

Supplementary Material to UrbanHeatOpt: A Software Framework for Supporting Municipal Heat Transition Planning

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Introduction

In this supplementary material, we provide additional details on the conceptualisation of the model, a comprehensive mathematical description of the optimisation model implemented in the software tool *UrbanHeatOpt* [1], as well as remarks on the spatial and temporal resolution of the data workflow and on the methodology for generating stochastic heat demand time series.

By addressing these key aspects, this supplementary material ensures full transparency of the underlying methodology, complementing the concise conceptual description in the main manuscript and the open-source code provided in the repository [1].

1 Optimisation Model

The optimisation model allows for finding optimal configurations of the municipal heating system (investment decisions) as well as simplified optimised operational results, i.e., energy flows, unit commitment, and storage usage. These results are an approximation to ensure computational tractability and to indicate a feasible layout. They can serve as an initial point for subsequent simulations of selected concepts with a higher level of technical detail.

1.1 Conceptual Description

General Objective The optimization model minimizes the annualized investment and operational costs (i.e., the total costs) of supplying heat to a community. In doing so, it selects among the various available options for providing heat. In the following, the different parts of the optimisation model are described conceptually to provide additional context alongside the mathematical formulation in Section 1.2.

Spatial and Temporal Dimension The spatial dimension is represented by heat nodes $n \in \mathcal{N}$, each describing a cluster of buildings with a heat demand or a heat generation unit $g \in \mathcal{G}$. The temporal resolution is given by the time index $h \in \mathcal{H}$, typically representing hourly values for a full year. However, other customised time steps and time horizons are also possible.

Heat Network Connections To cover the heat demand of a node $D_{n,h}$, the model can decide to connect the node to the heating network z_n^{DH} . Typically, buildings connected to the district heating network do not have an independent heating system; therefore, the complete heat demand of each hour must be supplied via the network. However, the binary parameter δ^{doubleH} allows, if set to 1, to relax this condition. For nodes not connected to the network, local heating costs (individual local heat boilers or heat pumps) are accounted for each unit of energy produced.

Pipe connections The binary decision variable $z_{n,m}^{\text{pipe}}$ (with m as an alias of n) indicates which candidate pipes $(n, m) \in \mathcal{P}$ are built. Here, $\mathcal{P}$ denotes the set of potential pipes represented as node pairs, enabling energy flow in the network. In addition, the continuous investment variable $x_{n,m}^{\text{pipe}}$ captures the size of the pipeline (i.e., larger pipe cross-section). Costs for pipe investments are accounted in two steps, $C^{\text{pipe,min}}$ for initial investment (i.e., construction work) and $C^{\text{pipe,slope}}$ for pipe (i.e., mass flow) sizing. The relation is further illustrated in Figure 1. The actual mass flow in the pipes, $\dot{m}_{n,m,h}$, for each pipe connection and each hour is determined by the model. Only the mass flows on the supply side are considered, since

this simplified approach captures the energy flows adequately. The return flows, which are symmetrically opposite to the supply flows, are not explicitly computed in order to reduce the computational burden.

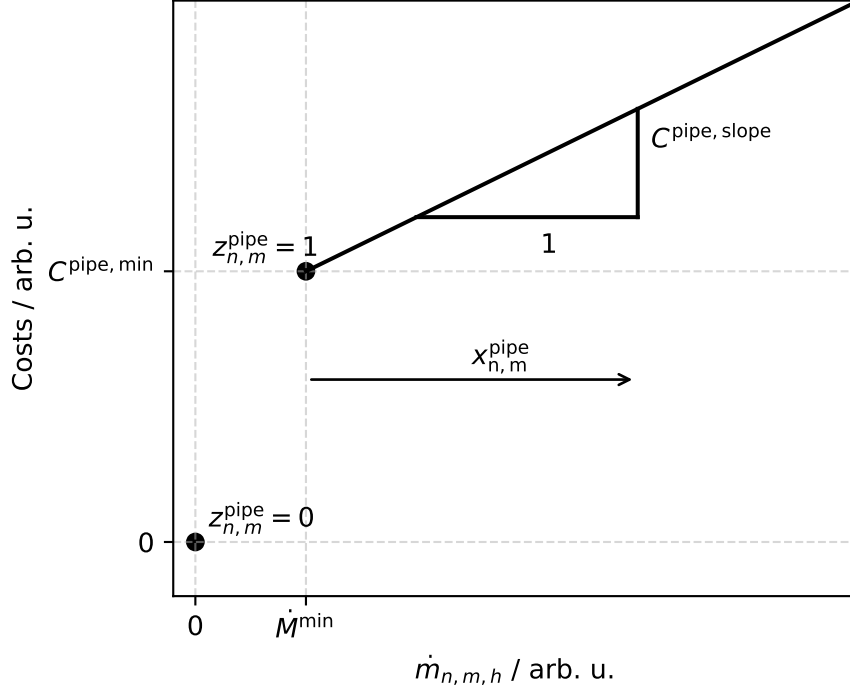


Figure 1: Schematic illustration of the cost accounting for piping: the binary variable $z_{n,m}^{\text{pipe}}$ indicates whether a pipe between nodes n and m is built. If a pipe is built the costs $C_{\text{pipe},\text{min}}$ (i.e., excavation and construction works) are incurred, and a minimum mass flow $\dot{M}^{\text{min}}$ is assigned. For larger mass flows, a linear cost relation is applied with slope $C_{\text{slope}}^{\text{pipe}}$ per unit of additional mass flow. This approach follows Ref. [2] in the literature.

Central Heat Generation Heat in the district heating network is supplied by generation units $g \in \mathcal{G}$, which are assigned to nodes n via the set $\mathcal{A}_n$ containing the heat generation units for each node. Three different technologies are distinguished, represented by the following subsets:

- Waste heat units ($w \in \mathcal{W} \subset \mathcal{G}$): Their hourly heat output is limited by an exogenous availability profile $\dot{M}_{w,h}^{\text{max}}$, reflecting process- or source-dependent variability. Within this range, from zero up to the maximum available heat, the model determines the actual amount of utilized heat. Unutilized waste heat is not further considered in the current formulation.
- Heat boilers ($b \in \mathcal{B} \subset \mathcal{G}$): Fully dispatchable units that can supply heat to the network on demand up to the installed capacity. Boilers provide system flexibility, covering residual demand not met by waste heat or storage.
- Thermal energy storage ($s \in \mathcal{S} \subset \mathcal{G}$): Storage units that can absorb heat (charging) and release heat (discharging). They buffer temporal mismatches between generation and demand, increase the utilization of waste heat, and reduce boiler operation. The maximum storage capacity is determined by the investment in storage volume x_s^{TES} .

Investments All heat sources are constrained by the corresponding investment decisions: x_g^{centr} for generation units and in addition x_s^{TES} for storage volume. In other words, the model has to invest in these units in order to utilise their heat supply.

All investments (in heat generation units, storage volume, district heating connections, and pipe connections), as well as operational activities (thermal heat production, pumping in the network), are associated with corresponding costs defined as input parameters. In the objective function, all costs over the chosen time horizon are aggregated and minimised, subject to the constraints, which represent technical limitations.

1.2 Mathematical Model Formulation

The following section provides the complete mathematical description of the implemented model, using standard notation and conventions from operations research.

Sets The sets define the basic framework of the model. They *enumerate*, for example, the time steps, heat nodes, or waste heat units. Please note that $\mathcal{S}$, $\mathcal{B}$, and $\mathcal{W}$ are subsets of $\mathcal{G}$, representing specific subtypes of heat generation units. For instance, the variable $q_{g,h}^{\text{centr}}$ is defined for all g -elements, but can also be restricted to subsets such as $q_{w,h}^{\text{centr}}$ when considering only waste heat units. Following common practice in operations research and to keep the notation concise, we refrain from defining and describing all variables redundantly for their respective subsets. Table 1 summarises all sets used in the model formulation.

Table 1: Sets for the model formulation

Name	Meaning	Symbol
n	Heat nodes	$n, m \in \mathcal{N}$
h	(Hourly) time index	$h \in \mathcal{H}$
pc	Pipe candidate connections	$(n, m) \in \mathcal{P}$
-	Set of nodes m connected to node n	Ω_n
hg	Heat generation units	$g \in \mathcal{G}$
tes	Thermal energy storage units	$s \in \mathcal{S} \subset \mathcal{G}$
hb	Heat boilers	$b \in \mathcal{B} \subset \mathcal{G}$
wh	Waste heat units	$w \in \mathcal{W} \subset \mathcal{G}$
hgn	Set of heat generation units (b, w, s) at heat node n	$\mathcal{A}_n$

Parameters Parameters define fixed values that serve as inputs to the optimisation model. In the present case, they either originate from previous processes in the data workflow (e.g., heat demand time series) or are specified by the user (e.g., most cost parameters). The domain of each parameter describes its potential range. For example, $\mathbb{R}_{\geq 0}$ denotes a range over non-negative real numbers (including zero).

Table 2 lists all parameters used in the model formulation.

Table 2: Parameters used in the optimization model. Note that (Latin) parameter symbols are denoted by uppercase letters, for better readability.

Name	Meaning	Symbol	Units	Domain
pCostHNS	Cost of heat not supplied	C^{HNS}	$\frac{\text{€}}{\text{kWh}}$	$\mathbb{R}_{\geq 0}$
pCostPumping	Pumping cost	C^{pump}	$\frac{\text{€}}{\text{m}^3 \text{ m}}^{(1)}$	$\mathbb{R}_{\geq 0}$
pTsupply	Supply temperature	T^{sup}	$^{\circ}\text{C}$ or K	$\mathbb{R}_{\geq 0}$
pTreturn	Return temperature	T^{ret}	$^{\circ}\text{C}$ or K	$\mathbb{R}_{\geq 0}$
pPipeCostIni	Initial pipe cost	$C^{\text{pipe,min}}$	$\frac{\text{€}}{\text{m}}^{(1)}$	$\mathbb{R}_{\geq 0}$
pPipeCostSlope	Pipe cost slope	$C^{\text{pipe,slope}}$	$\frac{\text{€ h}}{\text{m m}^3}^{(1)}$	$\mathbb{R}_{\geq 0}$
pMassFlowIni	Initial mass flow	$\dot{M}^{\text{min}}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
pAllowDoubleHeating	Allow double heating	δ^{DoubH}	-	$\{0, 1\}$
pTESlosses	Thermal energy storage losses	$\eta_{\text{TES}}^{\text{loss}}$	$\frac{\%}{\text{h}}$	$[0, 1]$
pCWater	Specific heat capacity of water	C_p^{water}	$\frac{\text{kWh}}{\text{m}^3 \text{ K}}$	$\mathbb{R}_{\geq 0}$
pHeatDemand	Heat demand per node and time step	$D_{n,h}$	kW	$\mathbb{R}_{\geq 0}$
pCostDHConnect	Cost of district heating connection	C_n^{DH}	€	$\mathbb{R}_{\geq 0}$
pMaxDHPower	Maximum district heating power	P_n^{max}	kW	$\mathbb{R}_{\geq 0}$
pCostLocalHeatProd	Cost of local heat production	C_n^{local}	$\frac{\text{€}}{\text{kWh}}$	$\mathbb{R}_{\geq 0}$
pPipeLength	Length of pipe connection	$L_{n,m}$	m	$\mathbb{R}_{\geq 0}$
pMaxWHMF	Maximum waste heat mass flow	$\dot{M}_{w,h}^{\text{max}}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
pCostCentrHeatProd	Cost of central heat production	C_g^{centr}	$\frac{\text{€}}{\text{kWh}}$	$\mathbb{R}_{\geq 0}$
pCostCentralHeatProdInv	Investment cost for central heat prod.	$C_g^{\text{centr,inv}}$	$\frac{\text{€}}{\text{kW}}$	$\mathbb{R}_{\geq 0}$
pCostTESInv	Investment cost for TES	$C_s^{\text{TES,inv}}$	$\frac{\text{€}}{\text{m}^3}$	$\mathbb{R}_{\geq 0}$
phWeight	Weight of the time step h	Δ	h	$\mathbb{R}$

⁽¹⁾ Costs are normalized per metre and multiplied by the pipe length in the objective function.

Variables In the context of the optimisation model, variables represent decision variables that are determined by the solver in order to minimise the objective function. The corresponding domain specifies the range of admissible values each decision variable can take. Table 3 summarises all variables used in the model formulation.

Table 3: Variables used in the optimisation model. Note that variables are denoted in lowercase letters.

Name	Meaning	Symbol	Units	Domain
vMF	Mass flow in pipes	$\dot{m}_{n,m,h}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
vHNS	Heat not supplied to thermal nodes	$q_{n,h}^{\text{HNS}}$	kW	$\mathbb{R}_{\geq 0}$
vLocalHeatProd	Locally produced heat	$q_{n,h}^{\text{local}}$	kW	$\mathbb{R}_{\geq 0}$
vMFConsumption	Mass flow consumed at node	$\dot{m}_{n,h}^{\text{cons}}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
vMFIInjection	Mass flow injected at node	$\dot{m}_{n,h}^{\text{inj}}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
vCentralHeatProd	Central heat production	$q_{g,h}^{\text{centr}}$	kW	$\mathbb{R}_{\geq 0}$
vCentralHeatProdInv	Investment in central heat production	x_g^{centr}	kW	$\mathbb{R}_{\geq 0}$
vTESLevel	TES state of charge (storage level)	$e_{s,h}$	m^3	$\mathbb{R}_{\geq 0}$
vTESCharge	TES charging	$\dot{m}_{s,h}^{\text{ch}}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
vTESDischarge	TES discharging	$\dot{m}_{s,h}^{\text{dch}}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
vTESCapacityInv	Investment in TES capacity	x_s^{TES}	m^3	$\mathbb{R}_{\geq 0}$
vPipeMassFlowInv	Investment in pipe mass flow capacity	$x_{n,m}^{\text{pipe}}$	$\frac{\text{m}^3}{\text{h}}$	$\mathbb{R}_{\geq 0}$
vDHconnect	District heating connection decision	z_n^{DH}	–	$\{0, 1\}$
vBinBuildPipe	Pipe construction decision	$z_{n,m}^{\text{pipe}}$	–	$\{0, 1\}$

Objective Function The objective function considers all costs within the system and provides the basis for the optimisation. To improve clarity, an auxiliary hourly cost expression is introduced, which captures the (operational) costs at each time step. This expression is then aggregated into the total cost function, which also includes investment costs.

Hourly Cost Expression The hourly cost function hOF_h sums up all cost contributions in a given time step h :

$$\text{hOF}_h = \sum_{n \in \mathcal{N}} C_n^{\text{HNS}} \cdot q_{n,h}^{\text{HNS}} + \sum_{n \in \mathcal{N}} C_n^{\text{local}} \cdot q_{n,h}^{\text{local}} + \sum_{g \in \mathcal{G}} C_g^{\text{centr}} \cdot q_{g,h}^{\text{centr}} + \sum_{(n,m) \in \mathcal{P}} C^{\text{pump}} \cdot L_{n,m} \cdot \dot{m}_{n,m,h} \quad \forall h \in \mathcal{H} \quad (1)$$

Total Cost Objective The optimisation model minimises the sum of all investment and operational costs:

$$\begin{aligned} \min \left(\sum_{n \in \mathcal{N}} C_n^{\text{DH}} \cdot z_n^{\text{DH}} + \sum_{g \in \mathcal{G}} C_g^{\text{centr,inv}} \cdot x_g^{\text{centr}} + \sum_{s \in \mathcal{S}} C_s^{\text{TES,inv}} \cdot x_s^{\text{TES}} \right. \\ \left. + \sum_{(n,m) \in \mathcal{P}} C^{\text{pipe,min}} \cdot L_{n,m} \cdot z_{n,m}^{\text{pipe}} + \sum_{(n,m) \in \mathcal{P}} C^{\text{pipe,slope}} \cdot L_{n,m} \cdot x_{n,m}^{\text{pipe}} + \Delta \cdot \sum_{h \in \mathcal{H}} \text{hOF}_h \right) \quad (2) \end{aligned}$$

Constraints Constraints introduce physical and technical boundaries to the optimisation model, which must be satisfied for each feasible solution. In this way, the fulfilment of system conditions is ensured.

Energy Balance Constraint The energy balance equation for every time step h and every heat node n ensures that the demand not covered by local heating must be supplied via mass flow consumption from the district heating network:

$$\dot{m}_{n,h}^{\text{cons}} = \frac{D_{n,h} - q_{n,h}^{\text{local}}}{(T^{\text{sup}} - T^{\text{ret}}) \cdot C_p^{\text{water}}} \quad \forall n \in \mathcal{N}, h \in \mathcal{H} \quad (3)$$

Maximum District Heating Power Constraint This constraint restricts the mass flow consumption from the district heating network to nodes where an investment z_n^{DH} has been made:

$$\dot{m}_{n,h}^{\text{cons}} \leq z_n^{\text{DH}} \cdot \frac{P_n^{\text{max}}}{(T^{\text{sup}} - T^{\text{ret}}) \cdot C_p^{\text{water}}} \quad \forall n \in \mathcal{N}, h \in \mathcal{H} \quad (4)$$

Mass Flow Balance The mass flow balance ensures that the sum of consumption (positive sign in this formulation), injection (negative sign in this formulation), and TES charging of each node n equals the inflows from minus the outflows to the network:

$$\dot{m}_{n,h}^{\text{cons}} + \sum_{s \in \mathcal{A}_n} \dot{m}_{s,h}^{\text{ch}} - \dot{m}_{n,h}^{\text{inj}} = \sum_{m \in \Omega_n} \dot{m}_{m,n,h} - \sum_{m \in \Omega_n} \dot{m}_{n,m,h} \quad \forall n \in \mathcal{N}, h \in \mathcal{H} \quad (5)$$

Mass Flow Injection The mass flow injected into the network equals the sum of all generation unit mass flows at the respective node:

$$\begin{aligned} \dot{m}_{n,h}^{\text{inj}} = & \sum_{w \in \mathcal{A}_n} \frac{q_{w,h}^{\text{centr}}}{(T^{\text{sup}} - T^{\text{ret}}) \cdot C_p^{\text{water}}} + \sum_{b \in \mathcal{A}_n} \frac{q_{b,h}^{\text{centr}}}{(T^{\text{sup}} - T^{\text{ret}}) \cdot C_p^{\text{water}}} \\ & + \sum_{s \in \mathcal{A}_n} \frac{q_{s,h}^{\text{centr}}}{(T^{\text{sup}} - T^{\text{ret}}) \cdot C_p^{\text{water}}} \quad \forall n \in \mathcal{N}, h \in \mathcal{H} \end{aligned} \quad (6)$$

Local Production Exclusion (No Double Heating) If no *double heating* is allowed ($\delta^{\text{DoubH}} = 0$), nodes connected to the district heating network cannot provide local heating. This reflects the practical assumption that buildings supplied by district heating typically do not retain individual heating systems:

$$q_{n,h}^{\text{local}} \leq (1 - z_n^{\text{DH}}) \cdot P_n^{\text{max}} \quad \text{if } \delta^{\text{DoubH}} = 0 \quad \forall n \in \mathcal{N}, h \in \mathcal{H} \quad (7)$$

Maximum Waste Heat Power The available waste heat mass flow $\dot{M}_{w,h}^{\text{max}}$ limits the power output of waste heat units in each time step:

$$q_{w,h}^{\text{centr}} \leq \dot{M}_{w,h}^{\text{max}} \cdot (T^{\text{sup}} - T^{\text{ret}}) \cdot C_p^{\text{water}} \quad \forall w \in \mathcal{W}, h \in \mathcal{H} \quad (8)$$

TES Discharge Conversion The TES discharge power is linked to its mass flow via the temperature difference and water's specific heat capacity:

$$q_{s,h}^{\text{centr}} = \dot{m}_{s,h}^{\text{dch}} \cdot (T^{\text{sup}} - T^{\text{ret}}) \cdot C_p^{\text{water}} \quad \forall s \in \mathcal{S}, h \in \mathcal{H} \quad (9)$$

Maximum Heat Generation by Investment The maximum heat generation of each unit is limited by its invested capacity:

$$q_{g,h}^{\text{centr}} \leq x_g^{\text{centr}} \quad \forall g \in \mathcal{G}, h \in \mathcal{H} \quad (10)$$

TES Capacity by Investment The maximum storage level is restricted to the invested TES volume:

$$e_{s,h} \leq x_s^{\text{TES}} \quad \forall s \in \mathcal{S}, h \in \mathcal{H} \quad (11)$$

TES Energy Balance The time-linking storage balance accounts for charging, discharging, and self-discharge losses. For the first time step, the level is linked to the end-of-horizon state (denoted by $|\mathcal{H}|$) to ensure cyclic behaviour:

$$e_{s,h} = \begin{cases} e_{s,|\mathcal{H}|} + \Delta \cdot \dot{m}_{s,h}^{\text{ch}} - \Delta \cdot \dot{m}_{s,h}^{\text{dch}}, & \text{if } h = 1, \\ e_{s,h-1} \cdot (1 - \eta_{\text{TES}}^{\text{loss}}) + \Delta \cdot \dot{m}_{s,h}^{\text{ch}} - \Delta \cdot \dot{m}_{s,h}^{\text{dch}}, & \text{otherwise} \end{cases} \quad \forall s \in \mathcal{S}, h \in \mathcal{H} \quad (12)$$

Maximum Pipe Mass Flow The mass flow through each pipe is limited by investments, consisting of a base capacity (smallest pipe diameter) plus additional increments via continuous investment. For more details see Figure 1.

$$\dot{m}_{n,m,h} \leq z_{n,m}^{\text{pipe}} \cdot \dot{M}^{\text{min}} + x_{n,m}^{\text{pipe}} \quad \forall (n,m) \in \mathcal{P}, \forall h \in \mathcal{H} \quad (13)$$

Logical Pipe Mass Flow Constraint This constraint restricts additional pipe capacity investments to pipes where the initial investment in the pipe has been made, where M (in m^3/h) refers to a *big M* constant:

$$x_{n,m}^{\text{pipe}} \leq z_{n,m}^{\text{pipe}} \cdot M \quad \forall (n,m) \in \mathcal{P} \quad (14)$$

2 Spatial and Temporal Resolution

The model formulation is generic and, therefore, not inherently limited to a specific spatial location, temporal resolution, or time horizon. The input data alone defines the concrete case study and the resulting outputs. However, the choice of specific resolution parameters has a notable impact on the obtained results, as well as on computational performance. The following paragraphs discuss these impacts and provide reference guidance for users.

2.1 Spatial Resolution and Clustering

Our software provides building-level resolution for obtaining heat demand and generating heat demand time series. This represents the maximum spatial resolution possible or meaningful to define. While it is theoretically possible (for small case studies) to perform the optimisation for individual buildings, the computational burden rapidly becomes prohibitive as the number of buildings increases. This is due to the complexity of the optimisation model, which simultaneously performs operational optimisation and generation expansion (investment decisions) over the complete time horizon.

To address this, a clustering procedure is introduced, which merges multiple buildings into a single heat node. While this approach inevitably introduces deviations at the level of individual buildings, it significantly improves computational tractability. By adjusting the number of clusters, users can balance spatial granularity against solver runtime: few clusters allow for quick exploratory runs, whereas more clusters enable higher-resolution analyses once all parameters are fixed.

The relationship between cluster size (i.e., inversely, the number of clusters) and output accuracy is complex and strongly dependent on the specific network topology, relative costs, and demand ratios. Therefore, no universal measure can be provided. It is the responsibility of the user to select a cluster size that aligns with the required spatial resolution for the case study, the size of the system, and the available computational resources.

2.2 Temporal Resolution and Time Horizon

The temporal resolution of the optimisation model is flexible. However, it is important to ensure that all input data share the same temporal resolution (e.g., outdoor temperature and waste heat profiles). While an hourly resolution is common in energy system modeling, finer resolutions such as quarter-hourly can be chosen for greater detail, or coarser resolutions such as two-hourly can be used to reduce computational time. Similar to spatial resolution, a finer temporal resolution increases detail but also slows down the calculations.

Regarding the time horizon, a full chronological year is typically selected. This ensures that all weather conditions within a given year are represented, and that long-term dynamics or seasonal effects are accounted for. Longer time horizons (e.g., two years) are technically possible, but it is generally recommended to compute each year separately if the impact of different weather years is of interest and to compare the results. If a shorter time horizon is considered (e.g., only the heating season), it is necessary to adjust all costs according to the selected period.

3 Stochastic Heat Demand Time Series Modeling

The modeling of heat demand time series is performed at the single-building level. In a preliminary step, certain parameters for each building (e.g., specific heat demand) are determined. Subsequently, an active occupancy profile – indicating when people are at home and active, rather than sleeping – is computed for each building using a Markov Chain Monte Carlo (MCMC) process.

Transition matrices derived from Time Use Surveys [3] drive this process, generating stochastic active occupancy profiles for individual dwellings. For a large number of buildings, these stochastic profiles converge toward the underlying distribution observed in the surveys. The occupancy information is then used to define the setpoint temperatures for each building, and the corresponding heat demand is calculated using a simplified thermal model.

This MCMC approach introduces a degree of randomness at the individual building level, reflecting real-world diversity in daily usage patterns. It thereby avoids unrealistic peaks in aggregated heat demand that would occur if standard load profiles were simply summed across buildings.

For further details on the underlying methodology, the reader is referred to [4].

References

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