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

Supplementary Material

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MODEL FORMULATION

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. In the following, the most important constraints regarding the selection of components and connections between process streams and utility levels are shown. The constraints are used to set up the utility system structure as shown in the simplified graphic in Figure 1.
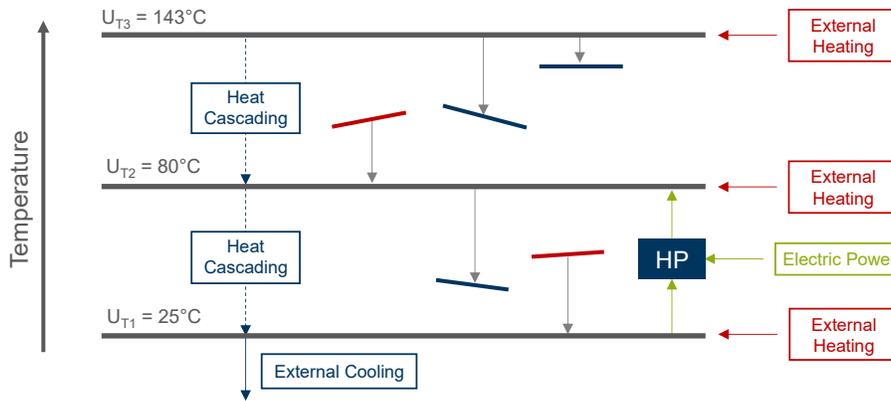

Figure 1. Exemplary structure of the utility system with heat cascading. Arrows depict energy flows in the utility system.

Binary activation variables for the utility system u_a determine the activation of N candidate temperature levels. For retrofit scenarios, fixed levels must be set to 1 as shown in equation (1).

$$u_a(fixed\ level) = 1 \tag{1}$$

The number of activated utility levels must not exceed the maximum number of allowed utility levels u_{max} as shown in equation (2).

$$\sum_{i \in N} u_{a,i} \leq u_{max} \tag{2}$$

Each hot stream i must be connected to exactly one feasible utility level u from the set of feasible candidate utility levels M_i. Equation (3) applies to all hot streams. The same logic applies to cold streams.

$$\sum_{u \in M_i} h_{i,u} = 1 \tag{3}$$

A utility level u can only be used if it is active. The energy balance for each utility level is shown in the following equation.

$$\sum_{u \in M_i} h_{i,u} = 1 \tag{4}$$

It considers heat supplied to the utility level u by hot streams ($\dot{Q}_{hot,u}$), heat supplied to cold process streams ($\dot{Q}_{cold,u}$), the sum of all heat extracted by heat pumps and supplied to other utility levels x ($\dot{Q}_{HP,u,x}$), upgrade heat from other utility levels w and provided by the heat pump to the utility level ($\dot{Q}_{HP,w,u}$), external heat supply ($\dot{Q}_{ext,u}$), heat cascaded down from the next higher utility level ($\dot{Q}_{cas,u-1}$) and heat cascaded down to the next lower utility level ($\dot{Q}_{cas,u}$). With heat cascading, the lowest temperature level must pass the heat surplus to cooling duty, and the highest utility level does not receive cascaded heat.

$$\dot{Q}_{hot,u} + \dot{Q}_{ext,u} + \dot{Q}_{HP,w,u} + \dot{Q}_{cas,u-1} = \dot{Q}_{cold,u} + \dot{Q}_{HP,u,x} + \dot{Q}_{cas,u} \tag{5}$$

COST CALCULATIONS

In the following, calculation of TAC is presented as this is the objective function in all case studies in this work.

CO₂-emissions

As costs for CO_2-emisison certificates are rising significantly and are expected to still rise in the future, we considered CO_2-emissions for the heat pump and natural gas boiler, e_{HP} and e_{NGB} respectively. External heat demand was assumed to be met by natural gas boilers. For the heat pump, we used emission factors for electricity $EF_{CO_2,el}$ assuming the compressor is driven by electricity (equation (6)). Likewise, the emission factor of natural gas $EF_{CO_2,NG}$ was used for calculating the emissions of the natural gas boiler (NGB), as shown in equation (7). The sum of CO_2-emissions by the heat pump and NGB account for the total CO_2-emissions, represented by e_{total}. Multiplying by annual operating hours t_{op} yields annual values.

$$e_{HP} = P_{HP,el} \cdot EF_{CO_2,el} \cdot \frac{t_{op}}{1000} \tag{6}$$

$$e_{NGB} = \dot{Q}_{NGB} \cdot \frac{1}{\eta_{NGB}} \cdot EF_{CO_2,NG} \cdot \frac{t_{op}}{1000} \tag{7}$$

Cost functions

The minimization of total annual costs (TAC) requires the consideration of operating expenditure (OPEX) as well as investment cost (CAPEX). We only considered heat pump investment costs as shown in equation (8) and use a constant specific cost factor $f_{inv,HP}$.

$$CAPEX = \dot{Q}_{HP,sink} \cdot f_{inv,HP} \tag{8}$$

We consider operational costs for CO_2-emissions, the required electricity of the heat pump, natural gas as well as costs for cooling water. The cost factor for CO_2-emissions is expressed in costs per mass of CO_2. The specific cost factors c_{el} and c_{NG}, for electricity and natural gas respectively, represent costs per unit of energy consumed, expressed in €/MWh. The cost factor for cooling water c_{cw} gives the costs per volumetric unit of water consumed. Thus, to determine the required amount of cooling water, we used the density (ρ_{cw}) and specific heat capacity ($c_{p,cw}$) of water as well as a maximum allowable temperature increase ΔT_{cw}. The cost functions for OPEX are shown in equations (9-12). Heat duties and electric power are given in kW.

$$OPEX_{CO_2} = e_{total} \cdot c_{CO_2} \tag{9}$$

$$OPEX_{HP} = P_{HP,el} \cdot c_{el} \cdot \frac{t_{op}}{1000} \tag{10}$$

$$OPEX_{NGB} = \dot{Q}_{NGB} \cdot c_{NG} \cdot \frac{1}{\eta_{NGB}} \cdot \frac{t_{op}}{1000} \tag{11}$$

$$OPEX_{cw} = \dot{Q}_{cw} \cdot c_{cw} \cdot \frac{1}{\rho_{cw} \cdot c_{p,cw} \cdot \Delta T_{cw}} \cdot 3600 \cdot t_{op} \tag{12}$$

The CAPEX was annualized using the annuity factor a (equation (13)) with interest rate $i = 0.07$ and depreciation time $n = 20$ in years. Subsequently, the TAC can be derived as shown in equation (14).

$$a = \frac{i \cdot (1+i)^n}{(1+i)^n - 1} \tag{13}$$

$$TAC = CAPEX \cdot a + OPEX_{total} \tag{14}$$

The values of the key parameters are shown in Table 1.

In Figure 2, the grand composite curve for the synthetic case study is presented. The pinch temperature is 75 °C. In Figure 3, the distribution of inlet and outlet temperatures as well as duties for hot and cold streams in the synthetic case study are presented.

Table 1. Values of key parameters in the different case studies.

| Parameter	Unit	Greenfield scenario Value	Retrofit scenario 1 Value/range	Retrofit scenario 2 Value/range	Retrofit scenario 3 Value/range
Utility system					
Utility levels	°C	variable	[13, 25, 80, 143, 214, 285, 1600], 1 level adjusted each run	[13, 25, 80, 143, 214, 285, 1600], 2 levels adjusted each run	[13, 35, 80, 134, 214, 285, 1600], fixed
System					
c_{cw}	€/m³ [4]	0.06	0.06	0.06	0.06
c_{el}	€/kWh	95.18 [1]	95.18 [1]	95.18 [1]	Base value: 95.18
c_{NG}	€/kWh	41.23 [1]	41.23 [1]	41.23 [1]	41.23 [1]
c_{CO_2}	€/t$_{CO2}$	83.59 [1]	83.59 [1]	83.59 [1]	Base value: 83.59
ρ_{cw}	kg/m³	997	997	997	997
$c_{p,cw}$	kJ/(kgK)	4.18	4.18	4.18	4.18
ΔT_{cw}	K	5	5	5	5
ΔT_{HX}	K	10	10	10	10
$EF_{CO_2,el}$	kg$_{CO2}$/kWh$_{th}$	0.435 [2]	0.402	0.435 [2]	Base value: 0.435
$EF_{CO_2,NG}$	kg$_{CO2}$/kWh$_{th}$	0.201 [2]	0.201	0.201 [2]	0.201 [2]
$f_{inv,HP}$	€/kW$_{th}$	750 [3]	750 [3]	750 [3]	Base value: 750
Min. heat pump sink duty $\dot{Q}_{HP,sink,min}$	kW	50	50	50	50
Compressor efficiency η_C	%	70	70	70	70
Natural gas boiler efficiency η_{NGB}	%	95	95	95	95
Annual operating hours t_{op}	h/a	8000	8000	8000	8000
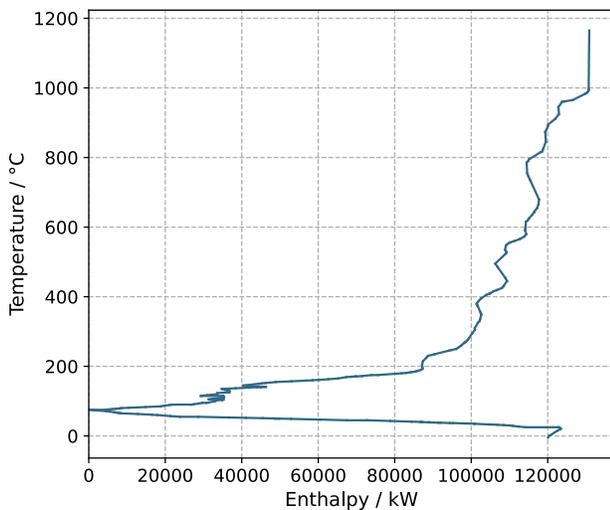
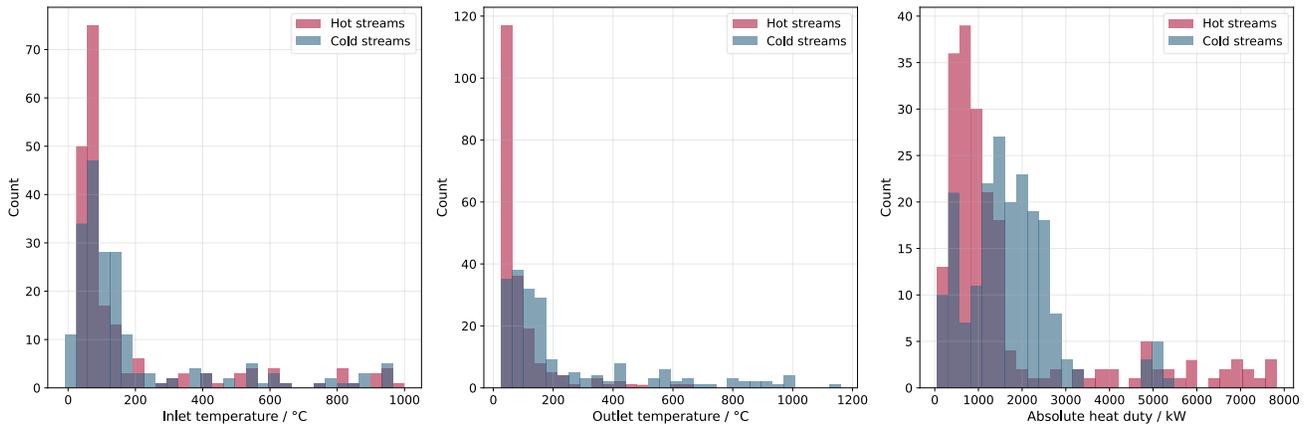**Figure 2**. Grand composite curve of the synthetic case study.

Figure 3. distribution of inlet and outlet temperature as well as required heat duty for hot and cold streams.

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