments mathematical programming models proved valuable since all these aspects can be accounted for in an objective function simultaneously.

Common formulations of DOO try to answer the subsequent question: *Which (mix of) energy conversion technologies, which capacities of those technologies and which energy carriers are needed in order to supply processes with a predefined amount of energy in a cost-optimal way?*

In case of thermal energy systems, also the qualities of heat (temperature and pressure of heat transfer media) are considered. The primary purpose of this kind of model is to obtain the optimal energy flow through the energy supply system with explicit consideration of different operating points, i.e., energy flows or mass flows are among the variables to be optimized. These varying operation points are imposed by the temporal resolution of the optimization. This dimension is typically introduced by a number of discrete time steps with a defined temporal resolution.

Although non-linear models are used for DOO, linearized models were shown to offer a good trade-off between accuracy and runtime for the purpose of energy supply system studies (Ommen *et al.* 2014).

Energy supply systems often use so-called superstructures, which represent the space of opportunity of available energy carriers, conversion technologies and excess heat potentials among which the model can select. The selection of available elements in this space can be subject to boundary conditions such as limited space for new plants, upper capacity limits for supply grids, etc.

Objective functions are typically economic in nature and seek to minimize total annualized costs (TAC) for investment and operational costs over a given depreciation period and a defined interest rate.

HENS is a wide and actively researched field, especially regarding different kinds of methodical implementations and computationally efficient mathematical programming formulations. In general, the question of optimal heat integration addressed by HENS-approaches can be stated as follows: *Given defined heating and cooling requirements for process streams (i.e., defined target temperatures and mass flow capacities), how can these requirements be satisfied by direct heat recovery from existing process streams with minimum overall costs?*

HENS approaches seek a way to optimize heat integration by placement of heat exchangers (HEXs) with optimized inlet and outlet temperatures within a set of available hot and cold streams.

Yee and Grossman proposed a MINLP model for simultaneous optimization of utility cost, HEX areas and stream matches based on a stage-wise representation, where “within each stage, potential exchanges

between hot and cold stream can occur” (Yee *et al.* 1990; Yee and Grossmann 1990). Even though an effective linearization of the proposed multi-stage structure exists (Beck and Hofmann 2018), the high number of binary variables in these problem formulations easily leads to a significant increase in combinatorial complexity and computationally demanding models. The resulting complexity can be somewhat reduced by definition of forbidden, restricted and required matches of streams. Also, instead of deterministic solvers metaheuristics such as genetic algorithms are applied to facilitate the solvability of HENS models (Xu *et al.* 2023).

Another actively researched aspect of HENS is the multi-period problem. Single-period HENS leads to optimal heat integration for only one operating point of the system (i.e., defined heat flow capacity and stream parameters). Extension to a multi-period problem is possible, but further increases the complexity of the model.

In conclusion, HENS models seek to optimize stage temperatures as continuous variables and stream matches as binary decisions, while heat capacity flow rates are considered constants. This is the case since simultaneous optimization of temperatures and mass flow would lead to a highly non-linear model. This issue of an integrated optimization of optimal heat integration and DOO is generally recognized (Martelli *et al.* 2017; Xu *et al.* 2023).

In practice, benefits of direct heat recovery are effectively reduced due to circumstances like long distances between potential stream matches as well as temporal dependencies of heat flows (e.g., batch-processes vs. continuous processes). Also, direct heat recovery might lead to a reduced flexibility of the overall energy distribution system operation, due to increased interdependencies of heat flows. In such cases, intermediate temperature heat distribution networks are a sensible way of providing processes in an exergy efficient manner. The required temperature levels for such distribution networks are predetermined by the processes themselves (start and target temperatures, heat transfer coefficients, etc.), thus making a continuous optimization of stream temperature for heat integration (as performed in HENS approaches) obsolete.

A way to account for exergetically optimized use of excess heat in distributed energy systems was proposed by Wang *et al.* (2018). They developed a model to optimize the utilization of energy by its quality (i.e., temperature level) employing a cascade of waste heat utilization technologies using a MILP formulation. They defined meaningful operating temperature ranges for different excess heat utilization technologies such as absorption refrigeration cycles, Rankine cycles, or organic Rankine cycles. By providing excess heat at different temperature levels (flue gas and low temperature heat) to this utilization cascade, the model allows for thermally optimized selection of waste heat utilization technologies by finding optimal waste heat recovery temperatures. For the purpose of keeping the model linear, they discretized the available excess heat mass flow. (Wang *et al.* 2018)

The present work proposes an adaption of the approach introduced by Wang *et al.* (2018) for utilization in state-of-the-art MILP DOO models. For this purpose, not temperature levels but energy flow rates (or mass flows, respectively) are continuous optimization variables, while temperature levels are considered constants. This model adaption provides a targeted and efficient approach, especially for heat supply systems and heat demands with existing temperature requirements.

The effectiveness of this formulation in terms of heat integration and reduced primary energy consumption is demonstrated in a case study conducted on the generalized energy supply system model of a pharmaceutical manufacturing facility.

2 METHODOLOGY

2.1 Design and operation optimization framework

The proposed formulation for temperature-discrete optimized heat flow is implemented as a component model, hereafter called *unit* model, in an existing in-house model library for commonly used components and plants of industrial energy supply systems. All units are formulated as mixed-integer linear programs. The unit models available in the model library can be categorized in:

- supply units (grid connection, photovoltaics, power-purchase agreements, ...)
- conversion and storage units (gas boiler, heat pump, electrode boiler, hot water storage, ...)
- demand units
- auxiliary units (units to model certain aspects of the system without physical counterpart)

The industrial energy system in question is modeled as a superstructure of interconnected units. All units are modeled as simplified and linearized models of the physical entity they represent. Units are subject to constraints, e.g., a heat pump has certain minimum uptime and downtime, minimum part load, ramping constraints, and contribute to the overall objective function. Energy supply units are associated with cost per unit of energy consumed but can also have power-related cost or a maximum supply capacity. So-called demand units represent predefined energy or mass flows with an associated temporal resolution.

Individual units expose so-called *ports* (e.g., for power, fuel, heat, etc.), which provide a way to interlink them within the superstructure via *nodes*. Nodes represent energy or mass balances and connect the unit ports in the model according to the energy and mass flows in the modeled industrial energy system. Units which are potentially added to the energy supply system can be associated with investment cost in the respective objective function.

The objective function is of economic nature and accounts for the TAC of the system. The overall objective is the sum of all the cost-related contributions of each unit. Its generalized form is stated in equation (1).

$$\min \text{TAC} = C_{\text{invest}} + C_{\text{energy}} \quad (1)$$

Where C_{invest} corresponds to the investment cost for new units and is subject to a certain depreciation period in years and an interest rate. C_{energy} corresponds to the cost of energy purchased from grid/energy supplier. The solution of the optimization problem provides information on optimal operation of each unit and on new units and their capacities.

2.2 Temperature-discrete heat flow optimization

2.2.1 Unit Model Description

The subsequently introduced formulation (referred to as “heat flow allocator” further on) allows an exergy-optimal allocation of temperature-discretized heat flows applied within the MILP DOO framework introduced in chapter 2.1. The heat flows provided as input to the heat flow allocator must either be cooled (utilization of model as *cooler*) or heated (*heater*) from a starting temperature to a target temperature. For this to happen, excess heat made available can be utilized from (*cooler*) or must be supplied to (*heater*) a predefined number of temperature stages. The optimal allocation of heat flows with regard to the objective function is subject of the optimization. A graphical representation of the heat flow allocator is shown in **Figure 1**. In the context of a model superstructure, each heat flow connected to a stage can be assigned to a heat distribution network with its associated temperature or even another heat flow allocator of the opposite type (heater-to-cooler connection).

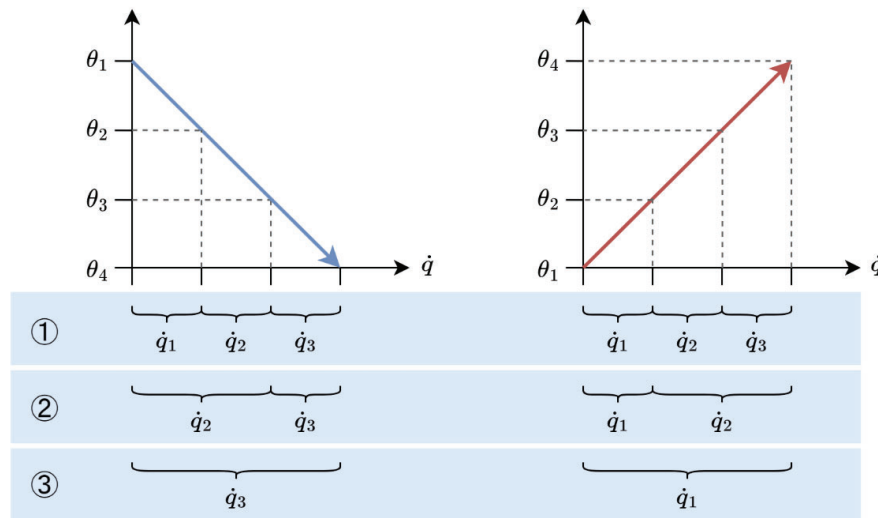


Figure 1: Temperatures θ vs. heat flow rates $\dot{q}_t$ for stages $i \in \{1, 2, 3\}$ at a given point in time. Cooling (left diagram) and heating (right diagram) of process streams (diagonal arrows, blue and red) indicated by temperature change from θ_1 to θ_4 . Heat flow rates $\dot{q}_t$ indicate the maximum available heat flow at stage i (shown in ① for stages 1-3). If heat is not utilized in higher-temperature stages, it can be used in lower-temperature stages (e.g., as shown in ② and ③).

2.2.2 Mathematical Formulation

Sets

The proposed formulation comprises of n different temperature stages described by set $I = \{1, \dots, n\}$ and is indexed by i . These stages are bounded by $m = n + 1$ temperature levels. Also, this problem is considered for a discrete number of time steps denoted by the set $T = \{1, \dots, o\}$, indexed by t .

Variables

To model the discretization, the heat flow allocator model uses of the following variables for every time step t :

- $\dot{q}_t$ total heat flow rate into/out of unit
- $\dot{m}_t$ mass flow rate corresponding to heat flow rate $\dot{q}_t$
- $\dot{q}_{i,t}$ heat flow rate at stage i
- $\dot{q}_{max\ i,t}$ maximum available heat flow rate out of/into stage i
- $\dot{q}_{res\ i,t}$ residual heat flow rate passed from one stage to the next

All variables are subject to a non-negativity constraint.

Parameters

The parameters used in the heat flow allocator model are:

- $\theta_{i,t}, \theta_{i+1,t}$ boundary temperatures of stage i
- $\Delta h_{i,t}$ difference in specific enthalpies in stage i between temperatures θ_i and θ_{i+1} (cooler unit) and θ_{i+1} and θ_i (heater unit), respectively (valid for sensible temperature change of the medium)

Depending on the actual implementation of this model, the enthalpy-based approach allows to account for different heat transfer media and different states of those media, e.g., sensible temperature change, condensation of flue gas, by using thermodynamic property databases.

Constraints

The following constraints are established, to model the desired behavior.

Equation (2) establishes a relation between mass flow rate $\dot{m}_t$ and heat flow rate $\dot{q}_t$:

$$\dot{q}_t = \dot{m}_t \sum_i \Delta h_{i,t} \quad \forall t \in T \quad (2)$$

Equation (3) describes the maximum available heat flow rate $\dot{q}_{max\,i,t}$ at stage i depending on the mass flow $\dot{m}_t$ for every time step t .

$$\dot{q}_{max\,i,t} = \dot{m}_t \Delta h_{i,t} \quad \forall t \in T, \forall i \in I \quad (3)$$

The heat flow $\dot{q}_{max\,i,t}$ can either be used in stage i or passed on to lower-temperature stages via the residual heat flows $\dot{q}_{res\,i+1,t}$ (cooler) or $\dot{q}_{res\,i,t}$ (heater), respectively. This cascade is modeled in the overall energy balance per temperature-discrete stage i (equation 4) and is depicted in **Figure 2**.

$$\dot{q}_{i,t} = \dot{q}_{max\,i,t} + \dot{q}_{res\,i,t} - \dot{q}_{res\,i+1,t} \quad \forall t \in T, \forall i \in I \quad (4)$$

In case of **optional** utilization of available heat (*cooler* unit), meaning that not all the available heat flow $\dot{q}_t$ has to be used in the cascade, this energy balance can be formulated as an inequality ($\leq$).

The residual heat flow entering the highest temperature stage as well as the heat flow exiting the lowest temperature stage must be set to zero since there is no residual energy flow into or out of those stages, respectively (equations 5 and 6).

$$\dot{q}_{res\,1,t} = 0 \quad \forall t \in T \quad (5)$$

$$\dot{q}_{res\,m,t} = 0 \quad \forall t \in T \quad (6)$$

Objective function

For the heat flow allocator model itself there is no associated contribution to the objective function considered for this work. The minimization of TAC of the system leads to an overall cost-optimal supply of energy including the exergetically optimal distribution of energy flows. However, by defining an associated contribution to the objective function, cost for e.g., integration of heat exchangers can be considered.

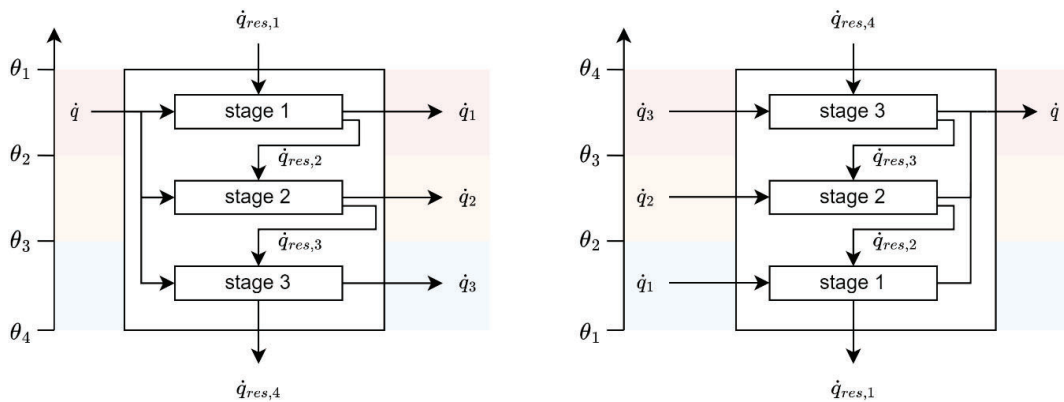


Figure 2: Visual representation of heat flows for *cooler* (left) and *heater* (right) instances of the heat flow allocator model in a simplified scheme with $n = 3$ stages for a given point in time. $\dot{q}$ refers the total heat flow into (cooler) or out of (heater) the unit, respectively. The heat flows $\dot{q}_i$, $i \in \{1,2,3\}$, refer the optimized heat flows out of (cooler) or into (heater) the unit at stage i , respectively. The heat flows $\dot{q}_{res}$ denote heat flows passed from stages with higher to stages with lower temperatures. The temperatures θ represent the upper and lower boundary temperatures θ_i and θ_{i+1} (cooler) as well as θ_{i+1} and θ_i (heater) of stage i .

2.3 Case Study – Pharmaceutical Energy Supply System

This case study compares the implications of the proposed formulation for exergy-optimal allocation of energy flows in a generalized energy supply system of a pharmaceutical manufacturing facility by showcasing the commonly applied process of generation of water for injection (WFI).

Production of WFI is a great example of a primary energy savings potential becoming accessible by a change of technology. Traditionally, WFI is created by evaporation and condensation in multi-effect distills and stored at a temperature of around 80 °C to avoid germination. WFI can either be used at this temperature for e.g., rinsing processes or is actively cooled for use at room temperature. While from an engineering point of view, this distillation-based production process is quite energy efficient, it still relies on high supply temperatures – in most cases provided by a fossil-fired steam utility.

WFI can also be produced via a sequence of water purification and filtration processes, a process which is already approved by most of the major regulatory authorities for pharmaceutical products. While this process does not need high temperatures in its production process, WFI still needs to be heated to approx. 80 °C regularly for either decontamination purposes or for hot application in processes.

2.3.1 Reference Energy System

Figure 3 shows the model superstructure of the energy system in consideration. While existing energy conversion and storage units (yellow arrows) can be used in all scenarios, the system can be extended by investment in new units (white arrows). This allows for a decarbonized and more efficient provision of energy via means of electrification (heat pumps and electric boilers) and heat integration measures. Heat integration is made possible via a cascade of **four heat distribution systems** with different temperatures, interconnected with heat pumps. Excess heat can be allocated to (*cooler* unit) or supplied from (*heater* unit) those heat distributions systems with the newly introduced heat flow allocator unit (light blue arrows). WFI can either be produced by means of membrane-based ultrafiltration or distillation.

2.3.2 Scenario Definition

The scenarios defined hereafter are designed to assess the impact of decarbonization and optimal allocation of heat flows on the commonly used process of WFI generation, by using the heat flow allocator model formulation. For this purpose, primary energy consumption, carbon emissions as well as TAC are compared to the status quo.

The status quo is represented by a *base* scenario, **without** any requirements regarding **decarbonization** and traditional WFI generation via multi-effect distillation. Furthermore, two additional groups of scenarios explore (1) a **fully decarbonized energy system**, in which WFI generation is either possible via the traditional distillation-based route (*distillation* scenarios) and (2) the energy efficient alternative process of filtration-based WFI generation (*ultrafiltration* scenarios).

In both of these two scenarios a commonly used problem formulation **without** optimal heat flow allocation (*reference*) is compared to the **newly introduced heat flow allocator formulation** (*optimal allocation*).

In the *base* scenario and the two *reference* scenarios, heat demand can only be met by sources that provide higher quality heat e.g., the use of low-pressure steam for sensible heating and evaporation of water. In contrast, the new heat flow allocator model allows for cascaded use of available heat sources e.g., preheating of water and subsequent evaporation with low-pressure steam.

In summary, the scenarios are as follows:

- *Base* scenario
- *Distillation* scenarios
 - Reference
 - Optimal allocation
- *Ultrafiltration* scenarios
 - Reference
 - Optimal allocation

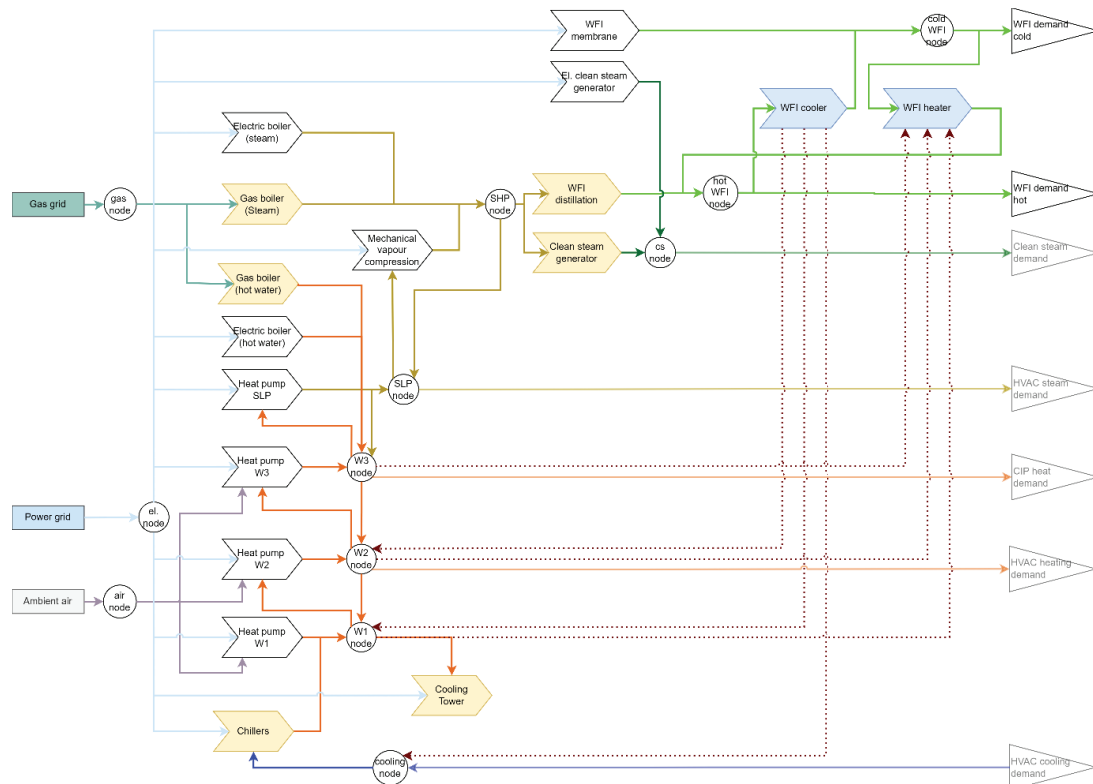


Figure 3: Energy flow sheet of the energy supply and distribution system of a pharmaceutical manufacturing facility. White arrows represent existing units, yellow arrows possible additions to the energy system. Light blue arrows represent the proposed heat flow allocator unit model. Dotted lines indicate heat flows from/to unit stages to/from available heat distribution networks (cold water, W1, W2, W3). The energy supply side is indicated on the left side, process demands on the right side. The conducted case study only considers hot and cold WFI demands (black triangles), further demands are indicated in grey color. Legend: SLP...steam low pressure, SHP...steam high pressure, HVAC...heating ventilation and air condition, CS...clean steam

2.3.3 Model Parameters

The model considers temporal profiles for 12 representative days scaled up to one year. These profiles include ambient air conditions and WFI consumption rate. Distillation-based WFI generation accounts for 2 GWh of natural gas consumption. All scenarios assume WFI demand at ambient temperature (20°C, 20% of total demand) as well as hot WFI demand (80°C, 80% of total demand). Electrical energy is assumed to be carbon neutral. Second law efficiency of heat pumps is assumed to be 50%. Membrane-based WFI generation consumes 6.75 kWh/m³ WFI according to Cataldo *et al.* (2020). In all optimizations a depreciation period of 10 years is considered. Investment cost and energy carrier cost are summarized in **Table 1**.

Table 1: Investment cost for energy conversion units (ECU) and cost of energy carriers

ECU / energy carrier	Costs	Unit
electric steam boiler	200	€/kW
electric hot water boiler	150	€/kW
hot water heat pumps	400	€/kW
steam heat pump low pressure	600	€/kW
mechanical vapor compressor	600	€/kW
natural gas	40	€/MWh
electricity	100	€/MWh

3 RESULTS

3.1 Impacts of Decarbonization

Full decarbonization of the energy supply system by means of electrification is possible and leads to a reduction in CO₂ emissions of 418 t_{CO2}/a in scenarios *distillation* and *ultrafiltration* compared to scenario *base*.

In the *distillation* scenarios high pressure steam at 180°C for WFI generation is generated by means of electric steam boilers, hot water and steam heat pumps and mechanic vapor compression with additional accumulated installed capacity of 0.96 MW_{th}. By using energy efficient ultrafiltration technologies for WFI generation (*ultrafiltration* scenarios), high temperature steam is not needed anymore, thus the accumulated installed capacities account for only 0.38 MW_{th}. The technologies for decarbonization chosen in the optimization are heat pumps and a small electric boiler for peak demands. In both cases, ambient air is used as source of low-temperature heat for heat pumps. Total annualized costs for energy and investments are shown in **Figure 4**. The chosen measures lead to a reduction in primary energy consumption by up to 76.6% in *ultrafiltration* scenarios and 45.8% in *distillation* scenarios (**Figure 5**).

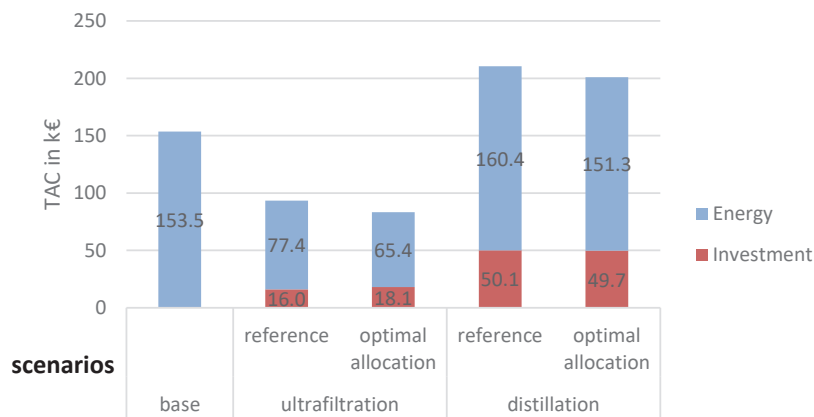


Figure 4: TAC for energy and investments for a depreciation period of 10 years. Scenario *base* represents the status quo of the fossil-fired energy system. Scenarios *ultrafiltration* and *distillation* assume a full decarbonization of heat supply. *Reference* cases depict the resulting TAC obtained with simple model formulation, *optimal allocation* cases depict TAC for optimally allocated heat flows obtained with the heat flow allocator model proposed in this work.

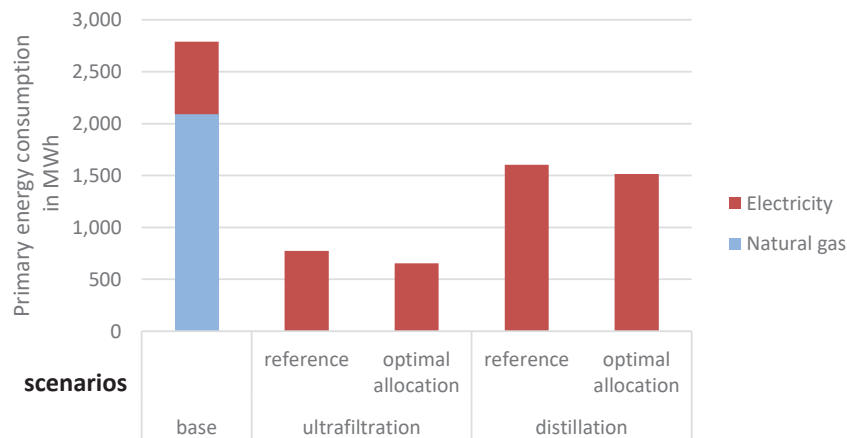


Figure 5: Primary energy consumption (PEC) in MWh per year. PEC is reduced by 72.3% (*reference*) and 76.6% (*optimal allocation*) in *ultrafiltration* scenarios and 42.5% (*reference*) and 45.8% (*optimal allocation*) in *distillation* scenarios.

3.2 Assessment of Proposed Model Formulation

A comparison of the results of the *reference* scenarios to the *optimal allocation* scenarios for both WFI generation technologies (*ultrafiltration* and *distillation*) shows that the proposed formulation indeed **allows to find a more exergy-efficient allocation of heat flows** within the modeled system. This is primarily reflected in reduced energy consumption in both *optimal allocation* scenarios compared to their *references*.

Moreover, in both *optimal allocation* scenarios additional heat pumps are integrated to supply lower-temperature heat distribution networks. In case of the *ultrafiltration* scenarios, these additional investments result in a marginally increased TAC compared to the *reference* scenarios. However, primary energy consumption in *optimal allocation* cases is decreased by 15.5% (*ultrafiltration*) and 5.7% (*distillation*) compared to the *reference* cases, respectively. In total, TAC for energy and investment costs are reduced in both *optimal allocation* scenarios compared to the *reference* scenarios due to increased exergy efficiency in heat provision (**Figure 4** and **Figure 5**).

Although the results are promising and the heat flow allocation model incorporates aspects of the real-world system not considered in simpler modeling approaches, e.g., in the *reference* scenario, further research is required to validate these findings.

4 CONCLUSION AND OUTLOOK

The proposed MILP heat flow allocator model adds functionality to commonly applied design and operational optimization superstructures by introduction of cascaded heat utilization. Typical energy flow-based optimization models do not generally allow for cascaded heat usage, and therefore do not adequately represent real life options for heat integration. This model overcomes these limitations and extends the solution space of the model to better reflect the physical system.

The case study conducted leads to the conclusion, that the proposed model allows to identify options for a more exergy-efficient allocation of heat flows within the modeled energy system resulting in a reduction in primary energy consumption of 5.7 to 15.5% (*optimal allocation* scenarios) compared to the system identified with the traditional model formulation (*reference* scenarios). However, the increase in exergy efficiency achieved with this model is dependent on the energy system in consideration. Furthermore, a detailed validation of the heat flow allocator model was beyond the scope of this paper and is still to be carried out.

High potential for the application of the new heat flow allocator model is expected in systems with multiple excess heat sources with large temperature ranges (e.g., flue gas condensation, heat recovery from compressed air generation) and heat sinks at different temperature levels in combination with several intermediate temperature heat distribution systems.

The proposed heat flow allocator model offers multiple options for further development. It can easily be extended to allow restricted, forbidden or required stream matches (i.e., utilization of heat) in certain temperature stages. Also, heat exchanger area calculation and an objective function to account for heat exchanger costs can be implemented by only minor additions to the model. From a research perspective a comprehensive comparison of results obtained with the proposed formulation with those of traditional HENS formulations would be beneficial.

NOMENCLATURE

CO ₂	carbon dioxide	
DOO	design and operational optimization	
ECU	energy conversion unit	
HENS	heat exchanger network synthesis	
HEX	heat exchanger	
MILP	mixed-integer linear programming	
MINLP	mixed-integer non-linear programming	
TAC	total annualized cost	
I	set of temperature-discrete stages	
T	set of time steps	
Δh	difference in specific enthalpy	(J/kg)
$\dot{m}$	mass flow rate	(kg/s)
$\dot{q}$	total heat flow rate into/out of unit	(W)
$\dot{q}_i$	heat flow rate out of/into stage i	(W)
$\dot{q}_{res}$	residual heat flow rate between neighboring stages	(W)
$\dot{q}_{max}$	maximum available heat flow rate	(W)
θ	temperature	(°C)

Subscript

i	temperature stage index
m	number of temperature levels
n	number of stages
o	number of time steps
t	time step index

REFERENCES

- Bashmakov, I.A.; Nilsson, L.J.; Acquaye, A.; Bataille, C.; Cullen, J.M.; de la Rue du Can, S. *et al.* (2023): Industry. In IPCC (Ed.): Climate Change 2022. Mitigation of Climate Change. Contribution of Working Group III to the Sixth: Cambridge University Press, pp. 1161–1244.
- Beck, Anton; Hofmann, René (2018): A Novel Approach for Linearization of a MINLP Stage-Wise Superstructure Formulation. In *Computers & Chemical Engineering* 112, pp. 17–26. DOI: 10.1016/j.compchemeng.2018.01.010.
- Cataldo, Alessandro Luigi; Sissolak, Bernhard; Metzger, Karl; Budzinski, Kristi; Shirokizawa, Osamu; Luchner, Markus *et al.* (2020): Water related impact of energy: Cost and carbon footprint analysis of water for biopharmaceuticals from tap to waste. In *Chemical Engineering Science: X* 8, p. 100083. DOI: 10.1016/j.cesx.2020.100083.
- Martelli, Emanuele; Elsidio, Cristina; Mian, Alberto; Marechal, Francois (2017): MINLP model and two-stage algorithm for the simultaneous synthesis of heat exchanger networks, utility systems and heat recovery cycles. In *Computers & Chemical Engineering* 106, pp. 663–689. DOI: 10.1016/j.compchemeng.2017.01.043.
- Ommen, Torben; Markussen, Wiebke Brix; Elmegaard, Brian (2014): Comparison of linear, mixed integer and non-linear programming methods in energy system dispatch modelling. In *Energy* 74, pp. 109–118. DOI: 10.1016/j.energy.2014.04.023.

- Wang, Xuan; Jin, Ming; Feng, Wei; Shu, Gequn; Tian, Hua; Liang, Youcai (2018): Cascade energy optimization for waste heat recovery in distributed energy systems. In *Applied Energy* 230, pp. 679–695. DOI: 10.1016/j.apenergy.2018.08.124.
- Xu, Yue; Liu, WeiWei; Zhang, Lu; Cui, GuoMin; Xiao, Yuan; Zhang, GuanHua; Yang, QiGuo (2023): A comprehensive review of recent advancements and developments in heat exchanger network synthesis techniques. In *Sci. China Technol. Sci.* DOI: 10.1007/s11431-022-2337-1.
- Yee, T. F.; Grossmann, I. E. (1990): Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis. In *Computers & Chemical Engineering* 14 (10), pp. 1165–1184. DOI: 10.1016/0098-1354(90)85010-8.
- Yee, T. F.; Grossmann, I. E.; Kravanja, Z. (1990): Simultaneous optimization models for heat integration—I. Area and energy targeting and modeling of multi-stream exchangers. In *Computers & Chemical Engineering* 14 (10), pp. 1151–1164. DOI: 10.1016/0098-1354(90)85009-Y.

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