Appendix A. Model formulation

Appendix A.1. Nomenclature of parameters and variables

Symbol	**Explanation**	**Unit**
Time-dependent variables		
$P_{\mathrm{grid},i}(t)$	Grid power to technology i	MW
$P_{\mathrm{bat,grid}}(t)$	Power from battery to grid	MW
$NG_{\mathrm{GB,in}}(t)$	Natural gas input to the gas boiler	MW
$H_{i,\mathrm{process}}(t)$	Heat flow from technology i to the process	MW
$H_{i,\mathrm{TES250}}(t)$	Heat flow from technology i to the TES at 250 °C	MW
$H_{\mathrm{GB,excess}}(t)$	Excess heat from the gas boiler	MW
$H_{\mathrm{ElB},i}(t)$	Heat from electric boiler to technology i	MW
$H_{\mathrm{HP},i}(t)$	Heat from heat pump to technology i	MW
$H_{\mathrm{HP,\ in}}(t)$	Heat from process heat source to heat pump	MW
$H_{\mathrm{MVR113},i}(t)$	Heat from MVR113 to technology i	MW
$H_{\mathrm{MVR120},i}(t)$	Heat from MVR120 to technology i	MW
$H_{\mathrm{TES120},i}(t)$	Heat flow from the TES at 120 °C to technology i	MW
$H_{2,\mathrm{H2E,H2B}}(t)$	Hydrogen from electrolyser to the boiler	MW
$H_{2,\mathrm{H2E,H2S}}(t)$	Hydrogen from electrolyser to storage	MW
$H_{2,\mathrm{H2S,H2B}}(t)$	Hydrogen from storage to the boiler	MW
$H_{\mathrm{H2B,\ process}}(t)$	Heat from hydrogen boiler to process	MW
$P_{\mathrm{bat},i}(t)$	Power from battery to technology i	MW
$SOE_i(t)$	State of energy of technology i	MWh
$b_1(t)$	Binary variable for battery charging	Binary (0/1)
$b_2(t)$	Binary variable for TES at 250 °C	Binary (0/1)
$b_3(t)$	Binary variable for TES at 120 °C	Binary (0/1)
$b_4(t)$	Binary variable for TES at 113 °C	Binary (0/1)
$b_5(t)$	Binary variable for the hydrogen storage tank	Binary (0/1)
$b_6(t)$	Binary variable for the connection to the power grid	Binary (0/1)
Sizing variables		
s_i	Size of technology i	MW_{th} or MWh
Time-dependent parameters		
$\mathrm{p}_{\mathrm{el,grid}}(t)$	Electricity price at time t	Eur/MWh
$\mathrm{p}_{\mathrm{NG,use}}(t)$	Price for using natural gas price at time t[3]	Eur/MWh

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[3]Includes price for CO_2 emissions

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Symbol	Explanation	Unit
$H_{\mathrm{dem}}(t)$	Heat demand of the process at time t	MW

Constants

s_{GB}	Gas boiler size	MW
r_{disc}	Discount rate	%
Δt	Time step duration	h
η_i	Efficiency of technology i	-
$\mathrm{COP}_{\mathrm{HP,Carnot}}$	Heat pump ideal coefficient of performance	-
$\mathrm{MinLoad}_{\mathrm{GB}}$	Minimum load factor for gas turbine	% of capacity
crate_i	Charge/discharge rate of technology i	MW/MWh
$\mathrm{cap}_{\mathrm{gr}}$	Grid connection capacity	MW
c_i	Capital cost of component i	Eur/unit
$\mathrm{Inf}_{\mathrm{i}}$	Installation or Lang factor of technology i	-
LT_i	Lifetime of component i	years

Appendix A.2. Mathematical formulations of the model for the electrification of the utility system

The following equations represent a mathematical formulation of the model for the electrification of the utility system with the 'High integration' heat pump, as it is the most complex model. All models are available on GitHub (see 'Data availability' statement).

Objective function.

$$min \sum_{t=0}^{t=16000} \text{OpEx}(t) + \text{CaPex}, \tag{A.1}$$

where

$$\begin{aligned}\text{OpEx}(t) =& \Delta t \cdot \Big(\text{p}_{\text{el,grid}}(t) \cdot (\sum_{i \in \{\text{process, bat, ElB, H2E, MVR}\}} P_{\text{grid, i}}(t) - P_{\text{bat, gr}}(t)) \\ &+ NG_{\text{GB,in}}(t) \cdot \text{p}_{\text{NG,use}}(t)\Big)\end{aligned}$$

and

$$\text{CaPex} = \sum_{i \in \{\text{HP, bat, ElB, SS-TES, LT-TES, H2E, H2B, H2S, MVR}\}} \frac{s_i \cdot c_i \cdot \text{Inf}_i \cdot r_{\text{disc}}}{1 - (1 + r_{\text{disc}})^{-\text{LT}_i}} \tag{A.2}$$

Heat balance equality constraints.

$$H_{\text{dem}}(t) = \sum_{i \in \{\text{HP, ElB, SS-TES, LT-TES, H2B, MVR}\}} H_{\text{i,process}(t)} \text{(A.3)}$$

GB constraints.

Heat generation constraint:

$$NG_{\text{GB,in}}(t) \cdot \eta_{\text{GB,th}} = H_{\text{GB,process}}(t) + H_{\text{GB,TES250}}(t) + H_{\text{GB,excess}}(t) \tag{A.4}$$

Maximum natural gas consumption constraints:

$$NG_{\text{GB,in}}(t) \leq H_{\text{dem,max}}/\eta_{\text{GB}} \tag{A.5}$$

Minimal load constraint:

$$NG_{\text{GT,in}}(t) \geq H_{\text{dem,max}}/\eta_{\text{GB}} \cdot \text{MinLoad}_{\text{GB}} \tag{A.6}$$

Electric boiler.
Heat generation constraint:

$$\sum_{i\in\{\text{process, TES250}\}} H_{\text{ElB},i}(t) = (P_{\text{grid,ElB}}(t) + P_{\text{bat,ElB}}(t)) \cdot \eta_{\text{ElB}} \tag{A.7}$$

Sizing constraint:

$$\sum_{i\in\{\text{process, TES250}\}} H_{\text{ElB},i}(t) \leq s_{\text{ElB}} \tag{A.8}$$

Heat pump.
Heat generation constraint:

$$\sum_{i\in\{\text{processT113, MVR113, TES113}\}} H_{\text{HP},i}(t) = \text{COP}_{\text{Carnot,HP}} \cdot \eta_{\text{HP}} \cdot \sum_{j\in\{\text{grid, bat}\}} P_{j,\text{HP}} \tag{A.9}$$

Heat source constraint:

$$\sum_{i\in\{\text{processT113, MVR113, TES113}\}} H_{\text{HP, i}}(t) \leq \frac{H_{\text{HP,in}}}{(1 - 1/(\text{COP}_{\text{Carnot,HP}} \cdot \eta_{HP})} \tag{A.10}$$

Sizing constraint:

$$\sum_{i\in\{\text{processT113, MVR113, TES113}\}} H_{\text{HP},i}(t) \leq s_{\text{HP}} \tag{A.11}$$

MVR113.
Heat generation constraint:

$$\sum_{i \in \{\text{processT120, TES120, MVR120}\}} H_{\text{MVR113},i}(t) = (P_{\text{grid,MVR113}} + P_{\text{bat,MVR113}})(t) \cdot \text{COP}_{\text{Carnot, MVR113}} \cdot \eta_{\text{MVR}} \tag{A.12}$$

Heat source constraint:

$$\sum_{i \in \{\text{processT120, TES120, MVR120}\}} H_{\text{MVR113},i}(t) = \frac{H_{\text{HP, MVR113}}(t)}{1 - 1/(\text{COP}_{\text{Carnot, MVR113}} \cdot \eta_{\text{MVR}}} \tag{A.13}$$

Sizing constraint:

$$\sum_{i \in \{\text{processT120, TES120, MVR120}\}} H_{\text{MVR113},i}(t) \leq s_{\text{MVR113}} \tag{A.14}$$

MVR120.
Heat generation constraint:

$$H_{\text{MVR120, process250}}(t) = (P_{\text{grid,MVR120}} + P_{\text{bat,MVR120}})(t) \cdot \text{COP}_{\text{Carnot, MVR120}} \cdot \eta_{\text{MVR}} \tag{A.15}$$

Heat source constraint:

$$H_{\text{MVR120, process250}}(t) = \frac{H_{\text{MVR113, MVR120}}(t) + H_{\text{TES120, MVR120}(t)}}{1 - 1/(\text{COP}_{\text{Carnot, MVR120}} \cdot \eta_{\text{MVR}}} \tag{A.16}$$

Sizing constraint:

$$H_{\text{MVR120, process250}}(t) \leq s_{\text{MVR113}} \tag{A.17}$$

Water electrolyser.
Hydrogen production constraint:

$$(P_{\text{grid,H2E}}(t) + P_{\text{bat,H2E}}(t)) \cdot \eta_{\text{H2E}} = H_{2,\text{H2E,H2B}}(t) + H_{2,\text{H2E,H2S}}(t) \tag{A.18}$$

Sizing constraint:

$$P_{\text{grid,H2E}}(t) + P_{\text{bat,H2E}}(t) \leq s_{\text{H2E}} \tag{A.19}$$

Hydrogen boiler.
Heat generation constraint:

$$(H_{2,\text{H2E,H2B}}(t) + H_{2,\text{H2S,H2B}}(t)) \cdot \eta_{\text{H2B}} = H_{\text{H2B,process}}(t) \tag{A.20}$$

Sizing constraint:

$$H_{\text{H2B,process}}(t) \leq s_{\text{H2B}} \tag{A.21}$$

Battery.
State of energy:

$$\text{SOE}_{\text{bat}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\text{bat}}(t-1) + \eta_{\text{bat}} \cdot \Delta t \cdot P_{\text{grid,bat}}(t-1) - & \\ \frac{1}{\eta_{\text{bat}}} \cdot \Delta t \cdot \sum_{i \in \{\text{ElB, HP, MVR113, MVR1120, H2E, grid}\}} P_{\text{bat},i}(t-1), & \text{otherwise} \end{cases} \tag{A.22}$$

Maximum charge constraint:

$$P_{\text{grid,bat}}(t) \leq \frac{s_{\text{bat}}}{\eta_{\text{bat}}} \cdot \frac{\text{crate}_{\text{bat}}}{\Delta t} \cdot b_1(t) \tag{A.23}$$

Maximum discharge constraint: Discharging for $t = 0$:

$$\sum_{i \in \{\text{ElB, HP, MVR113, MVR1120, H2E, grid}\}} P_{\text{bat},i}(0) = 0 \tag{A.24}$$

Discharging for $t > 0$:

$$\sum_{i \in \{\text{ElB, HP, MVR113, MVR1120, H2E, grid}\}} P_{\text{bat},i}(t) \leq s_{\text{bat}} \cdot \eta_{\text{bat}} \cdot \frac{\text{crate}_{\text{bat}}}{\Delta t} \cdot (1 - b_1(t)) \tag{A.25}$$

Sizing constraint:

$$SOE_{\text{bat}}(t) \leq s_{\text{bat}} \tag{A.26}$$

Thermal energy storage 250.
State of energy (SOE):

$$SOE_{\text{TES250}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\text{TES250}}(t-1) + \\ \Delta t \cdot \left(H_{\text{GB,TES250}}(t-1) + H_{\text{ElB,TES250}}(t-1) - \frac{H_{\text{TES250,process}}(t-1)}{\eta_{\text{TES}}} \right), & \text{otherwise} \end{cases} \tag{A.27}$$

Maximum charge constraint

$$H_{\text{GB,TES250}}(t) + H_{\text{ElB,TES250}}(t)(t) \leq \frac{s_{\text{TES250}} \cdot \text{crate}_{\text{TES}}}{\Delta t} \cdot b_2(t) \tag{A.28}$$

Maximum discharge constraint: Discharging for $t = 0$:

$$H_{\text{TES250,process}}(0) = 0 \tag{A.29}$$

Discharging for $t > 0$:

$$H_{\text{TES250,process}}(t) \leq \frac{s_{\text{TES250}} \cdot \eta_{\text{TES}} \cdot \text{crate}_{\text{TES}}}{\Delta t} \cdot (1 - b_2(t)) \tag{A.30}$$

Sizing constraint:

$$SOE_{\text{TES250}}(t) \leq s_{\text{TES250}} \tag{A.31}$$

Thermal energy storage 120.
State of energy (SOE):

$$SOE_{\text{TES120}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\text{TES120}}(t-1) + \\ \Delta t \cdot \left(H_{\text{MVR113,TES120}}(t-1) - \frac{H_{\text{TES120,process}}(t-1) + H_{\text{TES120,MVR120}}(t-1)}{\eta_{\text{TES}}} \right), & \text{otherwise} \end{cases} \tag{A.32}$$

Maximum charge constraint

$$H_{\mathrm{MVR113,TES120}}(t) \leq \frac{s_{\mathrm{TES120}} \cdot \mathrm{crate}_{\mathrm{TES}}}{\Delta t} \cdot b_3(t) \tag{A.33}$$

Maximum discharge constraint: Discharging for $t = 0$:

$$H_{\mathrm{TES120,process}}(0) + H_{\mathrm{TES120,MVR120}}(0) = 0 \tag{A.34}$$

Discharging for $t > 0$:

$$H_{\mathrm{TES120,process}}(t) + H_{\mathrm{TES120,MVR120}}(t) \leq \frac{s_{\mathrm{TES120}} \cdot \eta_{\mathrm{TES}} \cdot \mathrm{crate}_{\mathrm{TES}}}{\Delta t} \cdot (1 - b_3(t)) \tag{A.35}$$

Sizing constraint:

$$SOE_{\mathrm{TES120}}(t) \leq s_{\mathrm{TES120}} \tag{A.36}$$

Thermal energy storage 113.
State of energy (SOE):

$$SOE_{\mathrm{TES113}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\mathrm{TES113}}(t-1) + \\ \Delta t \cdot \left(H_{\mathrm{HP,TES113}}(t-1) - \frac{H_{\mathrm{TES113,process}}(t-1) + H_{\mathrm{TES113,MVR113}}(t-1)}{\eta_{\mathrm{TES}}} \right), & \text{otherwise} \end{cases} \tag{A.37}$$

Maximum charge constraint

$$H_{\mathrm{HP,TES113}}(t) \leq \frac{s_{\mathrm{TES113}} \cdot \mathrm{crate}_{\mathrm{TES}}}{\Delta t} \cdot b_4(t) \tag{A.38}$$

Maximum discharge constraint: Discharging for $t = 0$:

$$H_{\mathrm{TES113,process}}(0) + H_{\mathrm{TES113,MVR113}}(0) = 0 \tag{A.39}$$

Discharging for $t > 0$:

$$H_{\mathrm{TES113,process}}(t) + H_{\mathrm{TES113,MVR113}}(t) \leq \frac{s_{\mathrm{TES113}} \cdot \eta_{\mathrm{TES}} \cdot \mathrm{crate}_{\mathrm{TES}}}{\Delta t} \cdot (1 - b_4(t)) \tag{A.40}$$

Sizing constraint:

$$SOE_{\text{TES113}}(t) \leq s_{\text{TES113}} \tag{A.41}$$

Hydrogen storage.

State of energy:

$$\text{SOE}_{\text{H2S}}(t) = \begin{cases} 0, & \text{if } t = 0 \\ SOE_{\text{H2S}}(t-1) + \left(H_{2,\text{H2E,H2S}}(t-1) - \frac{H_{2,\text{H2S,H2B}}(t-1)}{\eta_{\text{H2S}}} \right) \cdot \Delta t, & \text{otherwise} \end{cases} \tag{A.42}$$

Charge constraint

$$H_{2,\text{H2E,H2S}}(t) \leq s_{\text{H2S}} \cdot b_5(t) \tag{A.43}$$

Discharge constraint: Discharging for $t = 0$:

$$H_{2,\text{H2S,H2B}}(0) = 0 \tag{A.44}$$

Discharging for $t > 0$:

$$H_{2,\text{H2S,H2B}}(t) \leq \frac{s_{\text{H2S}} \cdot \eta_{\text{H2S}}}{\Delta t} \cdot (1 - b_5(t)) \tag{A.45}$$

Sizing constraint:

$$SOE_{\text{H2S}}(t) \leq s_{\text{H2S}} \tag{A.46}$$

Grid connection capacity.

Maximum inflow constraint:

$$\text{cap}_{\text{grid}} \cdot b_6(t) \geq \sum_{i \in \{\text{ElB, bat, HP, H2E, MVR120, MVR113}\}} P_{\text{grid},i}(t) \tag{A.47}$$

Maximum outflow constraint:

$$P_{\text{bat,gr}}(t) \leq \text{cap}_{\text{gr}} \cdot (1 - b_6(t)) \tag{A.48}$$