Contribution of storage technologies to renewable energy hubs

Master Project

Author:
Jules MATHIEU

Supervisors:
Prof. François MARÉCHAL
Dorsan LEPOUR
Jonas SCHNIDRIG

Industrial Processes and Energy Systems Engineering
Ecole Polytechnique Fédérale de Lausanne

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Abstract

A holistic approach, considering all the energy needs of a territory, should be adopted in the challenge of the energy transition. Synergies between the different end-use demand sectors must be developed, in order to optimize the efficient use of resources. The multi-energy system of the future will be integrated and coordinated, with renewable energy sources and decentralized capacities. Indeed, in a context of increasing urbanization worldwide, decentralized renewable capacities appear to be the key driver to decarbonize urban environments and foster the emergence of *renewable energy hubs*. Mutualized infrastructures need to be deployed at every stage of these hubs: from energy harvesting, transport, and storage; to mobility services and goods production. The most suited scope to study the deployment and promotion of these local capacities and shared infrastructures appears to be the district perspective. The financial and environmental benefits of a district integrated approach for the mutualization of capacities have been proved, but their implementation mechanisms remain understudied. The aim of this study is to characterize the contribution of storage technologies to ensure the energy balance of a territory, assess the associated investments to be made, and discuss the techno-economic and environmental performance of the whole system.

Firstly, a district is defined as a renewable energy hub, by identifying the energy needs of the residents and the potential of endogenous resources. Then, a Mixed Integer Linear Programming (MILP) model is developed to offer a multi-objective optimization of energy resources at district-level. Finally, a characterization of the storage technologies available under the horizon 2050 is conducted and a set of technological solutions is created to serve as input to the optimization model.

Although their robustness has not been assessed, the obtained results show several interesting impacts. First, storage implantation allows to foster Photovoltaic (PV) deployment until full penetration. Sides effects to this increased penetration are a growth of the exported electricity together with a reduction of the imports. While the the latter is beneficial, the export increase might put the electric grid at risk. Second, synergies between electric and heat storage technologies where demonstrated through an increased use of heat technologies. Lastly, long term storage was not demonstrated and additional work should be undertaken to validate the overall model.

Finally, once the developed model is corrected with the proposed improvements, it aims to be integrated in a global comprehensive model whose final purpose is to assess the optimal level of mutualization of energy conversion and storage capacities in urban areas.

Acknowledgments

Tout d'abord, je tiens à remercier tout particulièrement Dorsan et Jonas pour leur accompagnement et leurs si nombreux conseils donnés lors de ce projet. Je n'oublie pas François Maréchal avec qui chaque échange a été particulièrement passionnant et souvent source de refonte du projet.

Ensuite, c'est ici que s'achèvent mes études. Au moins pour un temps... Ma vision de l'ingénieur s'est précisée au fil de mes études grâce à de nombreux acteurs. Je tiens donc à remercier l'ensemble de l'UCBL et l'EPFL pour m'avoir inculqué la rigueur et la méthode nécessaires à l'approche de l'ingénieur. Je remercie ensuite l'ensemble de mes contacts privés et professionnels qui m'ont fait prendre conscience de la place et du rôle que l'ingénieur pouvait avoir dans l'évolution de la société.

Je remercie donc chacun de mes amis. Ceux avec qui j'ai pu découvrir la notion d'amitié, Ceux qui m'ont nourri de débats passionnés, Ceux qui m'ont montré le dévouement pour atteindre ses rêves. Ceux qui m'ont rappelé la valeur simple de la vie. Enfin une dédicace spéciale à tous ceux qui m'ont accompagné explorer la montagne.

Also to the other students from the "Science and Technology" MSc where I met friends with an important sensitivity to climate change and with urge to change the world to a better place. So thank you to all of you ! For the record, I hereby promise to come back to Switzerland to see those of you who will still be there. For the others, I count on you to host me if I come to visit. Otherwise my door will always be opened !

Enfin même si aucun mot n'existe pour souligner son importance, merci à ma famille qui m'a, à maints égards, permis d'arriver là !

Jules Mathieu

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Acronyms

ADEME (ADEME) Agence de l'environnement et de la maîtrise de l'énergie
AEL (AEL) Alkalyne Electrolyzers
AWHP (AWHP) Air Water Heat Pump
BC (BC) Base Case
BE (BE) Break-Even
BESS (BESS) Battery Energy Storage System
CAPEX (CAPEX) Capital expenditure
CH4S (CH4S) CH4 Storage
COP (COP) Coefficient of Performance
DHN (DHN) District Heating Networks
DHW (DHW) Domestic How Water
EH (EH) Electric Heater
EHV (EHV) Extra High Voltage
ETZ (ETZ) Electrolyzer
EV (EV) Electric Vehicle
FC (FC) Fuel-cell
GHG (GHG) Greenhouse Gases
GIS (GIS) Geographic Information System
H2 (H2) Hydrogen
H2B (H2B) Hydrogen Buffer
H2S (H2S) Hydrogen Storage tank
H2SLP (H2SLP) Hydrogen Storage Low Pressure tank
HP (HP) Heat-Pump
HS (HS) Heat Storage
HV (HV) High Voltage
ICT (ICT) Information and Communication Technology
IPESE (IPESE) Industrial Processes and Energy Systems Engineering
KPI (KPI) Key Performance Indicators
LHS (LHS) Latent Heat Storage
LI-ION (li-ion) Lithium-Ion
LV (LV) Low Voltage
MILP (MILP) Mixed Integer Linear Programming
MTZ (MTZ) Methanizer
MV (MV) Medium Voltage
OPEX (OPEX) Operational expenditure
P2G (P2G) Power to Gas
P2G2P (P2G2P) Power to Gas to Power
PEM (PEM) Polymer Membrane Electrolyzers
PTES (PTES) Pumped Thermal Energy Storage
PV (PV) Photovoltaic
RE (RE) Renewable Energy
RTE (RTE) Round Trip Efficiency
SBD (SBD) Smart-Building Design
SC (SC) Self-Consumption
SE (SE) Specific electricity
SH (SH) Space Heating
SHS (SHS) Sensible Heat Storage
SIA (SIA) Société suisse des Ingénieurs et des Architectes
SMR (SMR) Small Modular Reactors
SOC (SOC) State Of Charge
SOEFC (SOEFC) Solid Oxide Electrolyzer and Fuel Cell
SS (SS) Self-Sufficiency
TCHS (TCHS) Thermochemical Heat Storage
TD (TD) Typical Day
TES (TES) Thermal Energy Storage
TOTEX (TOTEX) Total expenditure
TSO (TSO) Transmission System Operator

Nomenclature

Parameter

η	Efficiency
η_l	Efficiency degradation
σ	Self Discharge
inv_2	CAPEX
$kWhn$	Unit nominal capacity
kWn	Unit nominal power
L	Lifetime
op_1	OPEX
T	Temperature of operation

Preface

This submitted thesis was written as partial completion of the "Energy Science and Technology" Master's degree within the Electrical and Micro-Engineering section, School of Engineering department, Swiss Federal Institute of Technology Lausanne (EPFL). The thesis was carried out during 18 weeks from September 13, 2021 to January 14, 2022 under the supervision of Professor François Maréchal and the two doctoral students Dorsan Lepour and Jonas Schnidrig.
During the project, an energy model was adjusted to integrate long term storage technologies. Simultaneously, a literature research allowed to characterise several storage technologies which were then added to the model. This tool was hence applied to an urban district to analyse impact of the added storage technologies to the energy independence of the district.

Sion, January 12^{th} 2022
Jules Mathieu

Chapter 1

Introduction

1.1 Background

Climate change existence and causality to human actions are not to prove anymore and its consequences are already visible through frequency increase of extreme weather events such as droughts, heavy precipitation or hot temperature episodes [2]. For instance, droughts events in drying regions are now likely to occur 1.7 times more compared to the 1850-1900 reference period. The new challenge is to mitigate those consequences by limiting global warming well below 2°C as settled in the Paris agreement's international objective [3]. This objective does not let room for inaction as it corresponds to about 20 years of global carbon budget at current Greenhouse Gases (GHG) emission rate.
In that context, low carbon technologies are foreseen to replace fossil fuel and fulfill the energy needs of an increasing population [4]. Renewable Energy (RE) as well as nuclear technologies meet this low emission criterion. However, Switzerland's population took the decision in 2017 to phase out nuclear power in the next decades [5]. Switzerland has a high hydraulic potential but already uses most of it as it provides 36 TWh electric - 12.3% of Swiss primary energy consumption - and only plans a 4% increase by 2035 [6]. The RE increase will thus be driven by PV panels, wind turbines and biomass.

Regarding the energy system structure, the development of RE is expected to lead parts of the currently centralized energy system toward a decentralized structure [7], i.e the energy is thought to be produced through a distribution of small producing units across the territory instead of a limited number of large power plants. The interest of decentralization compared to centralization are numerous. First, it allows to maximize the efficiency as both transmission losses are saved and synergies between energy vectors can be exploited. [8] illustrates the many hurdles faced by nuclear cogeneration and states that lower level of centralization - using Small Modular Reactors (SMR) - could help to overcome those. By contrast, inefficiencies from decentralized Power to Gas (P2G) plants can meet part of the heat demand while answering the electricity load, thus increasing the overall system efficiency. This efficiency improvement benefits to other system's elements as showed by [9] where heat from the P2G covers high temperature needs thus increasing the efficiency of the

Heat-Pump (HP) faced with lower temperature output's need.

The integration of non-controllable stochastic energy production into the energy network reduces its flexibility to balance load and supply. In the report [10] the French Transmission System Operator (TSO) "Réseau de Transport d'Électricité" highlighted storage transcription of flexibility requirements regarding the French electricity grid to ensure its continuous operation. There are already 3 time-related power and capacity reserves to ensure the grid safety on a very short period (reserves can be activated in 30s for the first to 15minutes for the third) [11]. However, in a scenario characterized by a high share of non-controllable electricity sources, the report quantified the necessity for short to long term energy storage able to provide up to 47 GW flexibility and about 50 TWh to cover the seasonal unbalance [12]. This only concerns the French electricity sector whereas electricity is expected to represent 55% of the overall primary energy need in 2050 [10]. Yet, this raises the question of the integration of this storage in the overall energy structure and among other, its position in the electricity network as regards the tension level.
Still considering the electricity layer of the energy system, [13] pointed out the network limitations linked to the high penetration of PV due to the top-down layout of the grid. Upgrading cost of the Medium Voltage (MV) grid are expected to be the highest. The authors also demonstrate that the integration of storage capacity could help to integrate high share of PV in the electricity system.

Overall, the energy system is expected to transition from a centralized fossil-fuel based system towards a decentralized one characterized by high level of stochastic renewable production where the energy balance will have to be ensured by the integration of storage capacities. This study thus seeks to explore the possible configurations of such a system, with a particular focus on the storage technologies to be deployed in the future.

1.2 State of the art

Multi-energy carrier in holistic energy hub

The concept of "energy hub" was first developed in [14] and [15] as a framework where energy carriers can be converted and stored. This framework acts as an interface between the different connected loads and energy infrastructures. This formulation is particularly useful to exploit the different synergies between carriers and loads altogether. For instance, it allows to collect the inefficiencies under heat form from an energy carrier conversion to fulfill part of the heat demand. In addition, energy hubs have an intrinsic advantage of an increased reliability due to redundant connections inside and with the other energy hubs.

District characterisation - Qbuilding

Qbuilding, partly described in [16], is a Geographic Information System (GIS) based model whose main function is to collect and combine several GIS databases in Switzerland in an energy oriented perspective. In this project's standpoint, Qbuilding contains layers of information characterizing the building stock of the selected area (building area, use allocation, potential for PV capacities, etc.). In addition, Qbuilding also extracts information from energy norms and standards (Société suisse des Ingénieurs et des Architectes (SIA)), allowing to statistically quantify the buildings energy needs [17].

Regarding its operation, Qbuilding can be used as a black box receiving a spatial area located in Switzerland as an input. Outputs are then provided as "geopackage" or "comma separated values" files which must be filtered and aggregated into a single file before being sent to the modelling software.

Modelling

Smart-Building Design (SBD) is a MILP optimization model developed by Luise Middelhauve and Paul Stadler at Industrial Processes and Energy Systems Engineering (IPESE) [18, 19]. It optimises the investment and operation of an energy system designed to meet the demand of a building. The objective can be an energy or cost related one and the decision variables are the investment and operation decision for each technology unit. The tool allows for multi-objective optimization using epsilon constraints, and additional constraints may be enabled to meet precise requirements (e.g. limitation of CO2 emissions, or off-grid building).

The main strengths of SBD are on one hand the inclusion of a heat cascade to model the discrete temperature levels associated to conversion and storage units; and on the other hand the thermal requirements are not defined as fixed profiles but are independently modelled (space heating, space cooling, domestic hot water needs), based on the energy signature of the building envelop and the residents behavior [18].

Regarding MILP modelling complexity, the computational load increases exponentially with the number of nodes (e.g. technologies and buildings) it embeds as each node possesses its own set of variables and constraints. Energy modelling over districts is thus computationally expensive and several solution to reduce the complexity have already been proposed. First, some studies proposed to reduce the size of the time series using clustering techniques [20, 21]. Similarly spatial aggregation can also help to reduce the model complexity [22].

Energy storage

The planned necessity of an important storage capacity in the next decades (section 1.1) pushed the scientific sector to prolific research over the numerous storage technologies as well as the operation of decentralized energy systems. BESS have - thanks to the Electric Vehicle (EV) deployment - already achieved technical and commercial maturity. Due to their dynamic response and high power to capacity ratio, they are able to provide frequency shaving (i.e second to minute scale) in top of the electricity storage [23] [24]. Then, P2G benefits from much supports in the political sphere with at least 37 governments proposing strategies specific to the development of the hydrogen sector [25]. P2G allows for long term energy storage under chemical form as well as other uses than electricity, for instance in the mobility sector. In addition to those two sectors already commercialised or close to, scientific literature proposes technologies as PTES designed to store electricity under heat form. This technology is well suited for medium term storage as its Round Trip Efficiency (RTE) is between BESS and P2G. Moreover, [26] also states it can compete with other large scale technologies in terms of costs.

Regarding the thermal storage segment, [9] highlighted the differences between electrical and thermal load profiles leading to potential for thermal storage deployment. At building scale, domestic hot water tanks are already well known but new technologies are currently being developed such as LHS which displays higher energy density and nearly constant storage temperature [27].

1.3 Literature gap

Studies using optimization techniques often fix the costs of the energy exchanges between the district and the different energy networks [28]. But as an energy system design is strongly dependent on its interface conditions (price and availability of resources being the most impactful parameters), the result of the optimization is only insightful for those boundary conditions. Since these interface conditions cannot be foreseen with precision, especially in the long term, it is of interest to study energy systems robust to boundary parameters variations and to include resilience as a key criterion.

Moving on now to consider the impact of energy prices onto the energy hub under study, retail cost gives an actual value to the consumed energy. In an ideal market, it should correspond to the cost of producing and bringing the energy to the energy hub interface. In the energy hub perspective, this price can motivate the implantation of local generation if its energy levelized cost is cheaper. Then, if some extra energy is freely available, it can be interesting to store it for later use as long as the total cost of producing and storing this unit of energy is lower or equal to its network retail cost.

Regarding the feed-in cost, which is usually lower than the retail-cost, the same reasoning could be applied. However, in a energy hub seeking to minimize its Total expenditure (TOTEX), the decision of storing an extra energy unit produced instead of selling it is answered by its capacity to store and deliver this unit at a cheaper cost than the difference between the retail and feed-in cost. However, as previously discussed, the higher efficiency achieved by the decentralization of the system as well as the electric network limitation push for maximisation of internal energy use. Hence, considering a zero feed-in cost would allow to maximise the internal cost-effective energy use and limit the exported energy.

As of today, the only storage technologies featured in SBD include BESS as well as SHS dedicated to domestic hot water or space heating. As explained in the previous section, storage technologies for longer periods than daily storage will be needed in future energy hubs with important levels of renewable penetration. Integrating long term storage into SBD could enable this efficient software to model future comprehensive energy systems. Moreover, as part of [28] thesis plan, this adapted version of SBD could easily model the district-level behaviour and further adaptations of it could model region- to country-level territories.

1.4 Contribution

1.4.1 Problem Statement

The previous section highlighted storage necessity in the future decentralized energy grid as well as several weaknesses in the current energy models partly solved by the SBD optimisation software. The problem statement this project aims to answer is proposed hereafter:
Adaptation of the SBD *optimization model to explore the relation between electricity supply cost and penetration of renewable generation and storage capacities, in a future urban district.*

1.4.2 Energy hub level

Due to its historically centralized generation capacities, the current electricity grid has been built as a top-down infrastructure from the large power plants to the end-of-line consumers. Its design was not made to withstand high power levels on the Low Voltage (LV) layer. Renewable generation and especially PV might lead to reach these limitations leading to important upgrading costs [13]. According to [29], when increasing renewable generation, MV networks represent the largest share of the overall upgrading costs. Hence, it is of interest to design grid friendly structures at the MV/LV interface while still allowing high-penetration of renewable to reach the carbon neutrality objective [4, 30]. Regarding heat, District Heating Networks (DHN) seek to minimize losses through network distance minimization, in the same manner the electricity grid does [13]. The electricity definition is thus congruent with the heat considerations.

As a result, the district is defined by the set of buildings linked to a MV/LV electric transformer. The energy hub then embeds this defined district as well as the conversion and storage implemented technologies. The district thus represents the demand units as well as the external constraints through temperature and solar irradiation.

1.4.3 Stand-point

The perspective taken is located at the MV/LV transformer interface for electricity and district's boundaries for other energy vectors. In the case of a decentralized system, the manager of the district has complete autonomy on the two decision variables represented by investments and operation decisions. The main objective the manager seeks to minimize are district's TOTEX. His decisions are affected by both the energy needs of the district and the energy tariffs at its interface.

1.4.4 Research questions

Turning now to the core of the project, the problem statement is further precised through the following research questions :

- How to select the examined district ?
- What are the characteristics of the defined district ?
- How to adapt the SBD model to integrate long term energy storage ?
- How to adapt the SBD model to answer the demand of a district instead of a single building ?
- Which storage technologies are compatible inside such district ?
- How to characterize the different storage and conversion technologies ?
- How to model the different storage and conversion technologies ?
- How is the evolution of the electricity price impacting the renewable generation ?
- What are the interactions between renewable generation and storage deployment ?
- What are the synergies between storage technologies ?
- What is the robustness of the optimal solution regarding technology uncertainty ?

1.4.5 Objectives

In order to answer the previously presented questions, the following steps will be applied :

1. Use Voronoi partition of Switzerland to delimit LV districts;
2. Extract a district and its features using Qbuilding model;
3. Identify and characterize storage technologies suited to the district scale;
4. Model the different technologies in such a way that the key characteristics are captured;
5. Annualize the energy balance through TD serialization to allow long term energy storage;
6. Determine Key Performance Indicators (KPI) allowing to compare the performance of several scenarios;
7. Create plotting modules to allow the model user to quickly seize the behaviour of the modelled system;
8. Define a particular range of electricity cost values linked to changes in the penetration of renewable generation;
9. Analyze the robustness of the scenario through Sobol simulations over the different cost sets.

1.5 Project Background

This project has been realised as a Master Thesis within the IPESE laboratory under the supervision of Prof. François Maréchal and the two doctoral students Dorsan Lepour and Jonas Schnidrig.
This project was carried out in Sion with access to a 12 cores and 8 GB ram virtual machine. Additionally, an access to the AMPL software as well as Gurobi and Cplex licence were granted.

Chapter 2

Method

2.1 District definition

In the following section, the method to select the district to be examined is described and applied using Voronoi partitioning. Then, the Qbuilding software is used to extract the district typology.

2.1.1 Geographic breakdown

The article [13] derives a synthetic model of Switzerland distribution grid. The created model is based on the location of the Extra High Voltage (EHV)/High Voltage (HV) transformers location together with the assumption that electricity consumption follows heat needs. The combination of those two parameters with a maximal power threshold that a transformer can withstand allows to partition Switzerland into EHV regions in a first step. The procedure is then repeated twice using two lower power thresholds to derive HV and MV regions. The link between a transformer node and its region is a Voronoi partition consistent with an ideal power grid seeking to minimize transmission losses. A Voronoi partition corresponds to a set of convex regions constructed on a finite number of nodes - e.g MV/LV transformers - where the delimited space embeds all points closer to the reference node than the other nodes.

The fictitious position of the MV/LV transformers derived in this study is publicly available. A Voronoi partition was then used to construct LV regions corresponding to districts of this project. Figure 2.1 displays a map of Switzerland partitioned territory where each district is colored depending of the population density provided with the EHV transformer it is linked to. The reddish it is, the denser the EHV linked region is.

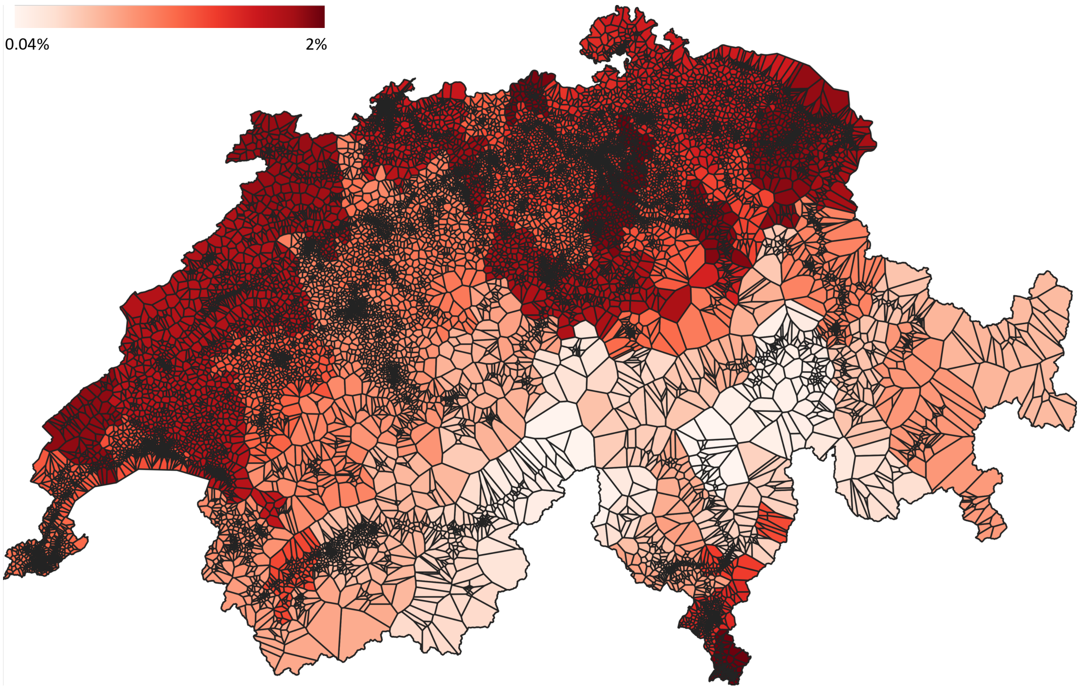

Figure 2.1: Switzerland map broken down along the LV districts with a population density scale (in % of the overall Swiss population)

2.1.2 Selection of one district and characterization

The previous section partitioned Switzerland into 17'638 convex districts whereas this project is focused on only one. Consequently, a single district was selected on the map in a subjective way although driven by some criteria. First, the one-building formulation described in section 2.2.2 requires the existence of a DHN to share heat flows between all the implementable technologies. The main selection criterion was thus a district with a built density high enough to motivate the interest of DHN. Hence an urban district. Second, the modelling of industrial high temperature needs is out of scope of this project (see section 2.2.1). It is thus needed to select a mostly residential and tertiary district.

The finally selected district together with its embedded buildings are displayed in figure 2.2.

Regarding its typology, this district includes 317 buildings where 92% of them correspond to individual housing, 4.4% to collective housing and the 3.6% left are distributed between industry, administrative and gathering places buildings. With respect to the overall built surface of 81'236 m2, shares are respectively 66%, 25% and 8%. Other characteristics of the district are presented in section 2.2.2.

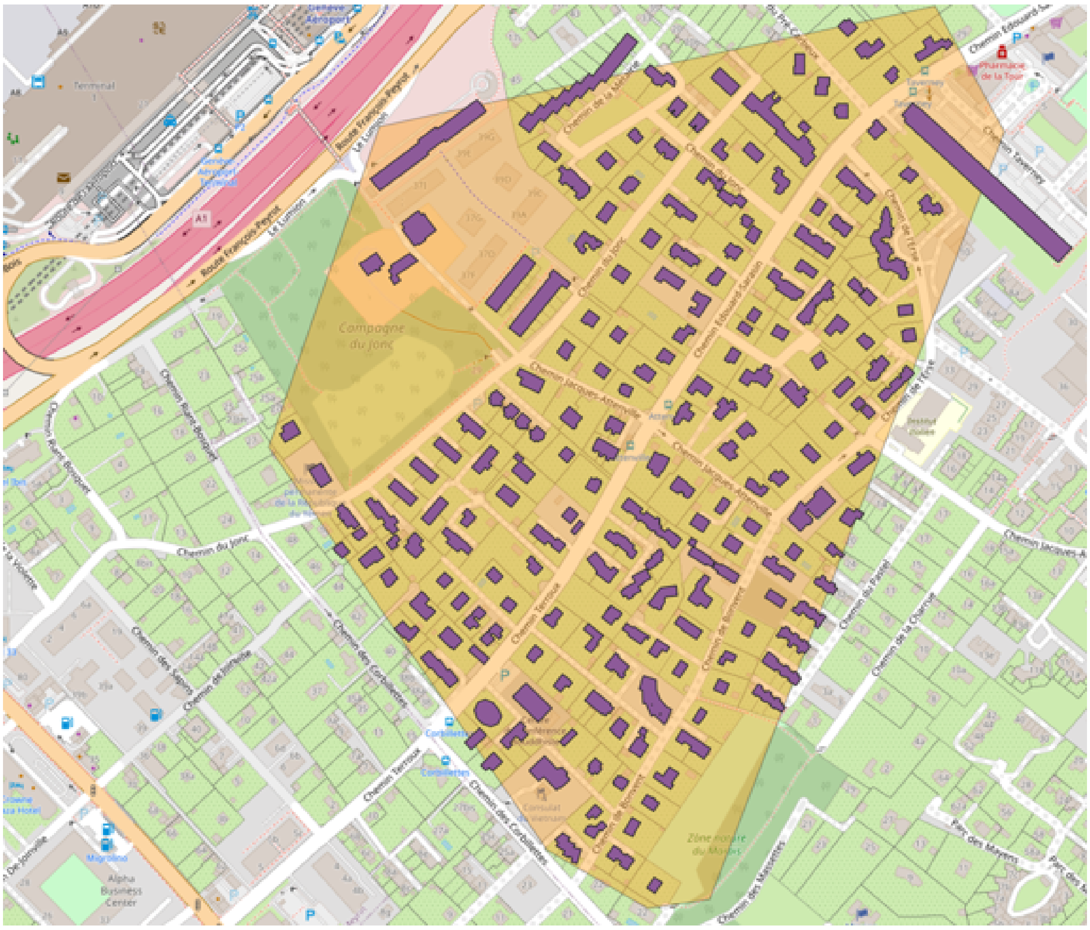

Figure 2.2: Visualisation of spatial boundaries of the districts as well as the set of buildings it is composed of.

2.2 Optimization model

This section focuses on the adaptation of the SBD model to allow the optimization of a territory's energy balance, including the implementation of storage technologies. It starts by integrating the TD serialisation to allow for inter-day energy storage. Then, it proposes a one-building aggregation of the overall district in order to reduce the computation load.

2.2.1 Hypothesis

In the section that follows, hypothesis settling boundaries of the model are discussed. A first set of boundaries concerns the energy needs which were not considered in this project's frame due to time constraints. These are mobility, cooling and Information and Communication Technology (ICT) related needs. On the other hand, covered services are Space Heating (SH), Domestic How Water (DHW) and Specific electricity (SE) needs.

The second set of hypothesis directly affects allowed energy flows and usable technologies and are further referred to as follows : the net-zero objective, the common technology restriction and the gas grid disconnection.

First, the net-zero objective is necessary to ensure a district compliant with the net-zero indicative target announced by the Swiss federal council in 2019 [31]. It implies a phase-out of petroleum products and plans DHN to mostly operate on HP technologies to cover their heat needs [30].

As concerns the common technology restriction, it aims to ensure that the model can be applied on most of the districts. Hence, technologies linked to specific territorial characteristics such as gas reservoir or hydraulic potential were disregarded. Heat pumps are not affected by this restriction as they can be air based when the geothermal potential does not justify an investment.

Third, the gas grid disconnection hypothesis is supported by efficiency considerations. An exergy perspective points out the interest of restricting gas for high temperature heat processes as proven in several energy system models results [30, 32, 33, 34]. As this district is mostly residential and high temperature needs are not characterized, it is more exergy efficient to use HP to provide residential heat instead of gas boiler, especially that the considered district is not in a heritage protection zone which could prevent HP use. However, in the frame of a country scale study where the biogas potential and high temperature heat consumption are characterized, this restrictive hypothesis should be revised as the maximisation of endogenous resources would then be at national scale.

Last but not least, the district is assumed to be connected to a DHN. This latter is a result of the one-building formulation further explained latter on. This formulation prevents to model the district down to the building level as regard decisions about storage and conversion technologies or DHN deployment. To allow for heat exchanges, DHN is thus considered as available but its costs are not modelled.

2.2.2 SBD adaptation to include storage

The following parts of this section move on to describe the process applied to fit SBD to allow long term storage as well as to model districts combining hundreds of buildings.

Daily optimization towards yearly energy balance

To be computationally effective, SBD is not operated on a full year but on a subset of TD resulting from a clustering step applied on the needs' yearly series, similar to [35, 36]. However, while this is actually effective regarding classic conversion technologies where the energy balance is subject to the same time frame as the power balance, it is not suited for inter-day storage.
[37] applied a method proposed by [21] to allow for long term storage while minimizing the computation complexity. The proposed concept keeps a TD based power balance but the energy balance is operated over a full year. In order to keep an energy to power relation which respects the laws of thermodynamics, the entire year is constructed back on a series of TD associated to each day of the

year. Days are thus associated with their most similar TD with respect to temperature and irradiation profiles.

The one-building formulation

So far, SBD is able to operate quickly on a set of a few tens of buildings. The selected district being composed of 317 buildings, an aggregation step was required to get the characteristic of an overall building representative of the entire district whose values were extracted by QBuilding. Results from this step are displayed in table 2.1. A weighted average based on building's share in the overall area was applied to intensives values (temperature or energy factors) while extensive values resulted from a simple sum. It must be highlighted that this aggregation step was created as a sub-function included in the pre-processing module of SBD. As a matter of fact, functions already available in SBD allowed to extract the energy signature for each building extracted by Qbuilding. The created module is thus interleaved between the SBD pre-processing function extracting energy signature of each district and the communication of the resulting building to the SBD solver. Moreover, this extra module create an automatic link between the Qbuilding district output and the final one-building typology provided to SBD

As concerns energy needs signature curves, they are generated by SBD based on the SIA norms which depend on the SIA2024 classification of the building [17]. Whereas several consumers grouped together should benefit from the overflow effect, profiles for each SIA category are identical. The resulting overall profile was a basic summation of each profile from each SIA category simply multiplied by its area in the overall district. In order to simulate this overflow effect, two different methods were applied on water and electricity needs. In both cases, the profiles shape has been changed while respecting the law of energy conservation.

Regarding water profiles, the french Agence de l'environnement et de la maîtrise de l'énergie (ADEME) organisation published an observation study where several residential buildings were monitored [1]. Figure 2.3 reproduces the observed profile for a building composed of 269 flats which was used to smooth the aggregated SIA profile. One might notice that the considered district includes a higher number of people with 1'958 people which is around trice as high as the number of people in this example. However, this profile is still considered as realistic as the overflow effect becomes linear with a low coefficient when passing the 200 flats threshold [1].

Parameter name	Meaning	Value	Unit
Ucoef	Thermal transmittance	1.65	[W/(K.m2)]
Ccoef	Thermal capacity	119.19	[Wh/(K.m2)]
edotel	Specific electric signature	13.94	[W/m2]
qdothw	Hot water signature	2.59	[W/m2]
SolarGainF	Fraction of house area subject to solar gains	0.08	ratio
Tinto	Reference indoor temperature	20.00	[°c]
hs_Tro	Reference return temperature of the heating system	47.01	[°c]
hs_Tso	Reference supply temperature of the heating system	61.33	[°c]
floor_n	Number of stories	3.68	[-]
hs_A	Reference energetic area	81’235.50	[m]
n_p	Number of residents	1’958.09	[-]

Table 2.1: Key characteristics of the district resulting from the aggregation of all district’s buildings

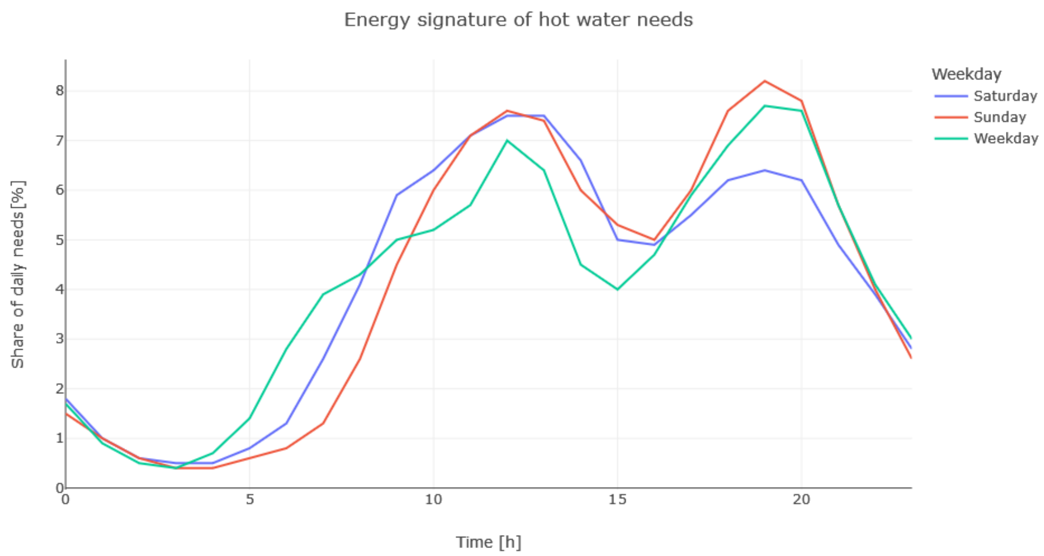

Figure 2.3: Hot water energy profiles for a building composed of 269 standard flats, reproduced from [1]

Concerning the electricity profile, no such curve was available. However, as displayed in figure 2.4, an important spike can be observed between 12 and 13h. Assuming that people generally eat between 12h and 14h, the applied method uses a Gauss distribution with a standard deviation of a hour to shift spikes of each building. As a result, 95% of buildings profiles are shifted between minus 2 and plus 2 hour from their original value while respecting the one-hour sampling frequency. In other words, each electric time value of a building is calculated through the following equation :

$$Final_t = Original_t * (1 - abs(SF)) + Original_{t\pm1} * abs(SF)$$

With SF the shift factor - from gauss distribution - and a negative sign instead of $\pm$ in case of a positive factor or the opposite with a negative one. Also, the day is considered as circular while applying the previous equation to ensure continuity around midnight and energy preservation.

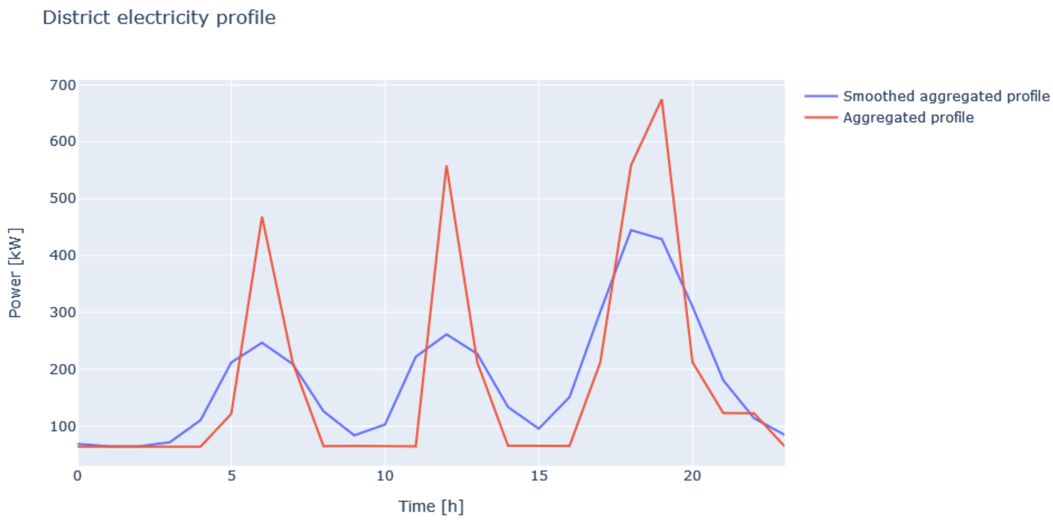

Figure 2.4: Aggregated electricity weekday profile of the district before and after the smoothing process

Last but not least, heat gains from electric needs are corrected to account for this new electricity profile and heat gains from human presence are kept as aggregation of SIA profiles.
The main drawback of the one-building formulation is the loss of the infra-district level of detail and modelling possibility. Every technology is thus modelled as if it were deployed at the district interface either as an aggregate of all units deployed inside the district or as a mega unit at the interface. However, a finer mesh model could allow to explore the interest of both possibilities or a mixed one as well as the actual operation of the DHN.

Structure modification to integrate storage technologies

SBD modifications to allow for the integration of storage technologies are presented in the following section. First, figure 2.5 presents all the modelled energy conversion and energy storage technologies, as well as their respective input and output layers. The H2 and CH4 layers were added to the model to allow for P2G storage chain.

Second, two additional curtailment variables were added, allowing electricity and heat curtailment. The existence of a third curtailment variable dedicated to PV panels in the original SBD model must be noted. The interest of the second electricity curtailment variable is then more in a informational purpose. The model is not expected to use it but it offers an extra level of freedom and the reasons for its use should be explored in case of utilisation. On the contrary, the heat curtailment variable is necessary due to the existence of the inefficiencies. Inefficiencies from the electricity related units are converted to heat from which a part is usable to fulfill heat related needs and the other part is considered to be lost in the environment. The boundary between usable and lost heat is defined first

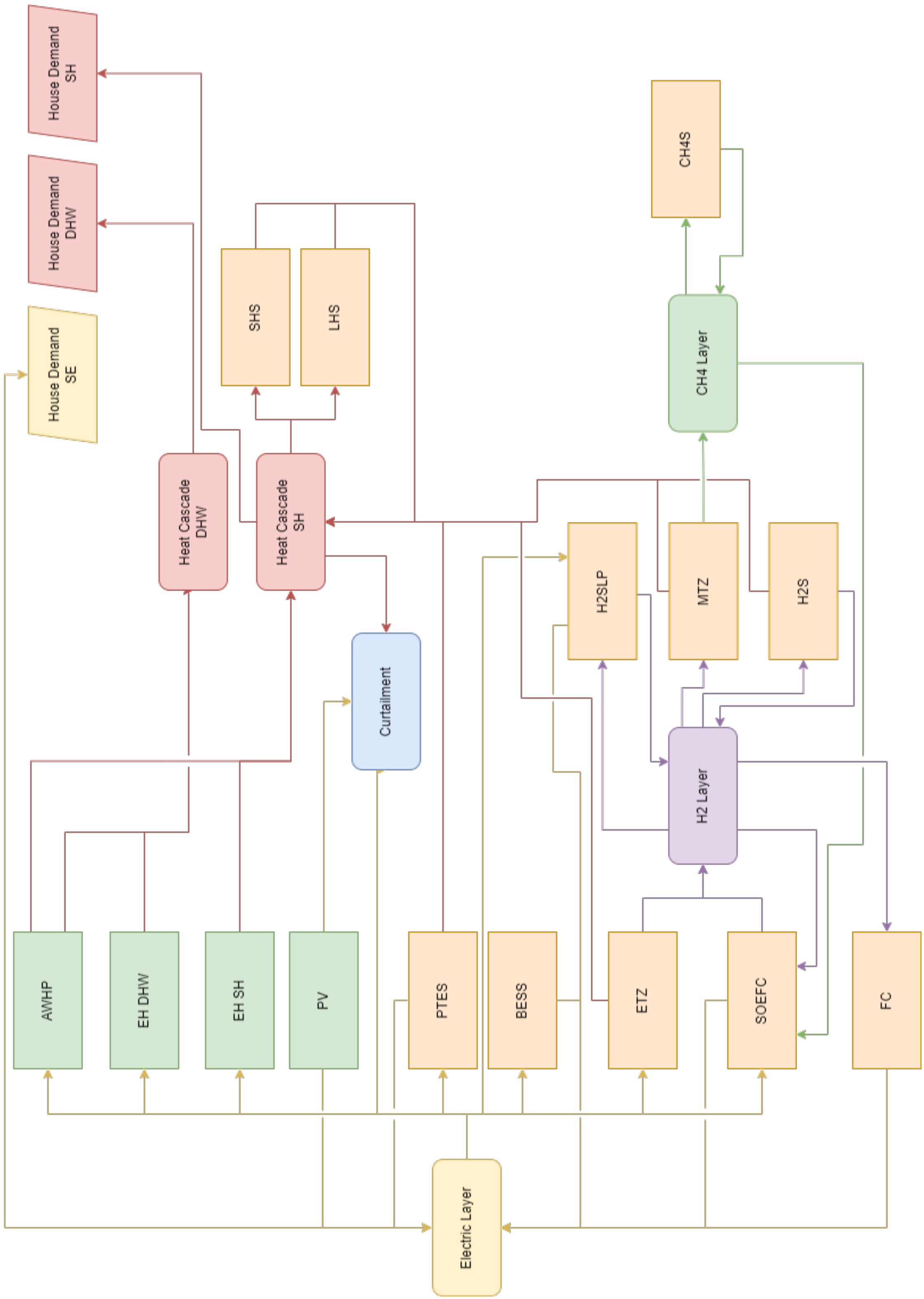

Figure 2.5: Presentation of the overall storage model structure. Definition of the acronyms can be found in the nomenclature section

by its exergy content (although one might increase this same exergy content using a HP) but also by the economical and technical interest of collecting those losses. For instance heat losses through pipes are difficult to collect if those pipes are not in an insulated room and the economical interest should be further examined before installing such a collection system. Eventually, this model gives the possibility to discard a certain heat fraction for each technology to represent those useless losses.

Third, a small fictitious cost is added to each flow entering storage or conversion technologies (apart from PV where it is the output flow which is "*taxed*"). This cost of 0.0001€ per kWh has a negligible impact to the overall system but prevents the use of inefficiencies as curtailment variables, preventing storage units from looping to curtail some energy as the curtail variables do not bear any operational cost. It must be noted that due to the MILP construction, a unit which is able to operate both ways is not restricted to a single direction at a specific time. Adding this restriction using binary variables would considerably increase the overall computation time. Fictitious cost is thus a way to prevent the looping of storage units when they should have no interest doing it. However, it might still be used to generate additional heat through the inefficiency without increasing the conversion power.

Fourth, the heat balance was modified to allow for heat curtailment. This modification was necessary due to ensure the possibility to discard useless heat from storage technologies. A closer look on the integration of each technology in the district would be necessary to select which type of unit could allow to release the heat. For instance, implantation of such technologies directly into buildings would add additional cooling demand in the cooling season.
Last, the SBD model has been modified to consider operational costs (related to as Operational expenditure (OPEX)) linked to maintenance of each technology in the overall TOTEX.

Objective function

The objective function is a TOTEX minimization. It is the sum of the OPEX and Capital expenditure (CAPEX) related to both storage and conversion technologies.
The OPEX includes all operational costs related to each technology as well as the small fictitious cost preventing loop behaviour.
The CAPEX is the actualised cost of all technologies scaled to one year of operation. The actualisation factor is computed with an actualisation rate of 0.02 and a project duration of 20 years. In addition, technology investments costs are all scaled to fulfil the project duration regarding to their own lifetime.
As previously highlighted, this TOTEX does not include DHN related costs.

Basic unit modification

The characterisation of future storage technologies in section 2.3 rise the need to update SBD units' parameters and costs to account for future improvements. As a results, the Air Water Heat Pump (AWHP) CAPEX have been set to 2376€/kWn [38, 39, 40, 41, 42, 43]. Additionally, PV CAPEX and efficiency were respectively set to 245€/kWn and 35% [44, 45].

KPIs definition

The following is a description of the different KPI. The KPI allow for analyzing and comparing the results obtained from different scenarios. While an exhaustive list is presented in table A.1, some key features are also discussed below.

The COP KPI allows to seize the electricity to heat conversion efficiency of the system. Its value gives the yearly average quantity of energy one can obtain under heat form for one energy unit of electricity. In another perspective, it allows to seize the importance of heat compared to electricity in the system. The higher the efficiency, the lower the heat importance. This electricity to heat factor is then used in other KPI to attribute more weight to value of electricity related KPI than heat related ones in overall KPI aggregating heat and electricity values.

The LC_U KPI gives the levelized cost of one kWh flowing out of the unit u. For technologies such as batteries, it directly reflects the cost of processing this energy unit by the technology. However, for technologies such as P2G, the specific cost of the overall chain is the combination of each technology LC_U and its efficiency. For instance, the following formulation can be used for the P2G process using the 3 following units : the electrolyzer ETZ, the H2 high pressure tank H2S and the standard fuel cell FC.

$$LC_{P2G} = \frac{LC_{ETZ}}{\eta_{H2S}} + \frac{LC_{H2S}}{\eta_{FC}} + LC_{FC}$$

Where η_{H2S} and η_{FC} are the energy efficiencies along the main vector (i.e. not the heat conversion efficiencies). The computation of the levelized cost on the energy output is the reason of the subscripted efficiency on the preceding technology LC.

Computation of Self-Consumption (SC) and Self-Sufficiency (SS) indicators are not straightforward and are computed in a multi-step manner explained in the following paragraph. First, SC refers to energy produced by PV panels (i.e. PV is the only renewable production technology the model is allowed to use) and either consumed to cover the district's needs or stored for later use. The two SC types are respectively referred to as "direct" and "storage" SC depending on whether the produced energy is directly used or stored for latter use. A second differentiating element is the energy vector provided (i.e heat or electricity as there is no other need type modelled). While electric SC is easy to grasp, the heat SC needs a conversion step. As a result, heat SC refers to heat provided to the district - to cover SH or DHW needs - by the PV panels through conversion or storage technologies. The computation of SC is a multiplication of the different ratios representing energy shares absorbed or returned by technologies on the considered pathway. In addition, only the time series with a non-zero PV production are considered.

As concerns SS, the same reasoning was applied apart from a few changes. First, instead of a PV production perspective, a district consumption perspective was taken. Electric SS refers to the share of district electric needs covered by PV production through direct generation or storage technologies. As regards heat, DHW and SH needs were aggregated as a total heat need. Then, the related SS refers to the fraction of heat demand covered by PV production through conversion or storage technologies. While it is assumed that all heat flowing out of storage technologies originates from PV production, the heat share flowing out of conversion technologies finally attributed to PV reflects the share of PV production in the electric production mix. It must be highlighted that the computation of SC and SS indicators is operated for each modelled hour and then averaged to obtain the overall indicators. This allows to get a resolution down to each typical day

KPI computation and presentation module

To efficiently compare and illustrate the characteristics of a given scenario, a post-processing module was created. It consists in a class with its set of methods which are able first to present in an interactive way the behaviour of the model for each time and each modelled TD. In addition, the set of KPI presented in the previous section is computed automatically.
Some plots are presented as examples in appendix A.1.

Allowing exploration of parameter spaces

So far, a model able to optimize a given district with one set of parameters has been created. To apply robustness assessment through Sobol analysis and explore multiples scenarios, the next step is thus the integration of such a model inside a wider frame, accepting varying parameters corresponding to specific scenarios. This would also enable the possibility to simultaneously apply the optimization process over several computing cores.
Similarly to the post-processing module, a new class was created with generic but over-writable characteristics of the district, together with a set of methods distributing the computations over the different computation cores as well as saving the overall results.

2.3 Storage technologies characterization

The previous section explained the modifications operated on the SBD structure. It is now necessary to select, characterize and model the different storage technologies. While each technology is fully described in its related *Rmarkdown* file (appendix B), some important criteria are highlighted in the present section.

2.3.1 Selection and characterization

Technology selection

Storage technologies can be grouped upon two usage criteria.
The first one is the storage duration or how many cycles a technology is designed to operate. This indicator allows to know to which energy balance the technology can answer, from the hourly balance to the yearly one, passing by the weekly or monthly ones (the grid frequency balance is out of scope in this study). Obviously, in a power perspective, a unit able to answer to the hourly balance could also answer to a longer period related balance but it usually comes with greater investment costs. On the contrary, seasonal storage technologies need to have a sufficiently low cost to provide energy at a competitive cost due to their low cycling potential (one to a few times a year) but often display limited power. In other words, the storage energy cost depends on the overall energy delivered (itself linked to the number of cycles and the efficiency) together with the per-unit investment cost.
The second criteria is the energy carriers the storage technology is able to handle. In the modelled system, only heat and electricity are considered regarding the final demand and are thus modelled. However, one could consider an hydrogen or a natural gas storage as a "km reservoir" to answer to the mobility demand. This grouping allowed to select a minimum number of technologies to be modelled in order to capture the different storage usage types. The following list presents the finally modelled technologies.

1. Electricity short-term (minutes to days) : BESS
2. Electricity medium-term (hours to weeks) : PTES, P2G (H2)
3. Electricity long-term (weeks to months) : P2G (H2 and CH4)
4. Heat short and medium-term : SHS, LHS

While this grouping is made to reflect storage uses, there is no clear definition of the different period boundaries. Technologies types are then expected to overlap as regard the behaviour of the model. As concerns modelling, further explained in the related section, each group displays specificities. While the most representative technology was selected in each category, the case of P2G is modelled allowing several pathways to explore. Regarding heat storage, two technologies are proposed to take full advantage of the heat cascade available in SBD.

Template

Reference year

As explained in the introduction, the considered district is a future district to allow simultaneously a new model not impacted by the technologies currently used in the district, as well as the expected cost and characteristics of storage technologies which are not competitive yet (apart from pumped hydraulic storage [26]) to be deployed. Hence, values extracted from the literature correspond to the expected values of mature technologies if a large scale production was to be implemented. These predictions place the set of values between 2030 and 2050 depending on the technologies.

Procedure

Two different phases into the development of a technology model can be identified. First, the characterization of the technology where literature values are extracted and key characteristics identified. Second, the modelling phase where key characteristics are modelled according to the needs and precision level of the model and where one final value inside the range is selected to represent the feature. In order to create a flexible database usable again for further projects, it was decided to create an independent *Rmarkdown* type file to summarize the overall process from the technology characterization to the final selection of parameters for the modelling. This *Rmarkdown* file is itself connected to a spreadsheet collecting all literature values in an easily exportable standardized format.

It must be pointed out that the undertook literature research is not extensive and only features values from recent work - most of the cited papers were published after 2017 - where reviews account for a significant number of the collected publications.

As regards monetary values, the actualisation step to express all cost on the same year basis was not applied for two reasons. First, it would have been time consuming given the important share of articles where the reference year was not provided. Second, the money-value variation in the last 5 years from which 71% of the studies were extracted is expected to be negligible compared to the uncertainty on the future cost values in the 2030-2050 period.

Quality criteria

Characterization of future technologies comes with important uncertainties which might impact the robustness of the overall results. To mitigate those impacts, it is needed to assess the variability of each parameter. The following assessment was applied on each selected value and is composed of 3 impact factors, themselves graded on a scale from 1 to 3 where 1 is the best score.

First, the **Literature Representation** grades the frequency that the parameter is cited in the literature. This scale is as follows :

1. Nearly all papers contain this value
2. About 1 out of 2 papers contains this value
3. Only a few papers contain this value

One might notice that those criteria (and especially the limit between two) can embed a large part of subjectivity. Henceforth, a conservative rule has been applied to select the higher integer when balancing between two.

Second, values cited in the literature can vary from one study to another. The **Range Size** thus reflects the size of the observed range as follows:

1. Range of values has a variation below 5% around the range midpoint (2.5% for efficiency)
2. Same but 10% (5% for efficiency)
3. Same but more than 20% (10% for efficiency)

The lower range permitted for efficiency variation reflects the usually lower changes efficiencies have compared to other parameters such as costs.

Third, despite being located in the future, some parameters could be more sensitive to technology breakthrough than others. A **Time Sensitivity** criterion thus reflects the value stability according to the following scale :

1. There are strong reasons to support that this value will not change with time (the value reached a theoretical plateau; the technology is already mature and deployed at large scale; . . .)
2. The value is a priory stable but one can not predict a breakthrough.
3. The value belongs to a technology still in R&D and there are large uncertainties about the long-term steady state value.

2.3.2 Modelling formulation

Basic technology structure

As displayed in figure 2.5, a generic storage technology can be seen as a standalone brick interacting with the model through the different layers to which it is connected. Those bricks can be activated by the model. In case of activation, decision variables are the unit size and its operation inside the range delimited by its size.

Specific implementation

As indicated previously, each storage technology is described in its related *Rmarkdown* file (appendix B). However, the final representation of each technology model together with values attributed to their parameters are highlighted in the following section.

BESS :

The BESS is a electrochemical storage system which stores energy under chemical form. It is an electric to electric system characterized by a high RTE as well as a low self-discharge. Its fragmentation into packs of several kWh makes it a very versatile technology which can either be installed as a large decentralized BESS unit at the district scale down to a centralized unit with a few stacks per building. Several different chemical formulation exist but the new breakthrough of Lithium-Ion (LI-ION) batteries in the electrical mobility segment will make them dominate the market in a few years [24]. Hence, LI-ION batteries were considered in the model and their main characteristics are presented in table 2.2.

One might notice that the RTE efficiency displayed in the figure is an average made over the lifetime of the technology (characterized by the bar over the RTE efficiency symbol. BESS is a technology whose efficiency reduces over time as illustrated by the "Efficiency degradation factor" from table 2.2. As a result, the average efficiency was computed and integrated in the model to reflect the average behaviour of technologies displaying this feature. Whereas the conservative option of taking the worst efficiency over the entire lifetime would be a way to ensure the system is able to meet the demand during all the lifetime, it does not reflect the time distributed deployment of the technologies which would reduce the probability to have all technologies similarly aged.

Additionally, a power limitation constraint needs to be applied on the input and output electric flows to ensure a high lifetime of the battery. This power limitation referred to as C-rate is the maximum power over the capacity of the battery. In other word, a C-rate of 2 means a the BESS would be fully charged/discharge in half-an-hour. The considered C-rate of 1 at the input and output is the maximum C-rate which can be applied on the model due to the time resolution of 1-hour.

Key criteria	Symbol	Value	Unit
RTE	η_{RTE}	86	[%]
Efficiency degradation factor	η_l	0.5	[%/year]
Hourly self-discharge	σ	0.008	[%/hour]
C-rate in	C_{in_max}	1	[kWin/kWhn]
C-rate out	C_{out_max}	1	[kWout/kWhn]
CAPEX	inv_2	206	[€/kWhn]
Opex	op_1	8	[$/kWhn]
Lifetime	L	16	years

Table 2.2: Key values characterizing the BESS model

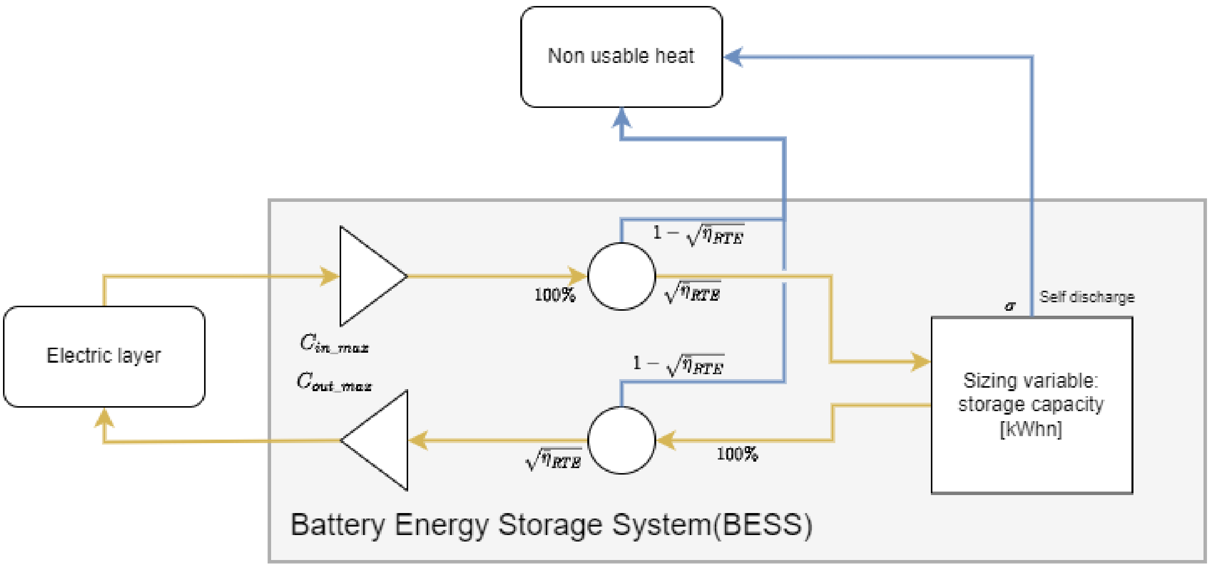

Figure 2.6: Representation of the modelled BESS system

PTES

PTES is an electricity to electricity storage system, where electricity is stored under heat form. Depending on the thermodynamic cycle it is based on, the working gas experiences a phase change to liquid (Rankine cycle) or remains gaseous (Brayton). The presented technology is based on a Rankine cycle. As concerns its components, electricity is first converted to heat using a HP, and stored into a hot or a cold reservoir. Next step is the discharge phase, where the working fluid - often CO2 - is evaporated and heated up thanks to the hot storage, before passing through the turbine where it produces electricity. Then the cold storage is used to condense back the leaving CO2 before entering the cycle again through a pump. This technology, still at pilot scale, is characterized by a low capacity

cost (compared to BESS), does not imply geographical constraints, and displays high RTE efficiency compared to other medium-term storage technologies as P2G.
Compared to BESS, in PTES systems the conversion technologies are not intrinsically linked to the overall capacity. As a consequence, there is a distinction between the values related to the conversion and the values related to the storage (all these key values summarized in table 2.3). This technology model thus features 2 sizing variables, as displayed in figure 2.7. An extra degree of freedom dissociates the input power from the output one, a decoupling that is owed to the separated compressor/-expander and pump/turbine equipment.

Key criteria	**Symbol**	**Value**	**Unit**
RTE	η_{RTE}	67	%
Self discharge	σ	1	%/day
Capex conversion	inv_2	574	€/kW
Capex storage	inv_2	17	€/kWh
Opex	op_1	11	€/kW
Opex storage	op_1	0.0026	€/kWh
lifetime	L	25	years

Table 2.3: Key values characterizing the PTES model

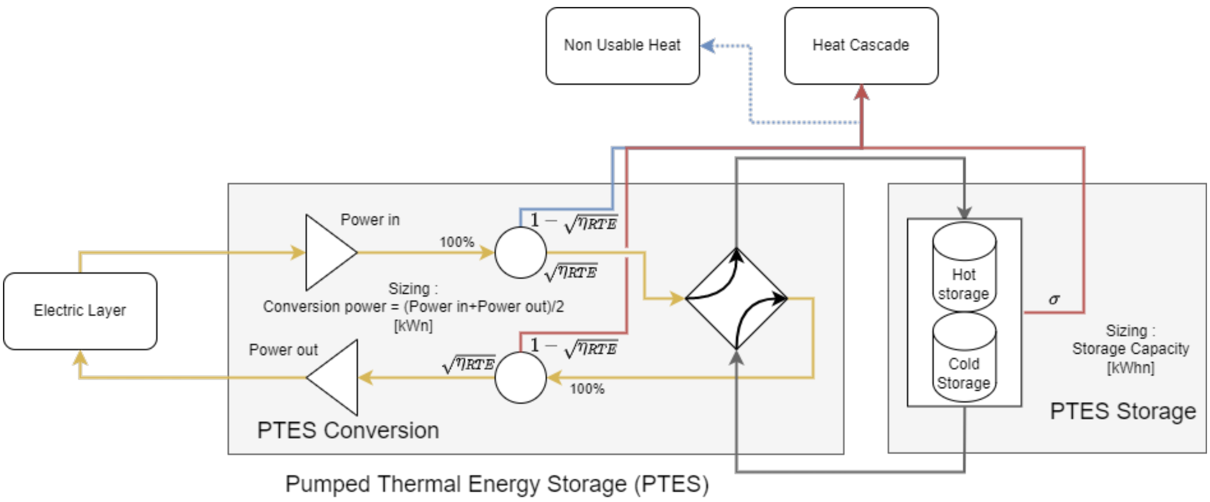

Figure 2.7: Representation of the modelled PTES system

P2G

Electrolyzers and fuel-cells

ETZ use electric potential to break the molecular bonds of water through an operation called "water splitting", i.e from H2O it produces O_2 and H_2 (although not written in stoichiometric proportions here). It must be highlighted that this reaction is a reversible one and devices performing water splitting are called electrolyzers, whereas the ones operating the other direction are referred to as fuel cells. SOEFC is an emerging technology, still at laboratory stage, which offers a single system that can operate both ways. This makes it very promising for the future implementation of Power to Gas to Power (P2G2P) [46]. Moreover, this technology also stands out by its high temperature operating range (650-1000°C) [47, 48]. The combination of those different elements motivated a specific modelling of this technology, regardless of the other electrolyzers and fuel cells.

As concerns standard catalytic electrolyzers, Alkalyne Electrolyzers (AEL) and Polymer Membrane Electrolyzers (PEM) represent the mains technologies. Although AEL have been already commercialised for many years, PEM which display a higher efficiency and a better dynamic than AEL, are expected to take some market shares in the following years [49, 50]. Both operate in the 20-100°c range and their main characteristics are similar, which led papers as [51] to consider both altogether when examining expected future characteristics. Those were thus modelled as a single technology.

The same reasoning was applied on FC. Overall, there are 3 technologies modelled: standards ETZ (figure 2.8), FC (figure 2.9), and SOEFC (figure 2.10).

Parameter	**Symbol**	**Values**	**Unit**
Power-to-H2 efficiency	η	76.00	%
Recoverable heat	η_H	14.00	%
Efficiency loss	η_l	0.12	%/1000h
CAPEX	inv_2	385€/kW for 1MV down to 269.5€/kW for 10MW	€/kWe
OPEX - Fixed costs	op_1	3.3	% of capex/year
Lifetime	L	10	year
Operating temperature	T	70	[°c]

Table 2.4: Key values characterizing the ETZ model

Parameter	**Symbol**	**Value**	**Unit**
Fuel-to-power efficiency	η_{out}	65.00	%/LHV basis
Fuel-to-heat efficiency	η_{in}	35.00	%/LHV basis
Efficiency loss	η_l	1.75	%/year
CAPEX	inv_2	1500	€/kW
OPEX - Fixed costs	op_1	3	% of capex per year
Lifetime	L	20	year
Operating temperature	T	70	[°c]

Table 2.5: Key values characterizing the FC model

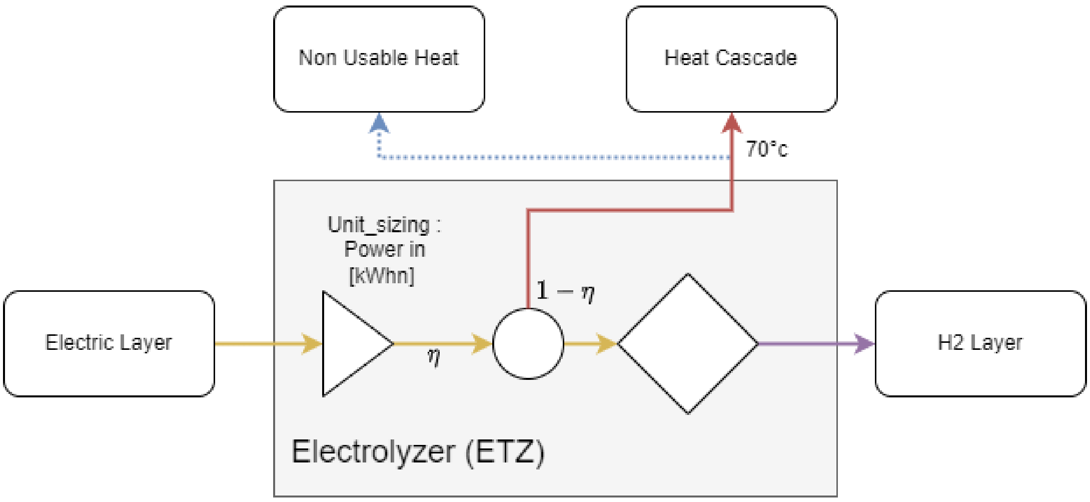

Figure 2.8: Representation of the modelled ETZ system

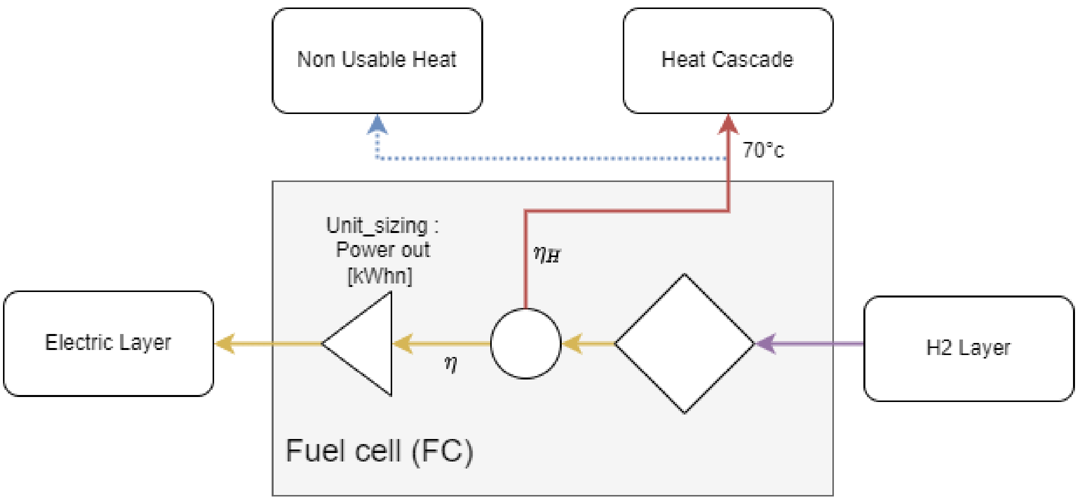

Figure 2.9: Representation of the modelled FC system

Parameter	Symbol	Value	Unit
Power-to-H2 efficiency	η_{in}	77.00	%
H2-to-Power efficiency	η_{out}	77.00	%
Power out limitation	$Pmax_{out}$	0.60	kWelout/kWn
Efficiency loss	η_l	0.50	%/1000h
CAPEX	inv_2	1500	€/kW
OPEX - Fixed costs	op_1	3	% of capex/year
Lifetime	L	10	year
Operating temperature	T	725	[°c]

Table 2.6: Key values characterizing the SOEFC model

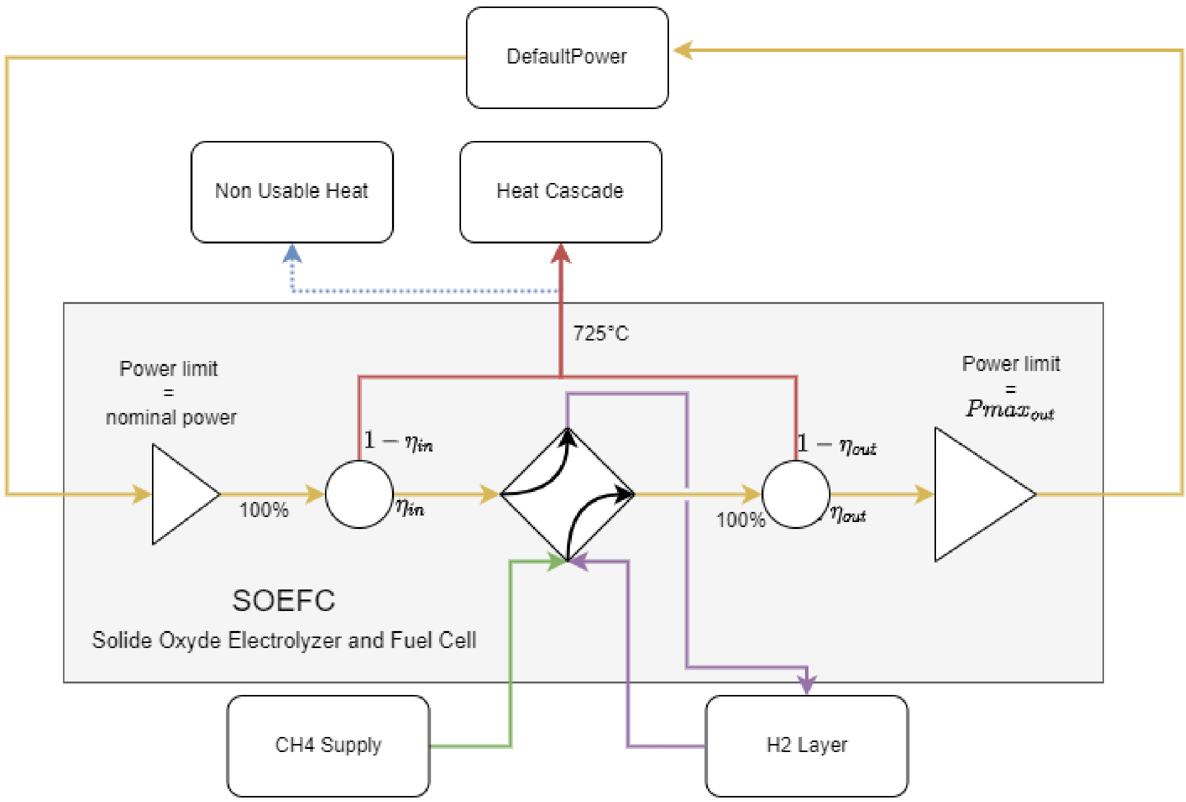

Figure 2.10: Representation of the modelled SOEFC system

Methanizer

Catalytic methanation is a highly exothermic process operated between 200-550°C which converts Hydrogen (H2) and CO2 into CH4 and O2 [52]. As stated in [51], MTZ suffer from a low dynamic and necessitate long periods of operation. As a result, MTZ are often combined with H2 buffers sized to store hours to days of their nominal H2 consumption.

A modelling method, proposed by [51], includes 3 different operating states, namely production, hot standby, and cold standby. This allows to precisely model the heat and electrical losses linked to each state. However, integrating such states in a MILP model would introduce 3 integer values for each period of the day and substantially increase the overall computing time.

Methanation needs a CO2 source which can be very energy intensive in case of direct air capture. However, considering the implementation of a CO2 tax high enough to motivate companies to capture CO2 instead of releasing it, it has been assumed that CO2 would be available for free for the operation of the methanizer, as those companies would otherwise have to cover the cost of storing this CO2.

Parameter	**Symbol**	**Value**	**Unit**
Conversion efficiency	η	78	%
CAPEX	inv_2	368.5	€/kW
OPEX - Fixed costs	op_1	3	% of capex/year
Lifetime	L	20	year
Operating temperature	T	400	[°C]
H2/CO2 ratio	-	0.198	kgCo2/kWhH2

Table 2.7: Key values characterizing the MTZ model

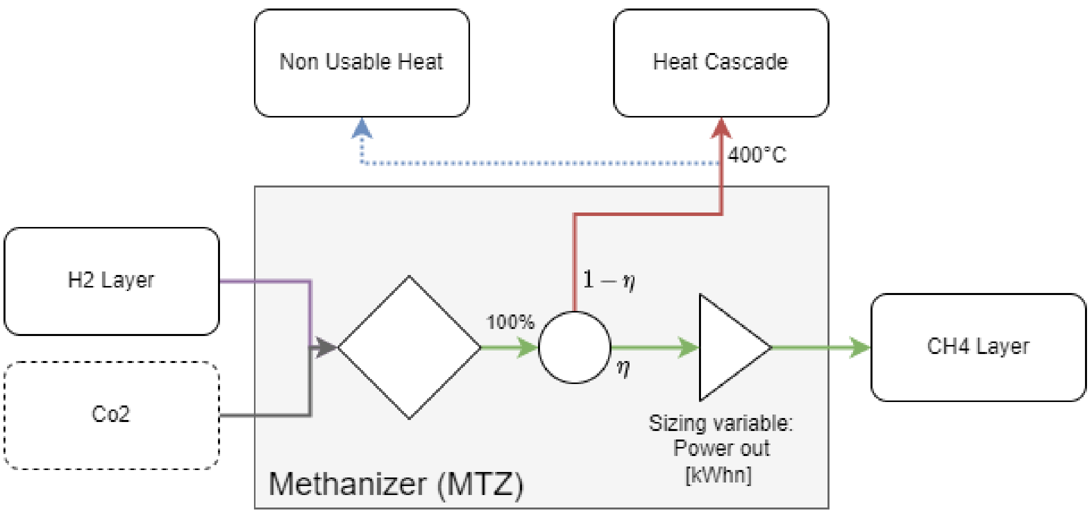

Figure 2.11: Representation of the modelled MTZ system

H2 and CH4 storage

Due to the decided territorial constraints stated in section 2.2.1, gas storage needs to be done in tanks. Despite the high energy content of H2 (120 MJ/kg) on a mass basis compared to CH4 (55 MJ/kg), H2 suffers from a low energy density at low pressure with an energy content of 12 MJ/Nm3 compared to the 38 MJ/Nm3 of methane. As a result, H2 is usually stored within high pressure tanks (350-700 bar) [53].

As regards H2 storage modelling, an electrical input is needed to compress the hydrogen to the 350 bar pressure level. This electric input can be then partly recovered through the expansion process. The electrical needs together with efficiencies and other key parameters are presented in table 2.8. Similarly to the PTES model, H2S has 2 sizing variables. One sets the maximal power of the compressor/expander, while the second variable fixes the overall capacity of the high pressure tank.

As indicated previously, the methanation process requires an Hydrogen Buffer (H2B) tank. Whereas H2 compression to high pressure level is needed to preserve space in case of large storage tanks and long time storage, H2 buffering only stores 1 day of methanizer H2 nominal consumption. A low pressure storage was thus considered to save energy losses due to compression efficiency. The literature research to characterize such a tank has been unsuccessful. As a result, characteristics of the H2S were used for the H2B, apart from the compression needs set to zero. Hence, figure 2.12 describing the H2S model is also valid for the H2B, apart from the electrical and heat related flows.

As concerns CH4S, the vessel's requirements are lower than for H2 due to the higher molar mass of this gas. Similarly to the H2B, CH4S can be considered to be storable at low pressure due to its higher energy content per volume unit, so that no compression step is needed.

Parameter	**Symbol**	**Value**	**Unit**
Compression electrical needs (350 bar)	$E_{el_{comp}}$	0.12	kwh_{el}/kwh_{H2}
Compression efficiency	η_c	85	%
Expansion efficiency	η_e	93	%
CAPEX	inv_2	13.5	€/kWh LHV
OPEX - Fixed costs	op_1	1.5	% of capex/year
Lifetime	L	60	year
Operating temperature	T	70	[°C]

Table 2.8: Key values characterizing the H2S model

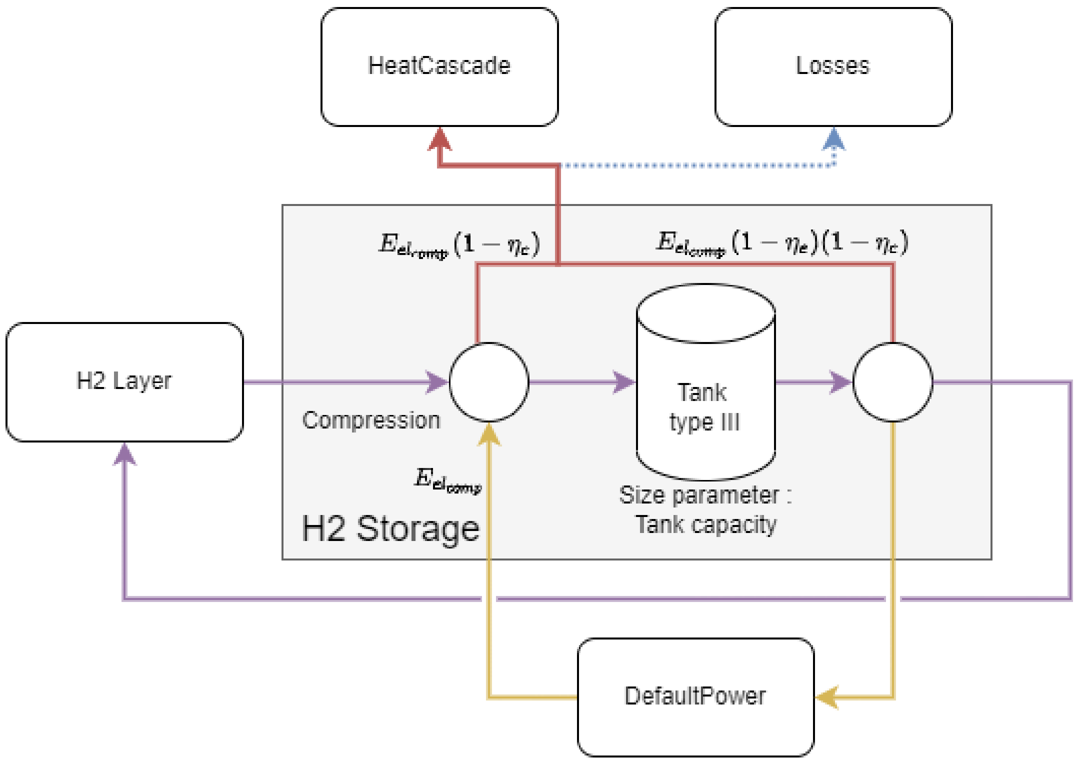

Figure 2.12: Representation of the modelled H2S system

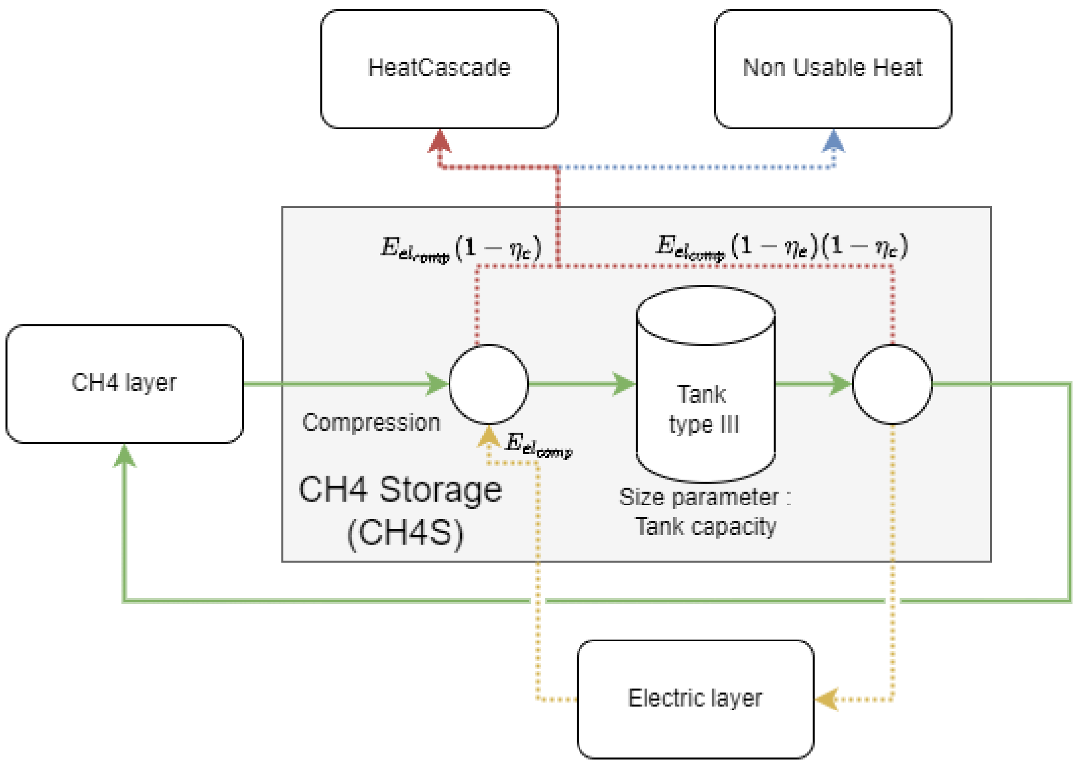

Figure 2.13: Representation of the modelled CH4S system

Parameter	Symbol	Value	Unit
Compression electrical needs	$E_{el_{comp}}$	0.00	%
CAPEX	inv_2	4.6	€/kWh
OPEX - Fixed costs	op_1	1	% of capex/year
Lifetime	L	60	year

Table 2.9: Key values characterizing the CH4S model

Thermal Energy Storage

Three different categories compose Thermal Energy Storage (TES), namely SHS, LHS and Thermochemical Heat Storage (TCHS). Due to its very low development stage, TCHS is left apart and not modelled in this study although it could present interesting properties for seasonal storage. This thanks to its high energy density and negligible self discharge [54].

SHS stores thermal energy into temperature difference in the storing medium. Compared to other TES types it offers a low investment cost, as water is the most used medium - for household application - and as it has been already used as housing hot water tanks for several decades [55, 56].

LHS is a novel technology still at pilot scale which stores energy into phase change. Compared to SHS technologies, it has a higher energy density together with very small temperature variation (i.e phase change occurs at constant temperature) [57]. This constant operating temperature prevents exergy losses (i.e stratification losses), characteristic of SHS systems [58]. Inside SHS tanks, exergy degradation mechanisms can effectively occur through conduction and especially convection taking place in the liquid storage. Thanks to the heat cascade present in SBD, such exergy considerations can be modelled supporting the creation of two different models for SHS and LHS as displayed in figures 2.14 and 2.15.

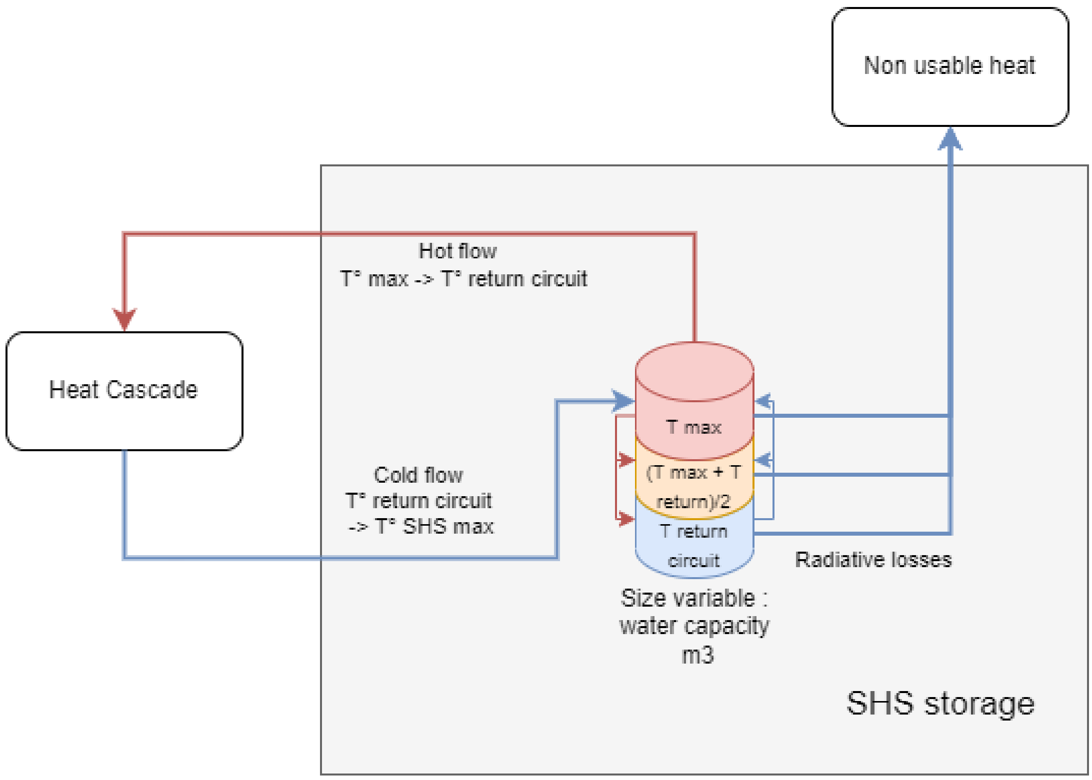

Figure 2.14: Representation of the modelled SHS system

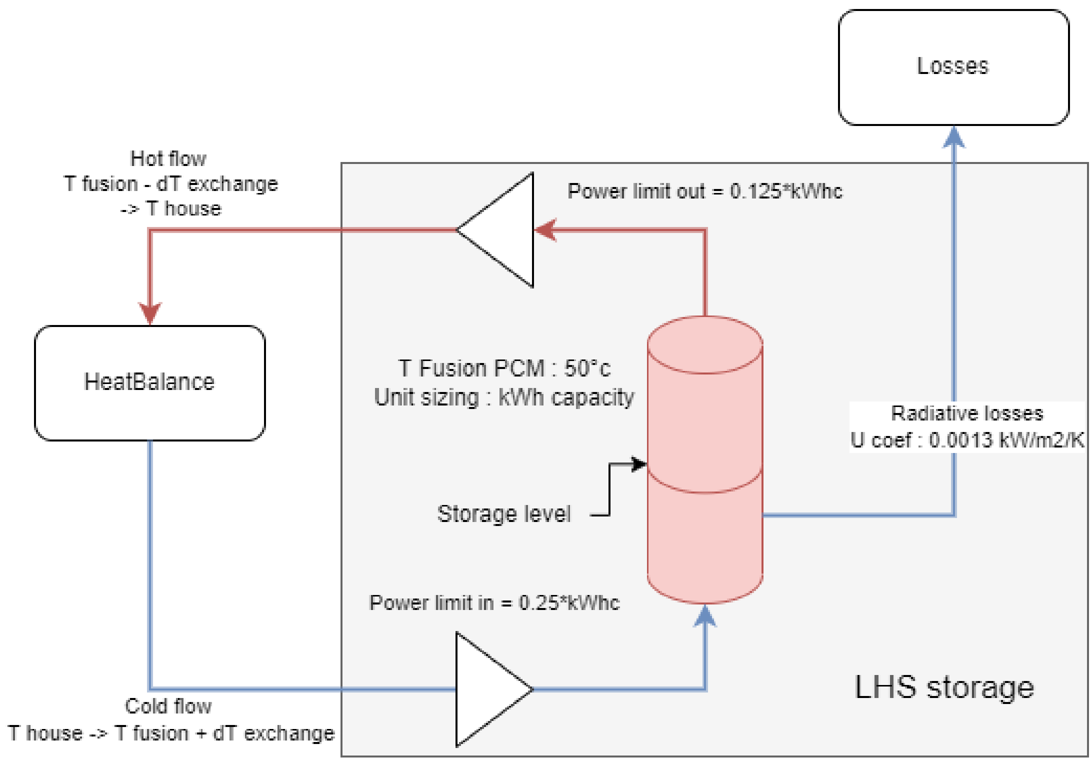

Figure 2.15: Representation of the modelled LHS system

Chapter 3

Results

In the chapter that follows, results from the different explored scenarios are presented. The adopted structure for their presentation is the following: first, the energy consumption of the district is characterized together with the external conditions applied to it. In a second section, the synergies between PV generation and storage are explored. In a third one, the exchanges between the overall energy hub and the electricity grid are investigated. Last but not least, the behaviour of each technology is assessed.

3.1 Optimization framework

This short section is a reminder of the framework derived in section 2. First, the optimization procedure is carried out as a TOTEX optimization based on the adapted SBD model. Modifications to the basic SBD structure and set of parameters have been discussed in section 2. More particularly :

- The district set of buildings and their demand profiles were detailed in 2.1.
- The modifications to the overall model structure and objective are the one discussed in 2.2.
- The added storage technologies are globally described in 2.3 and further detailed in appendix B.
- The only allowed units initially in SBD are the DHW, AWHP and Electric Heater (EH) whose costs were updated to corresponds to the expected future district.

3.2 District characterization

Figure 3.2 displays on the left side the annual energy consumption breakdown over the 3 modelled end-use demands: space heating (SH), domestic hot water (DHW) and domestic electricity (EL). The right side presents the same breakdown over the 10 typical days. It must be noted that the energy value per typical day only corresponds to the one consumed in one day. Hence, values have not been weighted by their annual frequency. The figure on the left side is thus not a simple average of these

10 typical days. As regards the orange dots, those represents the maximal PV electric generation considering surface limitations and the 35% nominal efficiency of PV panels. This maximal production was scaled down from the roof surface to the habitable one to be consistent with the final demand displayed on the figure. Of course, it does not integrate the conversion step from electricity to this final demand. As a result, even TD where the orange dot is below the sum of service as TD 4 has the potential to be self-sufficient if the heat need is covered by highly efficient systems like HP.

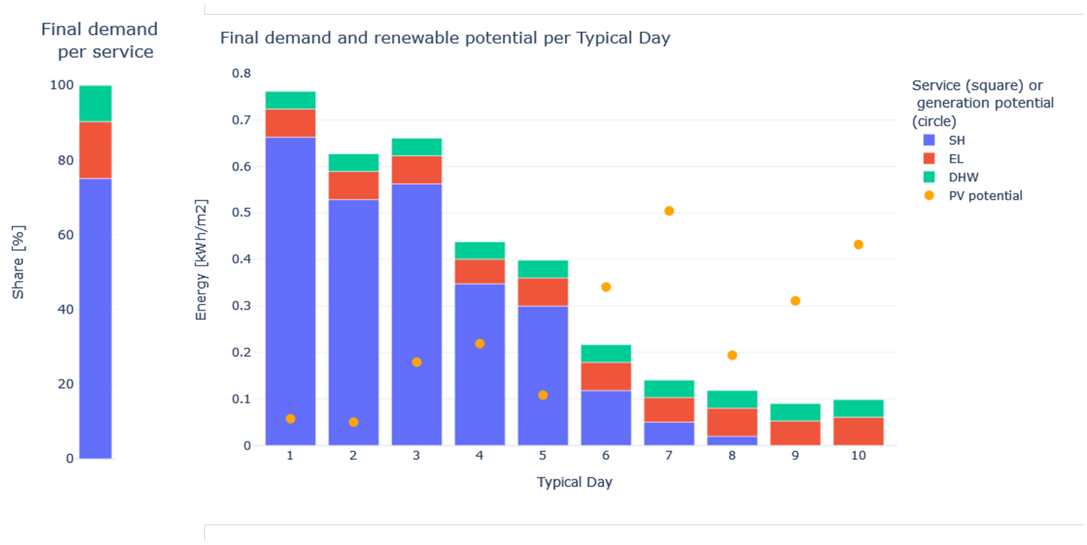

Figure 3.1: End-use demand of the district at yearly and typical day resolution

Figure 3.2 presents the external conditions the energy hub is exposed to (i.e. the global irradiance and the temperature) for each typical day. The irradiation is expressed per square meter exposed to sunlight and should thus not be confused with the habitable - or heated - surface of figure 3.2.

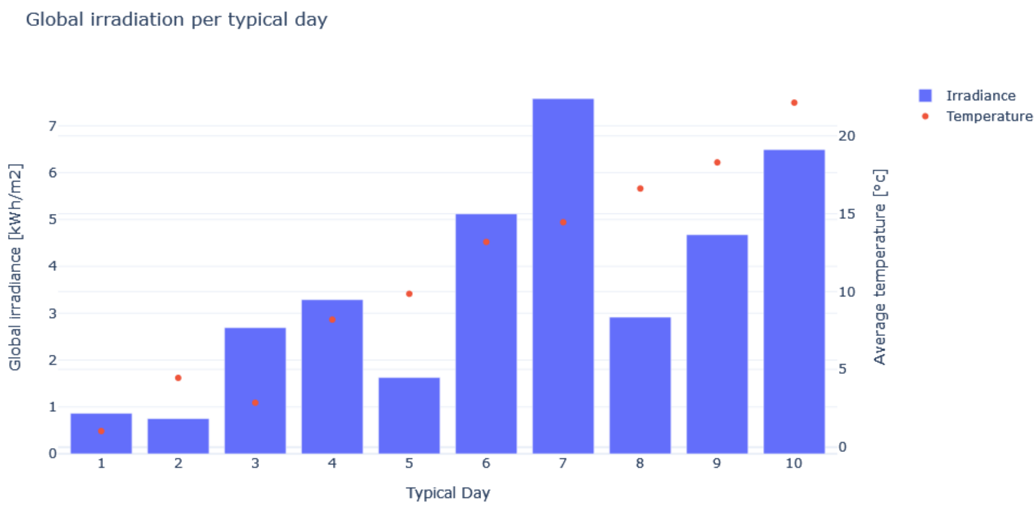

Figure 3.2: Global irradiance potential per typical day.

Figure 3.3 display the annual series of TD together with it associated potential energy balance. This *potential* energy balance results from the difference between the maximal PV generation of each TD considering maximal penetration constraints and the overall demand of each day. To reflect the higher energy efficiency one such system could achieve using HP to fulfil the heat demand, a Coefficient of Performance (COP) of 3 was applied to divide the heat demand. This is consistent with the overall mean COP noticed during the modelling of the system.

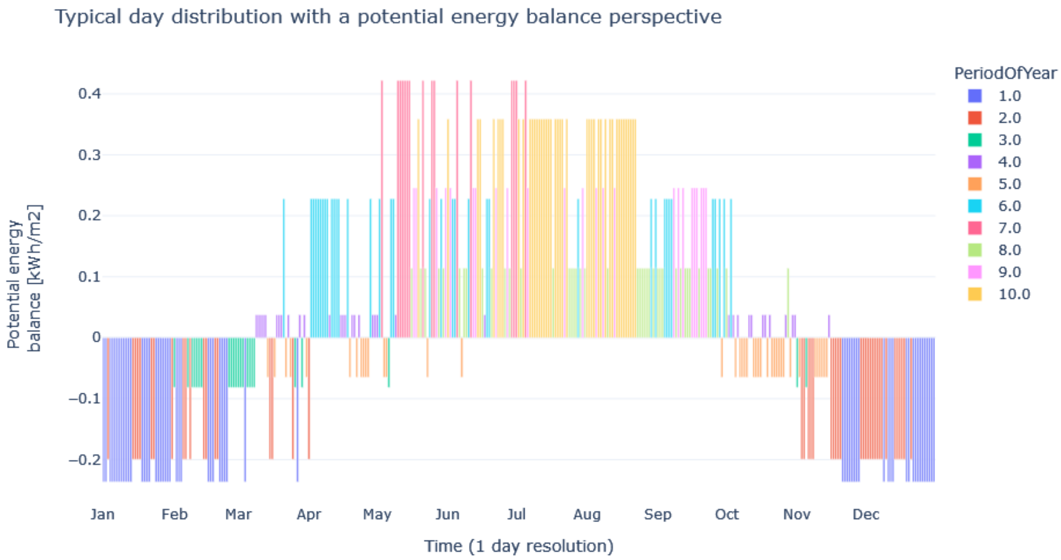

Figure 3.3: Typical day yearly distribution considering the potential energy balance

3.3 Synergy between generation and storage

Figure 3.4 shows the penetration of PV in function of the electricity cost for several scenarios restricting the number of storage technologies available. PV penetration is with respect to the maximal surface available, this latter corresponding to 70% of the roof surface. The explored scenarios are those whose technology break-even point was before the full penetration of PV in the no-storage case (i.e. 18 cts/kWh).

Figure 3.5 displays the size of conversion and storage technologies selected by the model depending on the electricity cost.

Figure 3.6 presents the values of the SC and SS indicators, depending on the electricity cost for two different scenarios. The two scenarios correspond to the case without any storage technology or with all technologies available.

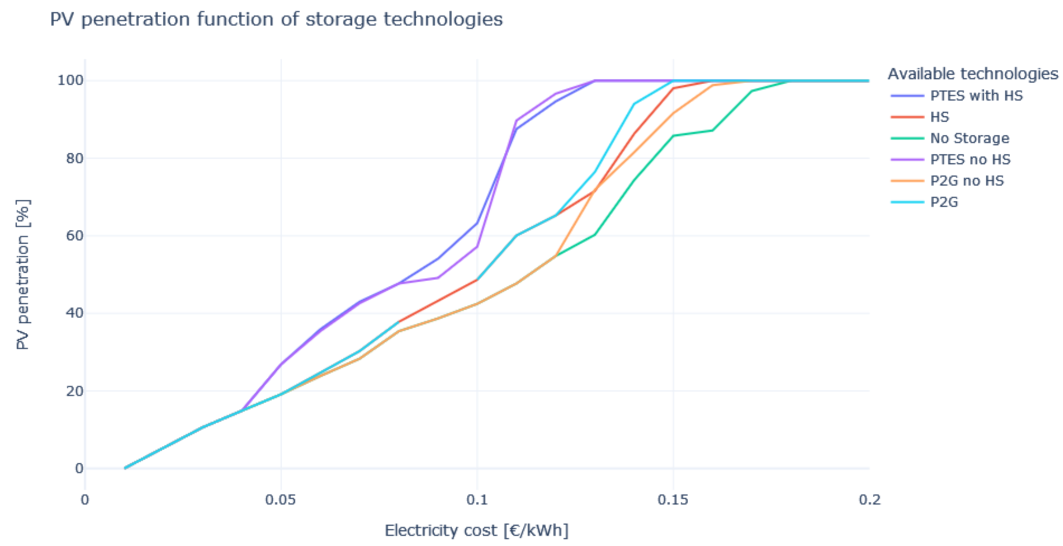

Figure 3.4: PV penetration for several scenarios in function of the electricity cost

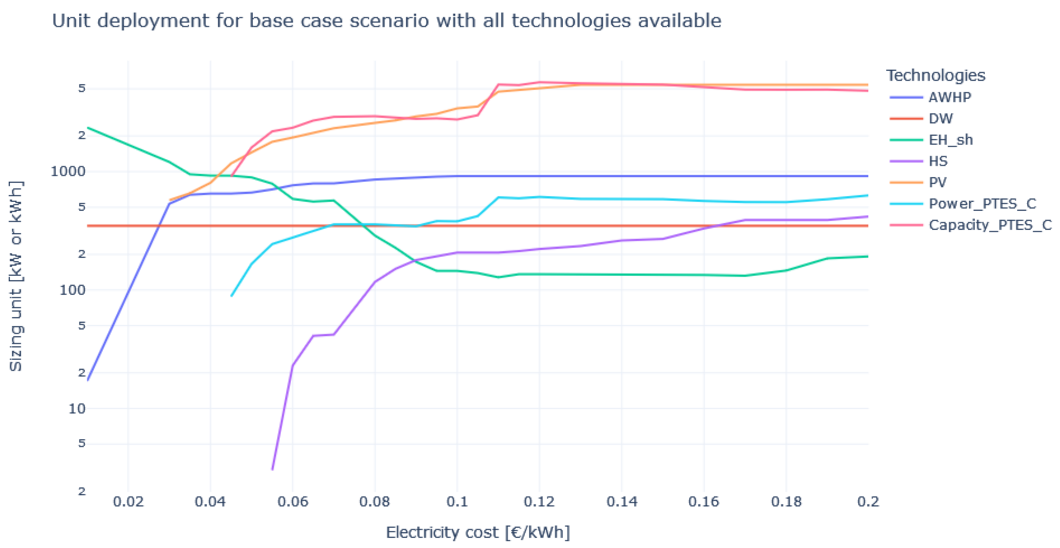

Figure 3.5: Deployment size of technologies selected by the model when all technologies are available

Figure 3.6: Main KPIs of the optimal solution when all technologies are available

3.4 Interactions depending on storage penetration

Figure 3.7 presents the energy hub electric imports and exports function of the electricity cost for two different scenario with and without storage. One can note that energy exchanges are scaled down per unit of surface area. This surface area is the overall heated surface. In addition, gaps can be noticed between 7 and 8 cts/kWh due to a modelling failure for the value 7.5 cts/kWh. Scenario with storage corresponds to scenario where all storage technologies available, even though PTES was the only technology to be selected by the model.

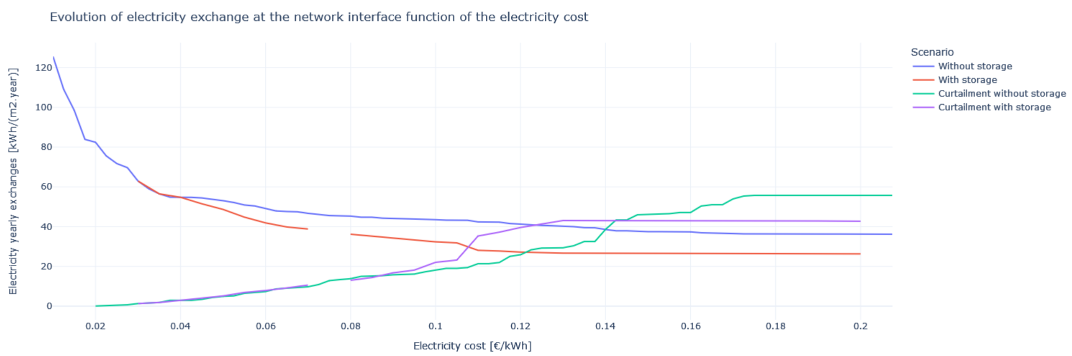

Figure 3.7: Energy exchanges at the energy hub electric interface

Figure 3.8 focuses on the import flows which are distributed over the 10 TD.

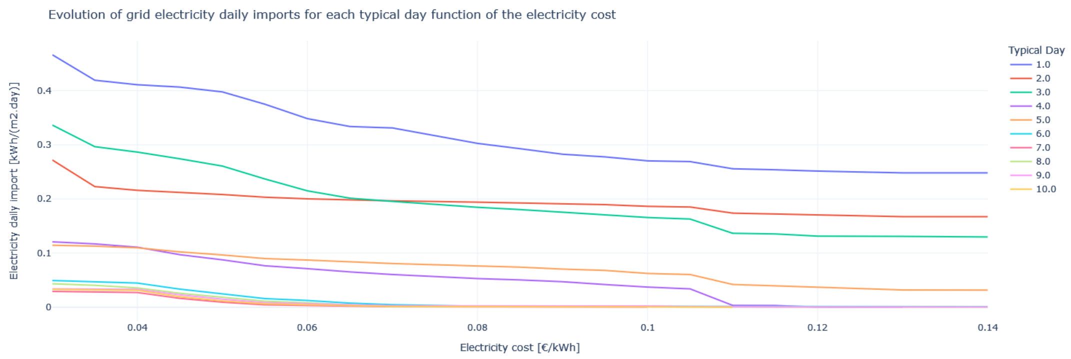

Figure 3.8: Electric imports from the energy hub broken down by TD

3.5 Technology characterization

Figure 3.9 presents the break-even costs where units start to be used for several scenarios with a 1 ct/kWh resolution (apart from the *all_tech* scenario which has a 0.25 resolution). All scenarios had the possibility to activate the Heat Storage (HS) technologies. The different scenarios and their available technologies are summarized in table 3.1.

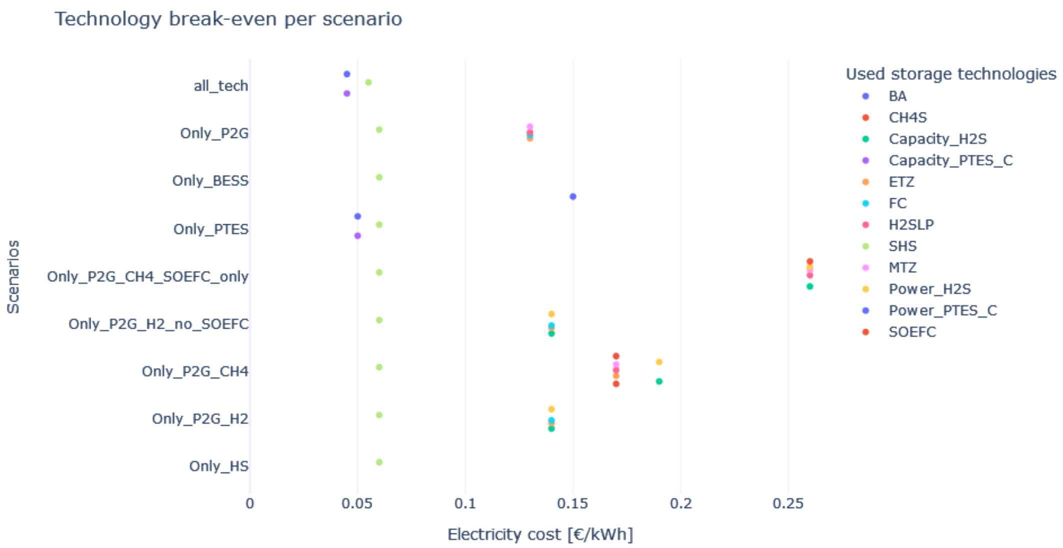

Figure 3.9: Break-even point for each unit, for different technology availability scenarios.

Scenario name	Available technologies
all_tech	SOEFC/FC/ETZ/MTZ/H2SLP/ H2S/PTES/BESS/SHS/LHS
Only_P2G	SOEFC/FC/ETZ/MTZ/H2SLP/ H2S/SHS/LHS
Only_BESS	BESS/SHS/LHS
Only_PTES	PTES/SHS/LHS
Only_P2G_CH4_SOEFC_only	SOEFC/MTZ/H2SLP/H2S/ /SHS/LHS
Only_P2G_H2_no_SOEFC	FC/ETZ/H2S/SHS/LHS
Only_P2G_CH4	SOEFC/ETZ/MTZ/H2SLP/H2S/ /SHS/LHS
Only_P2G_H2	SOEFC/FC/ETZ/H2S/SHS/LHS
Only HS	SHS/LHS

Table 3.1: Technologies available for each scenario

Figure 3.10 presents the average number of cycles per day made per technology for several scenarios. The number of cycles is computed on the power effectively entering the storage unit (i.e after inefficiencies) divided by the overall capacity installed. It must be highlighted that the capacity installed does not always correspond to the useful capacity. For instance, the State Of Charge (SOC) of BESS is limited to 80%. The beginning of the curve usually corresponds to the break-even cost of the technology (in the selected scenario).

Figure 3.11 presents the average number of cycles per year made per technology for two scenarios. The selected scenarios are the only two which made use of the inter-day storage. The energy taken into account is the one leading to an increase in the energy reservoir from one day to the following one. Gaps in the middle of the curve do not correspond to missing data but to energy cost where inter-day storage is not used anymore by the model.

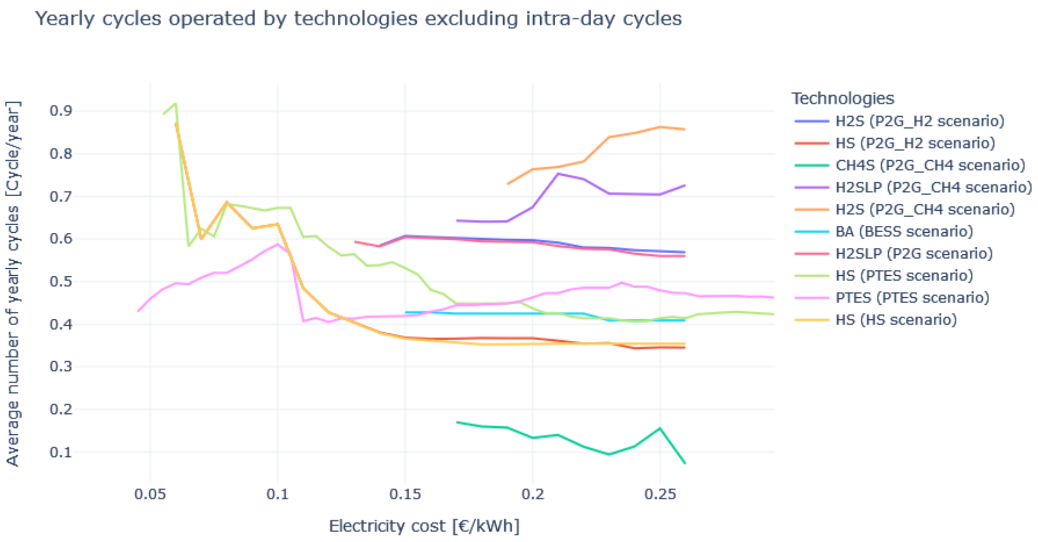

Figure 3.10: Evolution of the average cycle number a technology operates per day, depending on the electricity cost. Vertical axis is incorrectly labeled and should be "Average number of Daily Cycles [Cycles/Day]"

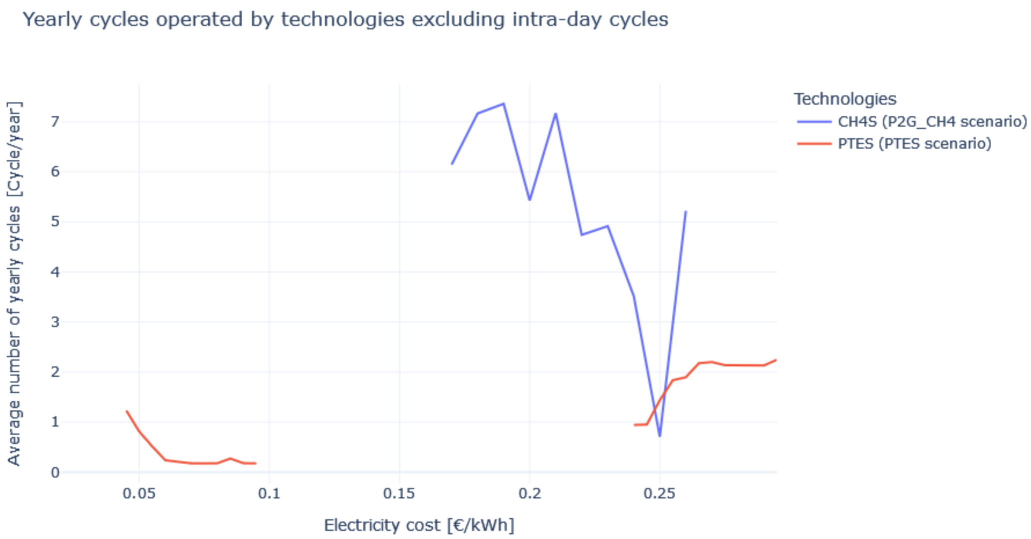

Figure 3.11: Evolution of the average cycle number a technology operates per year, depending on the electricity cost.

Chapter 4

Discussion

In the chapter that follows, the relations between the different groups showed in figure 4.1 are assessed. This will help answering most of the research questions that remain, summarized hereafter:

- How is the evolution of the electricity price impacting the renewable generation ?
- What are the interactions between renewable generation and storage deployment ?
- What are the synergies between storage technologies ?
- What is the robustness of the model regarding technology uncertainty ?

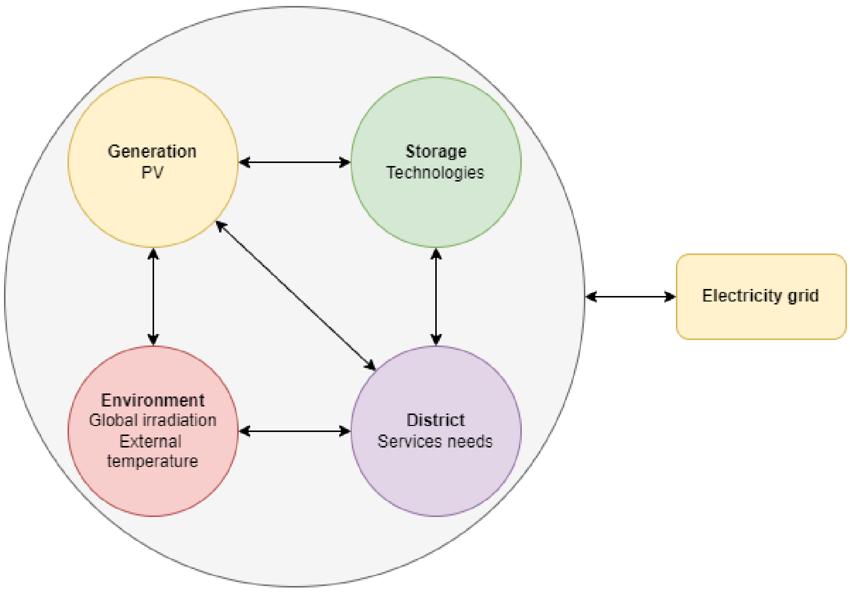

Figure 4.1: Diagram of the perspective taken over the district structure to analyze the results from the optimisation model

4.1 Generation and storage symbiosis

4.1.1 Storage and generation external influences

As displayed in figure 4.1, the generation and storage technologies groups are linked to the external environment (e.g. solar irradiance impacting PV production) and the district (e.g. loads to cover each service). First, figure 3.2 shows that the average external temperature increases with TD number and that irradiance seems to follow this tendency. However, for similar temperatures, high irradiance differences can be seen which likely corresponds to cloud coverage.
Figure 3.2 which displays the energy requirement to cover each service for each TD distinctively follows (with a negative correlation) the average temperature profile seen in figure 3.2. As regards DHW and electricity needs, those are nearly constant over the different TD.
It must be highlighted that global irradiance not only influences the PV production but also the solar gains received by the building. This is well illustrated by the difference in SH needs between TD 2 and 3 as well as between 6 and 7. In the first case, the TD with the lowest temperature has the highest irradiance and results in smaller SH needs than those of the second opposite configuration.

The yearly distribution of the 10 TD displayed in figure 3.3 also gives a time perspective on the energy unbalance over each TD. Although further described in section 3.2, it must be kept in mind that the energy balance presented in this figure is a potential one considering a full PV penetration as well as an electricity to heat efficiency (first law) of 3. However, it shows that 6 out of the 10 TD with a positive balance have the potential to be self-sufficient in a daily perspective. In contrast, this annual representation also highlights the net unbalance from November to April.

This discussion section is thus more a preamble to the overall modelling results as it underlines that storage and generation technologies can not be regarded as separated from the rest of the district as depicted in figure 4.1. It also highlights the potential for self sufficiency for 6 out of the 10 TD and the next results must be regarded in that frame.

4.1.2 Storage as PV penetration incentive

While PV excess production is a prerequisite for the interests of storage (without considering network limitations), the question of the benefits of storage to PV penetration remains. Figure 3.4 shows that storage does not impact the minimal electricity cost to deploy PV generation. However, it does show that integration of storage technologies allows to foster PV penetration whatever the technology type - although PTES is the one with the greatest impact. Moreover, the break-even costs for each storage technology can be seen through their separation with the main curve. As a result, break-even for PTES, P2G and HS seem to be respectively 4, 12 and 6 cts/kWh with a 1 ct/kWh precision. This is further confirmed by figure 3.9. Interestingly, while combination of P2G and HS seems to be only beneficial for PV penetration, this is not always true for PTES and HS. Indeed, from 11 cts/kWh and until full PV penetration, combination of PTES and HS technologies is below PTES alone.

It must be highlighted that the scenario with the combination of PTES and HS also corresponds to the scenario created by the model when all technologies are made available for its use. This scenario is thus further referred to as the Base Case (BC) scenario.

Figures 3.5 and 3.6 allow to further explore the reasons to a slower PV penetration with the combination of both PTES and HS technologies. First, 3.5 which displays the unit deployment function of the electricity cost exhibits a leap in PTES deployment between 10.5 and 11 cts/kWh. This gap is then transcribed in 3.6 where the SS indicator demonstrates a similar jump. However, this is not enough to cover the high increase in PV penetration happening at the same time and the SC indicator decrease. To conclude on the generation and storage relation, results showed interesting synergies between PV penetration and installation of storage technologies whereas the consequences of such synergy will be further explored in the next section.

4.2 Energy hub interface defuse ?

Turning now to the exchanges between the modelled energy hub and the electricity grid. The import curve in figure 3.7 highlights the impact of inefficient electrical heaters. Indeed, as no storage is deployed until the 4 cts/kWh threshold, the fast decrease of the imports is due to the shift from EH to AWHP, as displayed in figure 3.5. Then, starting from 0.04 cts/kWh, PTES storage has a negative effect on electricity imports and reduces the overall volume. One might notice the larger gap between the two curves around the 0.11 cts/kWh point, which is then reduced before reaching what seems to be asymptotic values.

As regards the exports, the impact of storage is not always beneficial. As a matter of fact, the positive effect storage has on PV penetration increases the curtailment needs. As curtailment can be seen as useless energy for the district, this would represent the energy quantity sent to the grid in the case of a 0 ct/kWh feed-in price. As long as the full PV penetration is not reached, storage could thus increase the energy amount sent back to the grid.

As highlighted in the previous section, the gap around the point 0.11 cts/kWh is still visible in the storage related curves. Figure 3.8 allows to further explore this leap in displaying two additional information. First, between 0.04 and 0.08 cts/kWh, the TD 6 to 10 see their imported energy reach zero. Then, from 0.08 cts/kWh onwards, TD 1 to 5 are the only ones needing imports. Second, the 0.11 cts/kWh leap displays different magnitude in import reduction for each TD. The two sunniest TDs 3 and 4 display a higher import absolute reduction than TDs 1, 2 and 5. The reason of these lower benefits for TDs 1, 2 and 5 might be an already complete exploitation of the daily PV potential as they present the 3 lowest irradiance profiles, in contrast to TDs 3 and 4 where this additional capacity even helped reduce TD 4 imports to zero.

To summarize, the deployment of storage capacities helps reducing the imports but has a negative impact on the energy volume to be exported as it drives the PV penetration up. The closer look at TD resolution showed that for a cost higher than 11 cts/kWh, the district is energy autonomous for 6 out of the 10 TDs which is consistent with the preliminary analysis demonstrated in figure 3.3. While a correlation between PV daily potential and import reduction was shown, the actual time behaviour of storage technologies will be addressed in the next section.

4.3 Storage technology behaviour

The objective of this section is to discuss the behaviour of each modelled technology and the observed synergies between these technologies.
Figure 3.9 starts by showing the Break-Even (BE) cost of deployed technologies in each explored scenario. Several observations can be made. First, PTES technology outperforms the other technologies whose main energy vector is electricity. Then, heat storage is deployed through theSHS technology while LHS seems to be of no interest in this model configuration.

As regards the P2G segment, several scenarios are explored. Interestingly, the "Only_P2G" scenario where all P2G related technologies are allowed deploys a MTZ unit without a CH4 tank. A more in-depth look showed this is to make use of the low pressure H2 tank storage (H2SLP) which benefits from a higher efficiency by avoiding the compression step. The Hydrogen Storage Low Pressure tank (H2SLP) thought as a buffer for the MTZ has a size constraint limit applied, this limits its size to one day of operation of the MTZ at nominal power. It is thus cheaper for the model to select a combination of H2SLP and MTZ CAPEX than to use the standard high pressure H2 tank (H2S).
The two scenario exploring SOEFC use show that SOEFC is not beneficial to the model for both H2 and CH4 production. However, as SOEFC is the only technology allowed to use CH4, the comparison between the two "P2G_CH4" scenarios shows that using a dedicated methanizer while using the SOEFC to reduce CH4 and O2 to electricity allows great improvements in the BE cost.

One might notice HS is allowed in every scenario. In contrast, all scenarios were also explored without HS technologies but no difference was noticed as regards the BE cost. As the resolution is rather low (1 ct/kWh), the two scenarios "Only_PTES" and "Only_P2G" were closer explored - with a 0.25 cts/kWh resolution - respectively in the 5 to 6 cts/kWh and in the 12 to 13 cts/kWh intervals. With and without PTES for the first case, with and without HS for the second one. This additional exploration did not show any difference in the BE cost whatever the storage status.

Turning now to the daily behaviour of each technology, figure 3.10 presents the average number of cycles operated daily per technology. As concerns HS, from 10 cts/kWh, its number of cycles decreases with the electricity cost until it reaches an asymptotic value. This decrease follows the size deployment shown in 3.5 for the PTES case. Even the part before the 10 cts/kWh seems to be correl-

ated to the unit size where the daily cycling increase occurs at a cost point translated as a deployment plateau.
Considering now the interaction with other technologies, HS behaviour seems to be positively impacted by PTES technology while the P2G impact is in the 0.02 cycle/year magnitude.
As regards the P2G scenarios, in the restricted to H2 case, a slow decreasing tendency is observed for the two used technologies. The CH4 is more complex as the number of cycles operated by the H2 tanks clearly increase while the CH4 tank which already operates only 7 to 8 times less cycles is on a downward trend. An hypothesis to this behaviour is that the size of the H2 tank acting like a buffer is nearly constant over the price increase but sees more H2 passing. On the contrary, the CH4 tank size increase to store more of the produced energy (as it is the cheapest gas reservoir). In addition, the 11 cts/kWh leap for PTES technology is again noticeable. The capacity increase which allowed to better treat PV production for the 5 first TDs is translated in a lower number of cycles.

For PTES case, additional answers are to be found in figure 3.11 where all technologies characterized by inter-day storage behaviour are displayed. First, it must be highlighted that the number of yearly cycles is fairly low compared to the annually achieved daily cycles, which might explain the chaotic behaviour of the CH4S curve. This is especially relevant compared to the overall CH4 capacity much lower than the PTES one (around one order of magnitude difference). Then, comparing the two figures 3.10 and 3.11, PTES evolution is split in three segments. The first one combines both an increase of the daily cycles and an opposite tendency on the yearly time scale. The second segment is characterized by daily storage only, which sees an upward slope with respect to costs. The last segment displays the return of inter-day storage, whose increase follows a small daily cycling decrease.

To conclude, some synergies between heat and electric technologies have been observed although not occurring with the same magnitude depending on the electric technology. The reason between those differences is still to be explored. In addition, a few technologies showed a inter-day storage behaviour and only on a small volume compared to intra-day variation which is not consistent with a clear seasonal storage. No inter-day specific technology was showed. Hence, the ability of the model to handle seasonal storage seems compromised, although further investigations are necessary to explore whether it is due to technology parameters or to model configuration. Moreover, some incongruous behaviour of the model were highlighted. For instance, the useless implementation of MTZ units to make use of low pressure hydrogen tanks, these latter being firstly designed to be used as buffer and not selected as possible long term H2 storage due to space considerations.

4.4 Limitations and recommendations

First, regarding the robustness of the results, the important part of robustness analysis through Sobol analysis has not been applied yet. The high uncertainty on technology parameters increases the overall incertitude over the different observed results, especially regarding the absolute values highlighted. Results from this project which can be seen as a first part toward a robust and comprehensive model should hence be seen as highlights of the model potential.

Second, these first results allowed to underline some issues in the model (e.g. the uselessness of MTZ deployment) which should be solved before pursuing with the next steps. Then, although not visible in the results, the operation time with all technologies activated is very long which is not the case with only a subset of the technologies are made available. The relation is not linear to the model complexity. Hence, these issues raised in the last weeks of the project need to be further explored and resolved before applying a high number of simulations as required to conduct a Sobol analysis.

Third, additional and deeper technology characterization with contribution of experts of each respective field could greatly reduce the uncertainty of the selected parameters. Moreover, some technology models do not reflect particular dynamic constraints. This is for instance the case of MTZ whose dynamic would require several operation states for a better modelling of linked losses. Use of integer variables would allow to model such states, but at a very intensive computational cost. Another formulation compatible with linear modelling would thus be of interest.

Fourth, only a subset of energy needs for residents of an area were modelled. In order to exhibit a full exploitation of synergies to answer various energy needs, a more complete list of energy needs must be modelled. A non-extensive list of those needs is: mobility, industrial energy needs through high temperature heat, ICT needs.

Fifth, there was no size restriction applied. However, CAPEX costs per unit size often depend on the scale of the deployed unit. It would thus be necessary to assess that the deployed size of each technology is congruent with its parameters. Moerover, the one-building formulation hid the actual implementation of technologies (district scale to building distribution). Some technologies would vary depending on the selected implementation. In particular, DHN was assumed to be available in the overall district and its costs covered outside this study scope. However, the size and actual implementation of such DHN should result from an optimisation decision, especially in low density areas.
Sixth, the modification of SBD with the removal of the extreme hours to preserve the energy balance leads the model to underestimate the maximal power requirement. A way to solve this issue would be to replace the previous hourly extremas by daily extremas which could be integrated into the TD annual series.
Last but not least, the restrictive gas grid disconnection hypothesis is unrealistic in the frame of a

country scale integration. Moreover, boiler technologies might be of great use to cover spike demand instead of inefficient EH. On additional step for integrating this model into a country scale model would thus be to model the potential use and restriction of the gas energy carrier.

Chapter 5

Conclusion

This project aimed to explore the interest of storage technologies for renewable sources integration and energy independence of a territory.

In a first step, the territory under investigation was delimited by the set of buildings connected to a single MV/LV transformer, and extracted using a Voronoi partitioning. Then, this so-defined district was characterized using the *Qbuilding* database. This characterization allowed to provide the *Smart Building Designer* (SBD) model with district typology and energy signature as well as external conditions.

A second step focused on the adaptation of SBD to model inter-day storage through the serialization of TD creating a yearly energy balance while conserving efficient daily based power optimization. Together with this structure modification, two additional modules were added to SBD to post-process the obtained results. The first one allows to compute a set of relevant KPIs allowing to differentiate performances of different scenarios. The second helps to quickly plots those results allowing the user to quickly grasp specificities of each scenario.

Simultaneously to the model development, a set of storage related technologies were selected and characterized through literature analysis. Then, this characterization allowed to create independent models for each storage technology in a comprehensive way. This comprehensive modelling allowed to make use of the inefficiencies under heat form to contribute to the balance of thermal related needs.

Last but not least, the model was applied on the selected district considering several scenarios to study the behaviour and interactions of the newly added storage technologies. Results obtained showed that storage technologies positively influence PV penetration while cost does not motivate maximal PV penetration. However, secondary effects regarding this improved PV penetration concern extra-production from PV which is also increased by storage and might put the network under higher pressure, compared to a scenario without storage. This is however not true anymore when full

PV penetration is reached.

Regarding storage behaviour, the model did not demonstrate long term storage. This can be either due to technology properties or model configuration and should be further explored later on. Lastly, some synergies between heat and electric storage have been demonstrated, illustrating the efficiency maximization benefit of decentralized generation and storage capacities.

Finally, the enhanced SBD model developed in this project needs an additional robustness analysis step to validate the obtained results, and still needs some extra adjustments. However, it already shows a high potential for exploration of storage benefits at district scale.

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Appendix A

Modeling details

A.1 Automatized plots

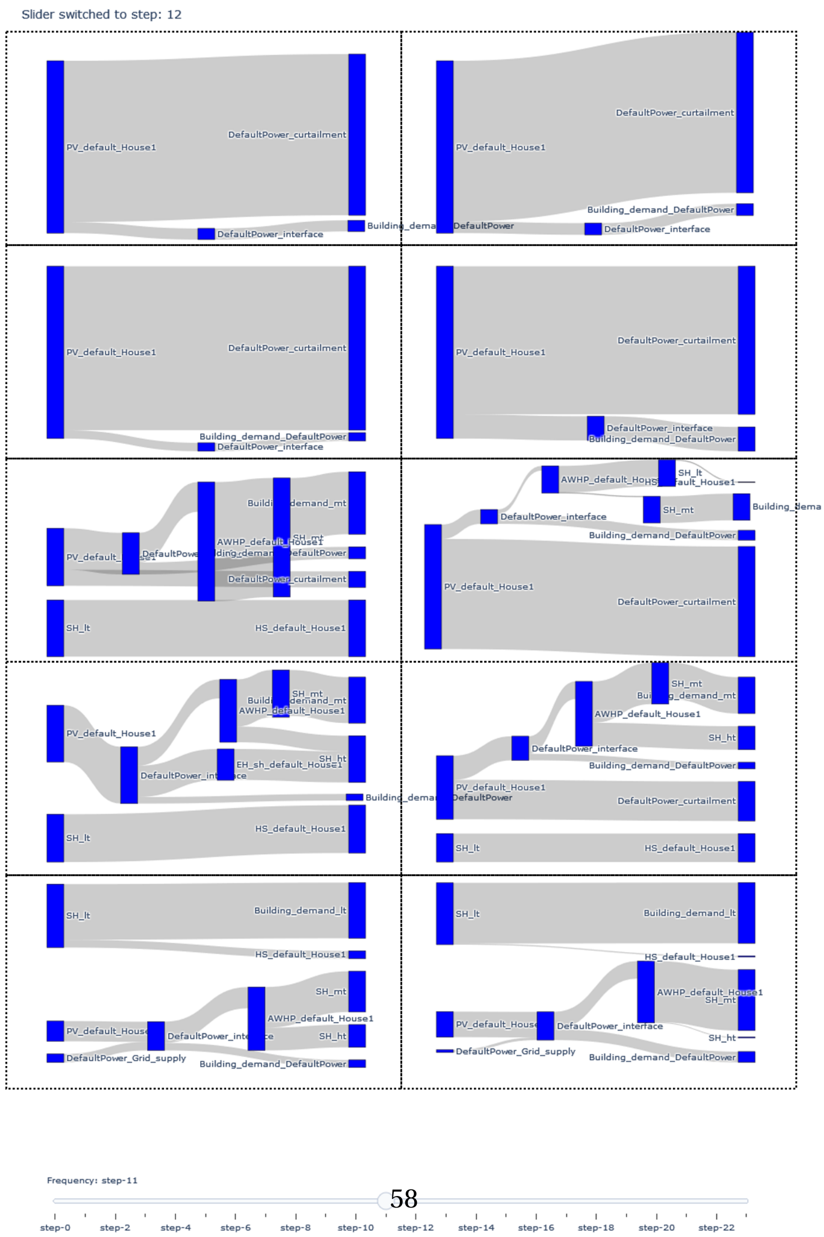

Figure A.1: Sankey plots describing the state of all TD composing the district at one hour selectable using the slider

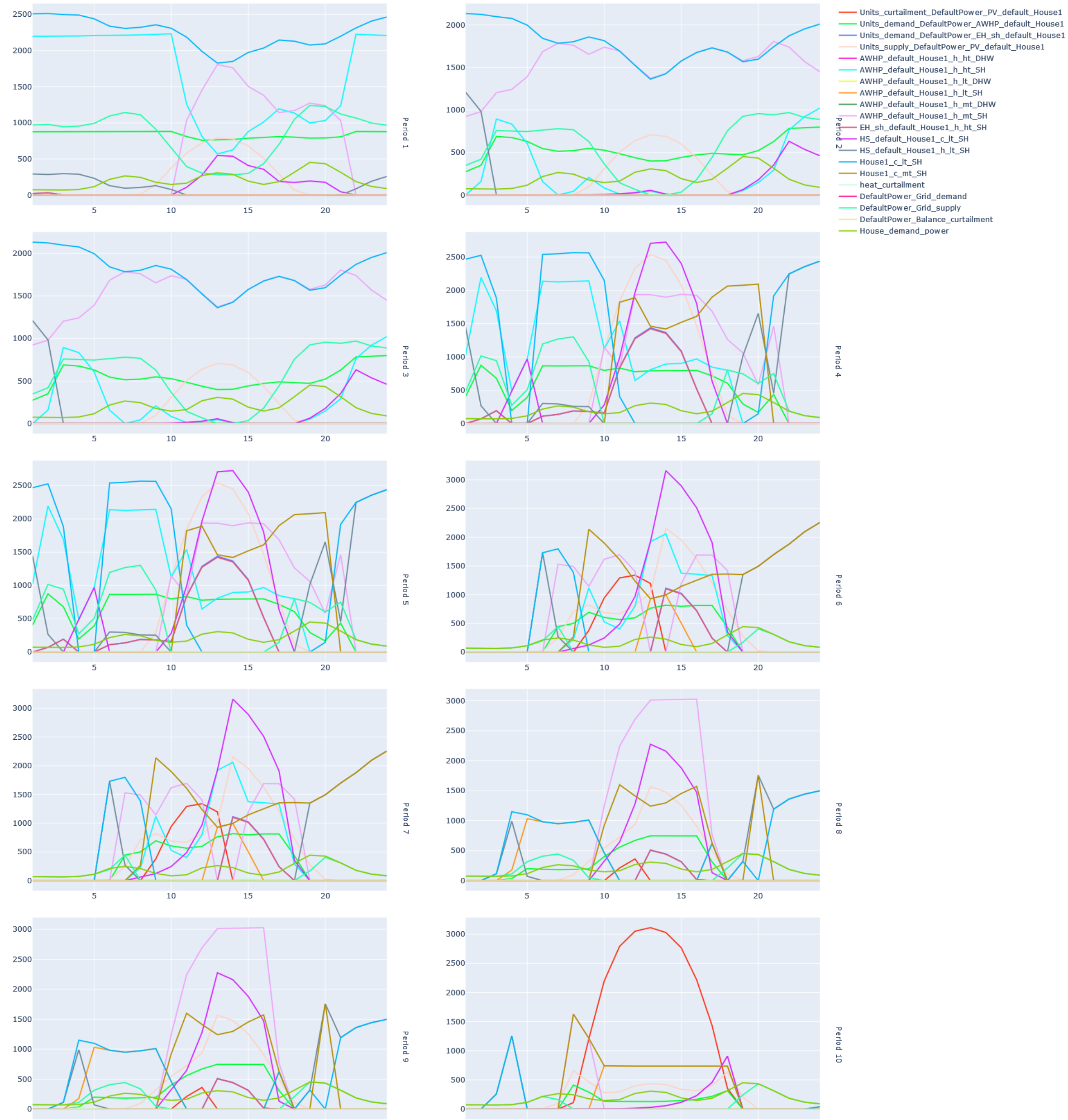

Figure A.2: Line plots describing the power flows of all TD composing the district along the day

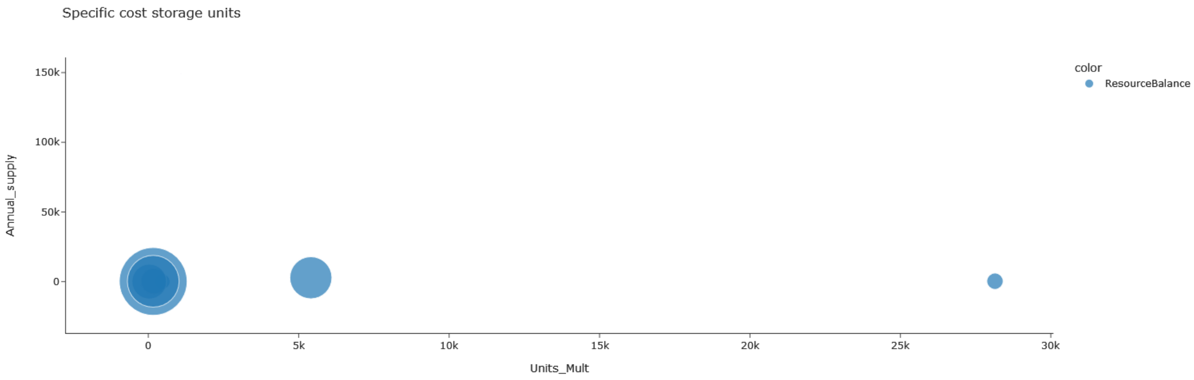

Figure A.3: Plots displaying the cost of processing the energy by the unit through circle diameter and which center is located depending on size and energy treated

A.2 KPIs

Acronym	**Name**	**Definition**
E_PV	Overall energy produced by PV	Overall energy produced by the PV over
E_PV_TDx	PV production per TD	Overall energy produced by the PV over
E_PV_TDx_y	PV production per TD over the year	Overall energy produced by the PV over
S_PV	Roof surface occupied by PV	Overall PV surface divided by the overal
E_C	Overall curtailed energy	Overall energy curtailed over a year/cap
E_C_PV_TDx	Curtailed energy per TD	Overall energy curtailed over each typic
E_C_PV_TDx_y	Curtailed energy per TD over the year	Overall energy curtailed over each typic
E_C_elec_TDx	Curtailed energy per TD	Overall energy curtailed over each typic
E_C_elec_TDx_y	Curtailed energy per TD over the year	Overall energy curtailed over each typic
LC_u	Specific cost of energy storage	Technology annualised cost divided by
Op_time_u	Time operating fraction	Annual count of non-zero hours over th
Op_time_d_u	Discharge time fraction	Annual count of discharging hours over
Op_time_c_u	Charge time fraction	Annual count of charging hours over th
Op_time_d_TDx_u	Daily discharge time fraction	Number of hours a technology have a n
Op_time_c_TDx_u	Charge time fraction	Number of hours a technology have a n
COP	Heat production efficiency	Weighted average (base on the electrici

COP_TDx	Heat production efficiency over TDs	
COP_u	Unit's heat production efficiency	
COP_TDx_u	Unit's heat production efficiency over TDs	
SC	Self consumption	(Overall PV production - PV curtaileme
SC_storage	SC linked to storage	Storage input over PV production
SC_storage_elec	SC linked to electric storage	Extra elec input from electric storage te
SC_storage_elec_TDx	SC linked to electric storage over TDs	
SC_storage_heat	SC linked to heat storage	Difference between
SC_storage_heat_TDx	SC linked to heat storage over TDs	
SC_direct	SC due to direct consumption	(Sum of district electric demand + elect
SC_direct_elec	SC due to direct electric consumption	Elec demand covered by PV divided by
SC_direct_elec_TDx	SC due to direct electric consumption over TDs	Elec demand covered by PV divided by
SC_direct_heat	SC due to direct heat consumption	
SC_direct_heat_TDx	SC due to direct heat consumption over TDs	
SS	Self sufficiency	
SS_storage	SS linked to storage	
SS_storage_elec	SS linked to electric storage	
SS_storage_elec_TDx	SS linked to electric storage over TDs	
SS_storage_heat	SS linked to heat storage	
SS_storage_heat_TDx	SS linked to heat storage over TDs	
SS_direct	SS due to direct consumption	
SS_direct_elec	SS due to direct electric consumption	
SS_direct_elec_TDx	SS due to direct electric consumption over TDs	
SS_direct_heat	SS due to direct heat consumption	
SS_direct_heat_TDx	SS due to direct heat consumption over TDs	
Mult_u	Unit Deployment	Installed capacity of a technology U
Mult_heat		Installed overall heat storage capacity
Mult_el		Installed overall electricity storage capa
		Number of cycles (energy flowing in ove

NCPY_heat	Unit Cycling	Number of cycles (energy flowing in ov
NCPY_elec		Number of cycles (energy flowing in ov

Appendix B

Storage technologies characterization

Lithium-ion storage

Jules Mathieu

January 13, 2022

Author : Jules Mathieu **Last modification date :** January 13, 2022 **Validation status :** Valid

1 Description

1.1 Nomenclature

Acronym	Meaning
BESS	Battery Energy Storage System
Li-ion	Lithium ion
DoD	Depth of Discharge
SoC	State of Charge
EV	Electric Vehicle
BMS	Battery management System
PCS	Power Conversion System
HVAC	Heating, Ventilating and Air Conditioning
DC	Direct Current
AC	Alternating Current
kWhn	Nomical Capacity in kWh

1.2 BESS short description

Battery Energy Storage Systems (BESS) are electrochemical devices composed of battery Packs - smallest component usually commercially available - regulated with BMS and coupled to the electrical grid through PCS. Each pack contains itself several modules themselves containing several cells. A cell is a typical battery composed of a cathode, anode, separator, and electrolyte. The cell integration into modules is done to achieve a specific voltage requirement. Then the number of Packs define the overall energy capacity and current - thus power - the BESS can achieve.

As of today, the main type of BESS installed are Li-Ion batteries according to (Tarvydas et al. 2018).

Figure 1.1 from (Killer, Farrokhseresht, and Paterakis 2020) represents an illustrative layout of a Li-Ion BESS which is also representative of other chemical based BESSs. Power Conversion System (PCS) ensure the link between the direct current BESS and the Alternating Current (AC) grid. The operation of the BESS is ensured by the Battery Management System (BMS) while the Heating, Ventilating and Air Conditioning (HVAC) system regulates its temperature.

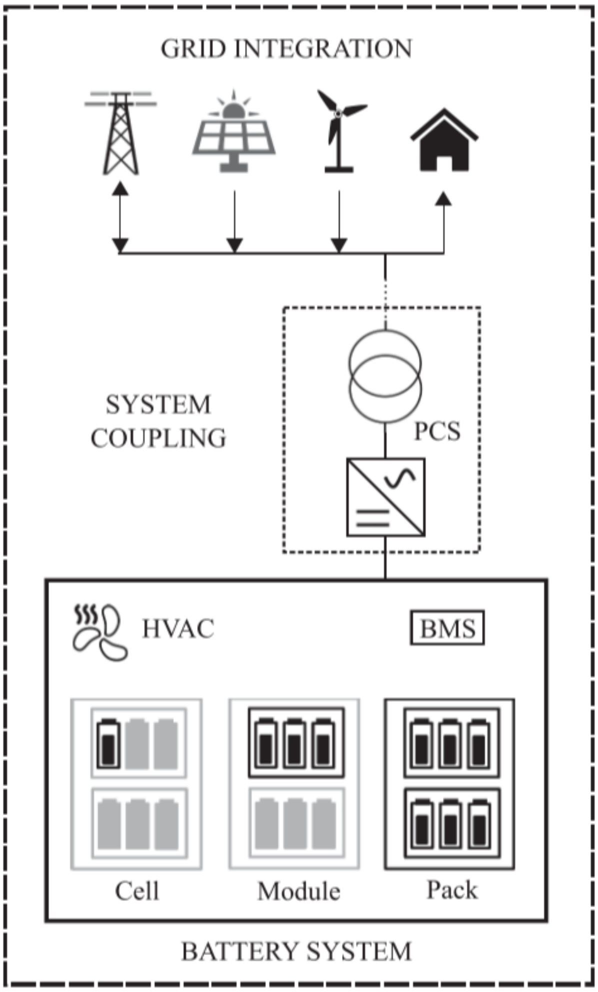

Fig. 1. Illustrative layout of a Li-ion stationary storage system interacting with loads, renewable energy sources, and/or the electric network.

Figure 1.1: Illustrative layout of a Li-ion stationary storage system from (Killer, Farrokhseresht, and Paterakis 2020)

When BESS is used as stationary storage system, it can be in a behind-the-meter or front-or-the-meter way. The former mitigates load and production peaks of the consumer who deployed it. In a grid perspective, this decreases his individual impact. On the contrary, the latter is used by the grid to regulate itself. Hence it can be used to smooth the consumption of several consumers (Killer, Farrokhseresht, and Paterakis 2020).

1.3 Li-ion Technology description

Li-ion batteries are a specific electrochemical technology part of the BESS segment. It displays several advantages over other BESS technologies as a high specific energy and power, a long lifetime as well as high round-trip efficiency (Killer, Farrokhseresht, and Paterakis 2020). The Li-ion market is driven by EV mobility and has been growing exponentially over the recent years (Tarvydas et al. 2018).

1.4 Specific key criteria

1.4.1 CAPEX and size

The CAPEX is strongly correlated to the BESS size as it can go from the 200-300€ range up to more than 1000€ for 5kWhn systems (Tarvydas et al. 2018; Vonsien and Madlener 2020).However the size/price relationship is not linear as many authors separate residential and utility-scaled BESS (Larsson and Börjesson 2018; Schopfer, Tiefenbeck, and Staake 2018; Vonsien and Madlener 2020). This stresses the need for a different approach of both scales.

1.4.2 C-rate

The C-rate is the ratio of the power to energy capacity. Thus, charging a battery with a c-rate equal to 2 means the battery will be full in half an hour. On the contrary, a 0.5 c-rate leads to a 2 hours-charging process. C-rate has an impact on BESS lifetime as the larger it is, the lower the lifetime. When it is not needed for power application, the c-rate is usually set to a maximum between 0.5 and 1C (Tarvydas et al. 2018).

1.4.3 Efficiency

Li-ion batteries are significantly affected by the temperature (Vonsien and Madlener 2020). Thus inducing the need of a regulation HVAC system, especially for district sized systems. In turn, HVAC also affects the overall efficiency (due to its specific electricity consumption). Of course, the C-rate also affects the efficiency which is hence lower for the power-designed BESS than for the energy-designed ones.

1.4.4 Lifetime and SOC

Battery lifetime depends on several parameters and is usually considered to happen when the maximal SOC reaches 80% of its original capacity. The main ageing parameters are linked to temperature, overcharge/discharge or high SOC storage (Wu et al. 2015). The two first can be avoided with sufficient HVAC management as well as max/min SOC limits. The high SOC storage it on its own directly linked to cost-efficiency as there is no well defined limit. Hence, the SOC limits must be found using specific properties of the BESS while optimizing the overall system costs. Doing so, (Vonsien and Madlener 2020) found an optimum SOC limit of 67%. However, as most of the literature cites 80% DoD lifetimes, a 80% DoD limit is considered.

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2 Characterization

2.1 Litterature overview

	Power/C-rate		**Efficiency**						**I**
Parameters	**Power in**	**Power Out**	**Round-Trip efficiency**	**Annual efficiency degradation**	**Storage Losses**	**CAPEX**	**CAPEX range**	**Year**	**OPE Fixe cost**
Abreviation	P_{in}	P_{out}	RTE	L_{RTE}	$L_{storage}$	C_{cap}	•	•	C_{Op}
Unit [-]	[kW/kWhn]	[kW/kWhn]	[%]	[%] of the efficiency	[kWh/h]	[€/kWhn]	[€/kWhn]	[year]	[$/kv year
Hydrowires	0.25	NA	86	5.0000000000000001E-3	NA	362[$/kWhn]	[308-419] [$/kWhn]	2025	8
Hydrowires	0.25	NA	86	5.0000000000000001E-3	NA	469[$/kWhn]	[393-581] [$/kWhn]	2018	10
Vonsien	0.5	1	NA	NA	NA	1466	[719-1570]	2016	NA
Schopfer	NA	NA	81	NA	NA	1000	NA	2018	NA
European Commisssion	NA	NA	NA	NA	NA	570	[250-1200]	2017	NA

	Power/C-rate		Efficiency						I
Parameters	**Power in**	**Power Out**	**Round-Trip efficiency**	**Annual efficiency degradation**	**Storage Losses**	**CAPEX**	**CAPEX range**	**Year**	**OPE Fixe cost**
European Commisssion	NA	NA	NA	NA	NA	206	[164-242]	2040	NA
European Commisssion	NA	NA	NA	NA	NA	313	[249-365]	2040	NA
Le Varlet	NA	NA	NA	NA	NA	NA	NA	2020	NA
Da Silva	NA	NA	NA	NA	NA	NA	NA	2021	NA

2.1.1 Resulting values

From the litterature overview, an AC-AC RTE of 86% as taken by (Mongird et al. 2019) is considered. This is above values usually taken in the litterature (Vonsien and Madlener 2020) of 95% both for DC charging and discharging the battery as well as for the AC-DC inverter leading to Schopfer efficiency of 81% (Schopfer, Tiefenbeck, and Staake 2018). Nevertheless, the selected value is realistic as (Mongird et al. 2019) value comes from real testing of grid-scale batteries. It is thus realistic to assume that in the following years, the efficiency gain will achieve at least a 86% average efficiency down to this scale.

As concern the annual RTE drop, (Mongird et al. 2019) was the only reference found giving a quantitative value.

The CAPEX is expected to decrease up to the [165-240]€/kWhn range in 2040 (Tarvydas et al. 2018). The mean value of 206€ is then adopted. Values for O&M comes from (Mongird et al. 2019), the only available source.

Lifetime of li-ion BESS is in the range 10-20 years but depends on several factors (see section 1.4.4). As underligned by (Tarvydas et al. 2018) which took the assumption of a 20 years lifetime, the majority of projects in the US DOE's database have a lifetime higher than 10 years. However it could be due to battery replacement to keep a minimal capacity. Litterature research carried out by (Vonsien and Madlener 2020) identified an average battery lifetime of 16 years with a overall cycling capacity of 4822 cycles. Those last numbers based on a compilation of studies seem more robust and were thus selected.

As regard the C-rate limitation, recommendation are scarce. Hence, based on the distribution of C-rate from real BESS projects, a limiting C-rate of 1C is fixed (Tarvydas et al. 2018).

Household/utility scale threshold is defined in accordance with (Killer, Farrokhseresht, and Paterakis 2020)'s definition being a limit of

50kWh capacity installed.

Table 2.1: Selected parameters about BESS technology

Key criteria	Symbol	Value	Unit	Literature Representation	Range size	Time robustness	Comments
RTE	$\bar{\eta}_{RTE}$	86.000	[%]	2	2	1	From the litterature overview, an AC-AC RTE of 86% as taken by (Mongird et al. 2019) is considered. This is above values usually taken in the litterature (Vonsien and Madlener 2020) of 95% both for DC charging and discharging the battery as well as for the AC-DC inverter leading to Schopfer efficiency of 81% (Schopfer, Tiefenbeck, and Staake 2018). Nevertheless, the selected value is realistic as (Mongird et al. 2019) value comes from real testing of grid-scale batteries. It is thus realistic to assume that in the following years, the efficiency gain will achieve at least a 86% average efficiency down to this scale.
Efficiency degradation factor	η_l	0.500	[%/year]	3	Irrelevant	2	As concern the annual RTE drop, (Mongird et al. 2019) was the only reference found giving a quantitative value.
Hourly self-discharge	σ	0.008	[%/hour]	Irrelevant	Irrelevant	Irrelevant	Value recovered from (Stadler 2019)
C-rate in	C_{in_max}	1.000	[kWin/kWhn]	3	Irrelevant	2	As regard the C-rate limitation, recommendation are scarce. Hence, based on the distribution of C-rate from real BESS projects, a limiting C-rate of 1C is fixed (Tarvydas et al. 2018)
C-rate out	C_{out_max}	2.000	[kWout/kWhn]	3	Irrelevant	2	As regard the C-rate limitation, recommendation are scarce. Hence, based on the distribution of C-rate from real BESS projects, a limiting C-rate of 1C is fixed (Tarvydas et al. 2018)
CAPEX	inv_2	206.000	[€/kWhn]	1	3	3	The CAPEX is expected to decrease up to the [165-240]€/kWhc range in 2040 (Tarvydas et al. 2018). The mean value of 206€ is then adopted.
Opex	op_1	8.000	[$/kWhn]	2	3	2	Values for O&M comes from (Tarvydas et al. 2018)

Key criteria	Symbol	Value	Unit	Literature Representation	Range size	Time robustness	Comments
Lifetime	L	16.000	years	1	3	1	Litterature research carried out by (Vonsien and Madlener 2020) identified an average battery lifetime of 16 years with a overall cycling capacity of 4822 cycles. Those last numbers based on a compilation of studies seem more robust and were thus selected.
GWP	NA	56.300	[kgCo2/kWhn]	3	Irrelevant	1	NA

Sensitivity code :

Literature Representation :

1. *Nearly all papers contain this value,*
2. *About 1 out of 2 papers contain this value,*
3. *Only a few papers contain this value*

Range Size :

1. *Range of values have a variation below 5% around the range midpoint (2.5% for efficiency),*
2. *Same but 10% (5% for efficiency),*
3. *Same but more than 20% (10% for efficiency)*

Time Sensitivity :

1. *There is strong reasons to support that this value won't change with time (the value reached a theoretical plateau, the technology is already mature and deployed at large scale …),*
2. *The value is a priory stable but can't prevent a breakthrough,*
3. *The value belongs to a technology still in R&D and there is large uncertainties about the final value..*

2.2 Modelling formulation

In order to use batteries in SBD. Several features needs to be modeled as constraints :

- The c-rate limitation as a limit onto the maximal power delivered/received by the BESS.
- The DoD limitation as a limit on the design capacity (we can't integrate it in the CAPEX because of the C-rate limit)
- The battery energy balance
- The RTE losses over the years
- The lifetime
- The size constraints as 2 different technologies (BESS for household or utility scaled)

As a result of the DoD limitation, we can operate the BESS in order to absorb the annual loss of capacity in the 20% margin. This last assumption results in keeping the capacity loss out of the model. Also, the transient response is far shorter than the time resolution of the model. Hence, there is no need to integrate it in the model.

2.2.1 Use limitation

Batteries are quite easy to deploy and do not suffer from restrictive limitations as regard the modelling and district's boundaries.

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Pumped Thermal Energy Storage

Author : Jules Mathieu **Last modification date :** January 13, 2022 **Validation status :** Valid

1 Introduction

1.1 Nomenclature

Acronym	Meaning
TES	Thermal Energy Storage
TEES	Thermo-Electrical Energy Storage
SBD	Smart Building Design
HP	Heat Pump
PTES	Pumped Thermal Energy Storage
CAES	Compressed Air Energy Storage
PHS	Pumped Hydroelectric Storage

1.2 Principle overview

Storing electricity through heat at low temperature is a relatively new concept developed either by ABB corporate research (Mercangöz et al. 2012) using transcritical Rankine cycles or by (Desrues et al. 2010) based on higher temperature Brayton cycles. Reason highlighted by (Morandin et al. 2012) are a common idea that the exergy is largely lost when converted to low temperature heat.

PTES systems presents the main advantage of getting rid of geographical constraints CAES and PHS suffers from. In addition, PTES has a great scale range potential and can provides small systems down to the 100 kW range (Mercangöz et al. 2012).

1.2.1 Rankyne based PTES

The suggested simplified concept depicted in figure 1.1 uses a Heat Pump (HP) with Co2 as the working fluid to convert electricity into hot and cold heat streams which are both stored in their respective storage tanks during charge step. Then, the discharge step consist in using the hot storage to evaporate the Co2 fluid before turbining it through a Thermal Engine (TE) to recover the electricity. The cold storage is then used to condense the CO2 before pumping it to the evaporator again.

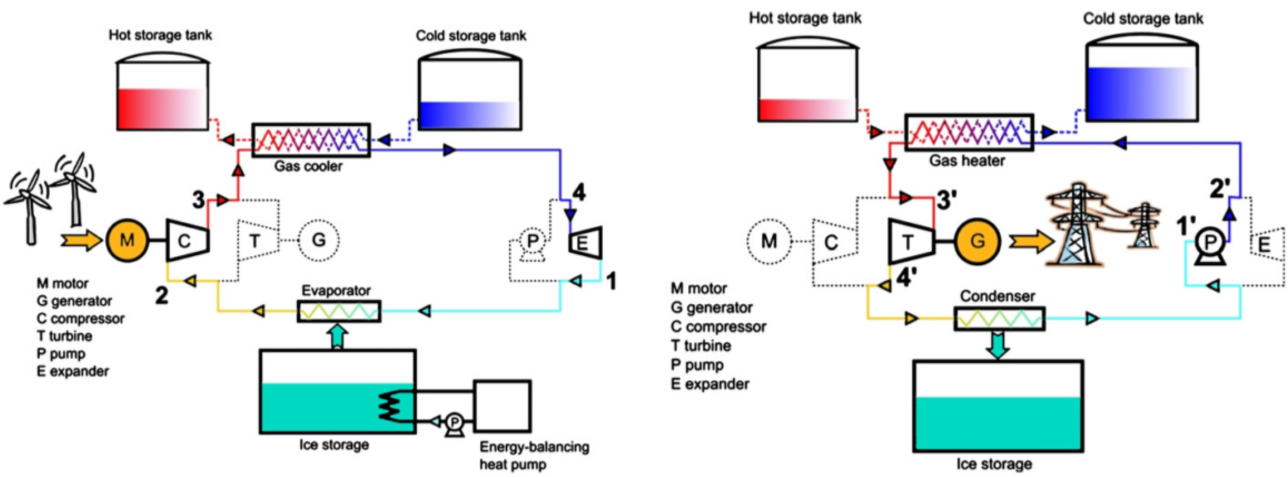

Figure 1.1: Basic schematic of the proposed concept from (Mercangöz et al. 2012)

1.2.2 Brayton based PTES

Brayton based PTES works similarly to the Rankine based one. The difference stands out in the working fluid used - mainly Argon - which does not experience phase change and stays under gas shape. This has the following effects on the thermodynamic cycle and its components : * The pump/expander devices are replaced by another compressor/turbine couple. * Hot and Cold heat exchanger are added to disregard the heat from the irreversibilities into the ambient.

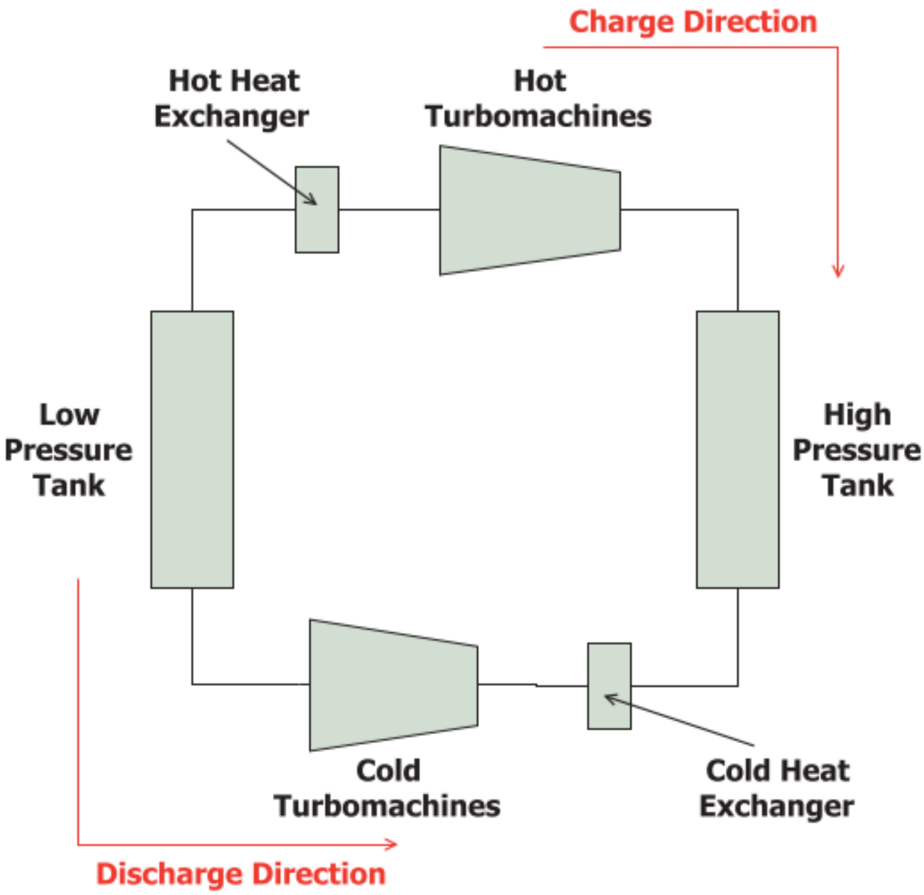

Figure 1.2: Basic schematic of the brayton cycle based PTES issued from (Benato and Stoppato 2018)

As regard large - over 10MW - energy storage plants, (Benato and Stoppato 2018) suggest Brayton based PTES should be preferred over other PTES configuration because of its reduced unit CAPEX as well as a more simple layout despite its lower round trip efficiency. However, (Mercangöz et al. 2012) also highlights the oversized storage needed by Brayton cycle in case of steady state operation.

1.2.3 Storage medium

Most of the studies use SHS storage for the hot storage due to it’s lowest cost (Benato and Stoppato 2018). On the contrary, cold storage often use LHS with ice as the main medium. Sometimes mixed with an adjuvant to reduce its eutectic temperature point, ice is the cheapest medium among PCMs (MacPhee and Dincer 2009).

1.3 Specific key criteria

1.3.1 Round trip efficiency

PTES systems offer a relatively high efficiency already above 53% (Mercangöz et al. 2012) and expected to reach the 70-80% range in the future (Benato and Stoppato 2018).

The losses of the overall system can be looked upon as the equipment irreversibilities on one side and the losses related to the thermodynamic design on the other. (Morandin et al. 2013) showed that the latter is mainly affected by the number of intermediate storages - it minimize the heat exergy degradation - and pressure levels.

Self-discharge losses rely on the thermal insulation of the different storage tanks. (Smallbone et al. 2017) estimated them to be in the order of 1% losses per day.

1.3.2 Charging/discharging time

Along the literature review, the different maximal charging time at nominal power crossed were in the range 2-8h, corresponding to medium time storage. This large variance is a result of the relative decoupling between storage volume and conversion power. Unlike electrochemical batteries, PTES hence has one additional freedom degree between power and capacity.

1.3.3 System dynamic

PTES systems have a short startup time - below 5 minutes - which allow them to meet the primary and secondary frequency regulation requirements (Mercangöz et al. 2012).

2 Characterization

2.1 Litterature overview

The literature overview is summarized in figure 2.1.

Table 2.1: Litterature about PTES technologies

Type	Working fluid	Material	Power in	Power out	RTE	CAPEX range	CAPEX conv	Year
•	•	•	P_{in}	P_{out}	RTE	•	•	•
[-]	[-]	[-]	[kW/kWhn or kW/kWn]	[kW/kWhn]	[%]	[€/kWhn]	[€/kWn]	[year]
Brayton	Argon based	•	1.25 (pin/pout ratio)	•	overall 72% 98% elec efficiency motor thermal store eff 98% mechanical eff 90% thermal eff of compression/expansion cycle 97%	13 hot : 11-17 cold : 2-4	overall scenario 1 :350 (but sum of below cost =400) HP : 166 TE : 64 other components : 170	2016
Brayton	Argon based	•	1.25 (pin/pout ratio)	•	0.67	17 hot : 11-17 cold : 2-5	? Info disappeared?	2016
Brayton	Argon based	•	1.25 (pin/pout ratio)	•	0.52	21 hot : 11-17 cold : 2-6	797 HP 294 TE 64 other components 439	2016
Brayton	Argon based	•	6-8h charge/discharge	in/out ratio = 1	66.7%, up to 70-80%	60	•	•
Rankine	Transcritical Co2 based	•	•	•	53% - 65.5%	•	•	•
Rankine	Transcritical Co2 based	•	50MW/ 3:13 to 4:10 h charging time	50MW/2h discharge time	48-64%	29.3-37.6 M$ (purchase cost only) Breking down th e 64% eff cost : 5.1M$ storage 8.3M$ Heat exchanger 20.8M$ Turbomachine + El.Equip	•	2009

Type	Working fluid	Material	Power in	Power out	RTE	CAPEX range	CAPEX conv	Year
Rankine	Transcritical Co2 based	•	•	•	51% range : [47-56%]	•	2000-6500	2012
•	•	•	•	•	65% range : [55-70%]	•	1200-2500	2012

2.1.1 Resulting values

Table 2.2 summarizes the finally selected values to be integrated into the SBD model.

Table 2.2: Litterature about PTES technologies

Key criteria	Value	Unit	Literature representation	Range size	Time robustness	Comments
RTE	67.0000	%	1	3	3	Medium scenario of (Smallbone et al. 2017), congruent to best performing technologies from other articles
Self discharge	1.0000	%/day	3	1	1	Dependent on the system insulation
Capex conversion	574.0000	€/kW	2	3	3	Value from (Smallbone et al. 2017) selected as it allows energy/power decoupling
Capex storage	17.0000	€/kWh	2	3	2	Value from (Smallbone et al. 2017) selected as it allows energy/power decoupling
Opex	11.0000	€/kW	3	Irrelevant	1	Only one value
Opex storage	0.0026	€/kWh	3	Irrelevant	1	Only one value which was considered as similar to CAES systems
lifetime	25.0000	years	3	Irrelevant	2	The low boundary value of the review was taken to take into account the other value together with the fact that the review is considered as the most representative.

The relative decoupling between power and capacity leads to different CAPEX regarding storage and conversion. Similarly, a better fit to the needs can be expected due to this extra freedom degree.

Sensitivity code :

Literature Representation :

1. *Nearly all papers contain this value,*
2. *About 1 out of 2 papers contain this value,*
3. *Only a few papers contain this value*

Range Size :

1. *Range of values have a variation below 5% around the range midpoint (2.5% for efficiency),*
2. *Same but 10% (5% for efficiency),*
3. *Same but more than 20% (10% for efficiency)*

Time Sensitivity :

1. *There is strong reasons to support that this value won't change with time (the value reached a theoretical plateau, the technology is already mature and deployed at large scale …),*
2. *The value is a priory stable but can't prevent a breakthrough,*
3. *The value belongs to a technology still in R&D and there is large uncertainties about the final value..*

2.2 Modelling formulation

In order to reflect the power/capacity decoupling, the system is modelled using 2 different technologies. The conversion technology is the set formed by the reversible HP and electrical engine/generator. It is characterised by its nominal power, cost and efficiency also including charging and discharging losses. The second technology is the set of hot and cold thermal storages. It has its own CAPEX and OPEX values and is subject to self-discharge losses.

2.2.1 Comparison with values from Energyscope and SBD

This technology does not exist in Energyscope.

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Power-To-Gas storage

Author : Jules Mathieu **Last modification date :** January 13, 2022 **Validation status :** Valid

1 Introduction

1.1 Nomenclature

Acronym	Meaning
DC	Direct Current
AC	Alternating Current
P2G	Power to Gas
H2	Dihydrogen
CH4	Methane
SNG	Synthetic Natural Gas
NG	Natural Gas
AEL	Alkaline Electrolysis
PEM	Polymer Electrolyte Membranes
SOEC	Solid Oxide Electrolysis
SOFC	Solid Oxide Fuel Cell
CHP	Combined Heat and Power
HHV	High Heating Value
LHV	Low Heating Value
AFC	Alkaline Fuel Cell
PAFC	Phosphoric Acid Fuel Cell
MCFC	Molten-Carbonate Fuel Cell

1.2 Power-to-Gas presentation

1.2.1 Electrochemical reactions

The following reactions for H2 electrolysis and SNG generation and their descriptions comes from (Götz et al. 2016).

1.2.1.1 H2 electrolysis

Water electrolysis reaction follows the equation (1.1). The massic HHV and LHV of this process are respectively equal to 39.4kWh/kgH2 and 33.3kWh/kGH2. This reaction is slightly endothermic and leads to larger heat losses which can be recovered to increase the overall process efficiency (overall efficiency is the sum of the electrical and thermal efficiencies). The reverse reaction happens when H2 reacts in a fuel cell.

$$H_2O(l) \rightarrow H_2(g) + \frac{1}{2}O_2(g) \qquad \Delta H_r^{0=} + 285.8kJ/mol \tag{1.1}$$

1.2.1.2 Hydrogen to Synthetic Natural Gas (SNG)

The following reactions occur in a methanizer whom active part can either be biological or catalytic. While the equations (1.2) and (1.3) directly form methane, the equation (1.4) refereed to as reverse water gas shift reaction needs to be combined with (1.3) to produce some. In contrast, the Boudouard reaction - equation (1.5) - leads to carbon poisoning drastically reducing the lifetime of the methanizer.

$$CO_2(g) + 4H_2(g) \rightleftarrows CH_4(g) + 2H_2O(g) \qquad \Delta H_r^{0=} - 165.1kJ/mol \tag{1.2}$$

$$CO(g) + 3H_2(g) \rightleftarrows CH_4(g) + H_2O(g) \qquad \Delta H_r^{0=} - 206.3kJ/mol \tag{1.3}$$

$$CO_2(g) + H_2(g) \rightleftarrows CO(g) + H_2O(g) \qquad \Delta H_r^{0=} + 41.2kJ/mol \tag{1.4}$$

$$2CO(g) \rightleftarrows C(s) + CO_2(g) \qquad \Delta H_r^{0=} - 172.5kJ/mol \tag{1.5}$$

1.2.1.3 SOEC co-electrolysis

It consists in the water electrolysis happening at the same time as Co2 reduction into CO. During this process, H2 can react with CO by-product to produce CH4 - equation (1.3). However, in order to avoid carbon poisoning which would drastically reduce the lifetime of the SOEC, the H/C ratio has to be high limiting the CH4 content of the generated gas (Clausen, Butera, and Jensen 2019). One should notice that water is under gas form for this reaction. Depending of the heat source to bring liquid water to gas, the power-to-gas efficiency can be noticeably improved.

$$CO_2(g) + 2H_2O(g) \rightleftarrows CH4(g) + 2O_2 \qquad \Delta H_r^{0=} + 708kJ/mol \tag{1.6}$$

1.2.2 Possible pathways

Following the previous equations, different pathways can be followed starting from a kWh of electricity. All of them start by an electrolysis step from which paths differ:

1. The electrolysis produces H2 which is then stored in a pressured tank to be used by a CHP fuel cell.
2. The produced H2 could also be directly injected into the CH4 gas grid up to 10% volume.
3. The produced H2 can be converted to CH4 in a methanizer although it necessitates a CO2 source. The latter can either be a biogas generation unit where H2 can be used to upgrade the amount of CH4 produced. Other sources are Co2 capture from intensive industrial processes or direct air capture of Co2 from the air. In the CH4 production case, a CH4 storage needs to be deployed. In addition, a h2 buffer tank needs to be deployed due to the lower dynamic response of the methanizer.
4. Using a SOEC electrolyzer with injection of Co2, SNG can directly be produced at a higher efficiency than the combination of electrolyzer and a methanation plant. However, the CH4 content is not sufficient for direct injection into the grid, leaving the choice between independent CHP use or SNG upgrade.

Then, following the 4 previous pathways, fuel cells can be used as CHP units to produce electricity and heat to households. Other uses are mobility (H2 and CH4) or industrial heat (CH4).

Those different pathways are presented in figure 1.1.

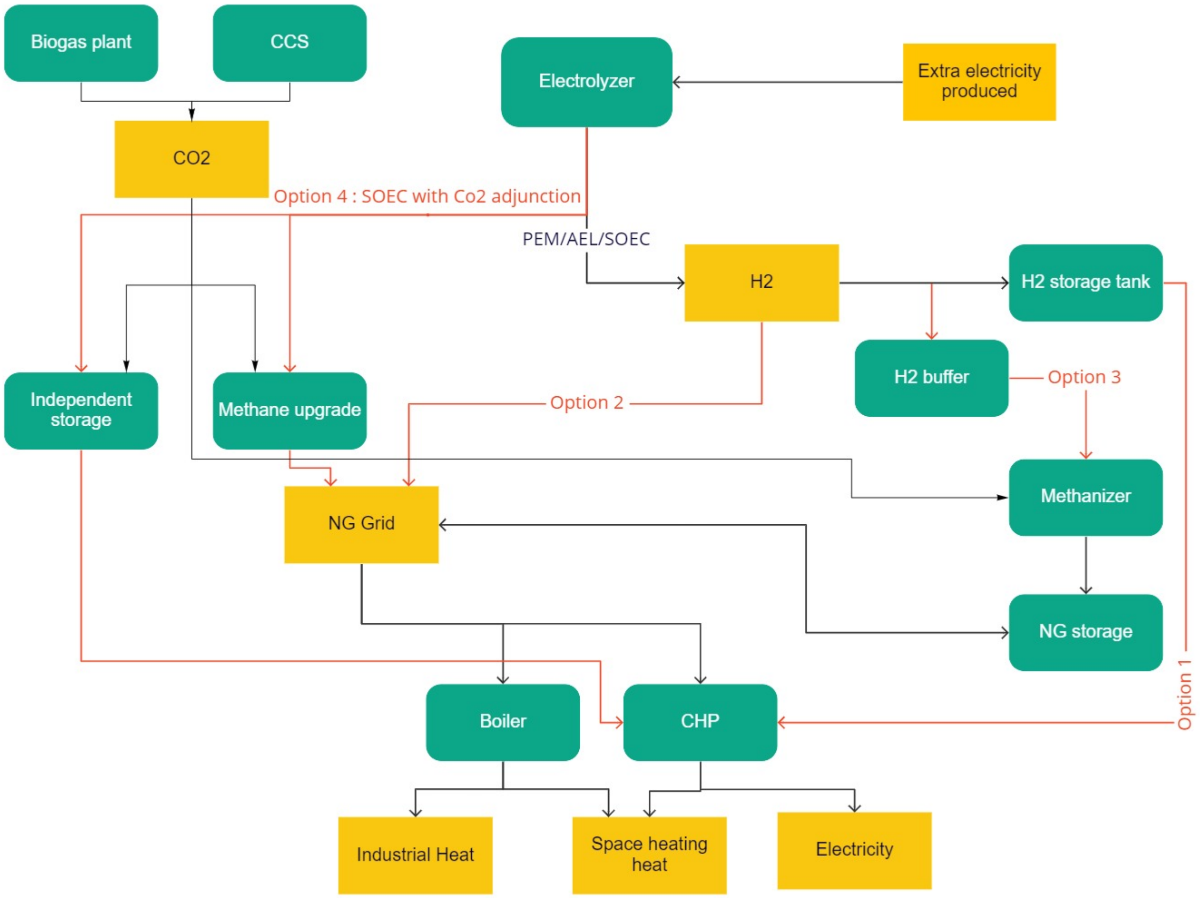

Figure 1.1: Representative flowchart of the possible pathways a P2G system allows

1.2.3 Electrolyser technologies

The following subsections presents the different electrolyzer technologies from already mature (AEL) to technologies still at pilot scale (SOEC).

1.2.3.1 Alkalyne - AEL

Already commercialised for many years, it is the most mature and well understood technology. In an AEL, an aqueous alkaline solution is used as the electrolyte. According to (Götz et al. 2016), AEL electrolyzers can be operated between 20 and 100% of the design capacity and can manage overload operation up to 150%. Compared to other technologies, AEL mains drawbacks are a long startup time - about 1h - as well as a lower efficiency. However, it displays a much longer lifetime than other fuel cell technologies as it could go up to 30 years (with a renovation of the stacks every 8-12y)(Götz et al. 2016). However, the lead of this technology is expected to decrease with the improvement of PEM fuel cells.

1.2.3.2 Polymer electrolyte membranes - PEM

PEM electrolysers are based on a solid polymer membranes. Their better design for dynamic operation make them well suited for energy storage coupled with fluctuating and intermittent power supply (Ruf et al. 2020). Additionally, they display a slightly better efficiency than AEL (Hu et al. 2020).

However, they still suffer from higher capital costs than AEL - see table **??** - although it is expected to decrease together with its commercial deployment as well as a lower lifetime

1.2.3.3 Solid Oxide Electrolysis - SOEC

SOEC consists of three main components which are two porous electrodes and a dense ceramic electrolyte capable of conducting oxide ions (O^{2-}). It typically operates in the 600 to 850°c range allowing for more favorable thermodynamics and kinetics than AEL and PEM electrolizers operating in the 20-100 range (Götz et al. 2016).

However, this technology is still at pilot scale even though it is on the verge of commercialization (Hauch et al. 2020). In order to further deploy this technology, several challenges remains (performance, degradation, and scale-up).

It must be noted that SOEC have the very interesting property to be able to operate both ways - as an electrolyser or a fuel cell. The reverse direction of equation (1.6) is happening when the SOEC is operating with CH4 or the reverse of (1.1) with H2.

1.2.4 Methanation

1.2.4.1 Processes

Several processes illustrated by figure 1.2 from (Götz et al. 2016) allows to convert H2 in CH4. (Thema, Bauer, and Sterner 2019) recorded similar number of projects using biological or catalytic technology - even though catalytic projects usually display a higher power - and can't predict which one is the most likely to outrun the other. Catalytic methanation typically operates at temperature between 250°c and 550°c and mainly use Ni as the catalyst. The methanation reaction being highly exothermic, there is strong needs of an effective heat management system. Then, the heat can be used latter on, either for the electrolysis step or to fulfil the demand.

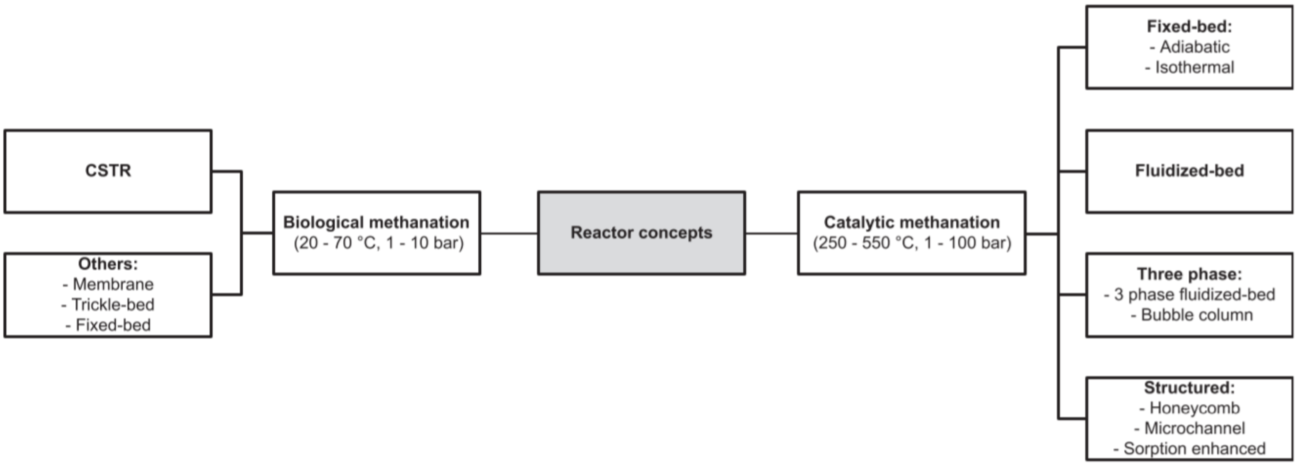

Fig. 4. Reactor concepts for the production of SNG.

Figure 1.2: Representative flowchart of the possible decisions a P2G system allows

As regards system dynamic, it must be noted that the methanation process needs a few hours to warm up when initially in cold state (Gorre, Ortloff, and van Leeuwen 2019).

1.2.4.2 CO2 sources

To convert H2 toward CH4, a CO2 source is needed.This can come from a CCS process or from a CO2 rich gas where the methanation acts as an specific heat upgrading process of the gas. At a district scale, biogas productions plants seem particularly well designed to this use(Götz et al. 2016). Although CO2 cost is currently rarely considered, the implementation of a CO2 price would result in a linear increase of P2G costs.

1.2.5 Storage technologies

1.2.5.1 H2 storage

Two different storage technologies are suitable for small-scale temporary storage. These are high pressure gas tanks or metallic hybride tanks (Götz et al. 2016). Inside the former category, tank III are able to store H2 up to 350bar while class IV tank can store it up to 700bars.

Additionally, up to 10% with respect to its volume, H2 can directly be ingested into the NG grid without any constraint on the equipments (Grond, Schulze, and Holstein 2013).

1.2.5.2 CH4 storage

Depending on the CH4 content, a gas with more than 80% CH4 is considered as SNG and can benefit from the SNG storage capacity far less expensive than dedicated storage. On the other hand, a CO2/CH4 gas should be stored in a dedicated cavern or tank (Gorre, Ortloff, and van Leeuwen 2019). Even though tank storage is much more expensive, cavern storage is driven by a scarce geological availability.

1.2.6 Fuel cell technologies

While SOFC/SOEC can be operated both ways, as a fuel cell and as an electrolyzer, efficiency reasons drove fuel cells to be usually made to only work in an unidirectional way. Exception are the regenerative fuel cells, the high pressure electrolyzers and off course the SOEC/SOFC ("Regenerative Fuel Cell" 2021). The different types of FC are showed in figure 1.3. FC systems in the 10kW-MW range are SOFC, PEMFC, AFC and PAFC. Two operating categories can be distinguished with SOFC operating around 650°c and AFC/PEMFC in the 0-100°c range (Sazali et al. 2020).

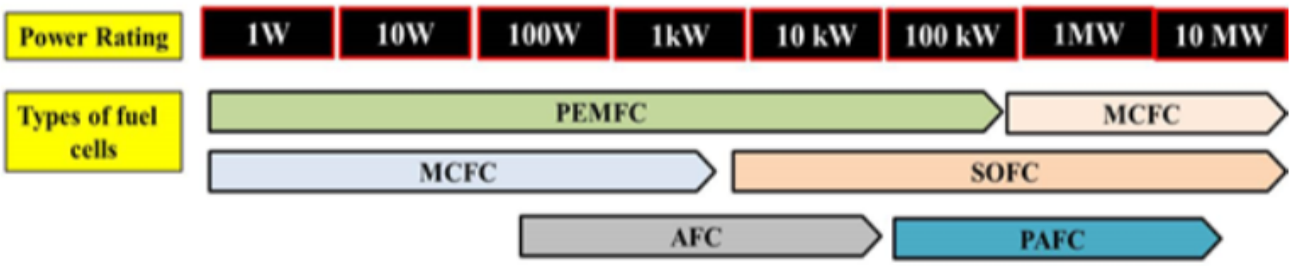

Figure 1.3: Figure presenting the different FC technologies issued from (Sazali et al. 2020)

In integrated energy systems, it can be interesting for a FC to be able to operate both on pure H2 or a combination of SNG and H2. Only a few FC technologies have this property among which SOFC and MCFC (Wang et al. 2020).

1.3 Specific key criteria (fuel cells and electrolyzers)

1.3.1 Electrolyse efficiency

The efficiency of an electrolyzer is best operating at part load rather than full load due to the current density going through the device. A study suggests the best operating load to be in the range 40-60% of nominal load with a gain of about 10% versus full load (Bartuccioli et al. 2014).

Regarding the typical efficiency of electrolyzer, it is in the range 60-75% for AEL and PEM technologies with an expected improvement to around 80% in the next decades (Gorre, Ortloff, and van Leeuwen 2019). In this respect, SOEC displays a remarkable potential of 75-79% with water at ambiant temperature up to 85-90% with 125°c steam (which could be provided by renewable sources). Then, thermal losses can be used for other thermal needs with a net advantage regarding exergy potential for SOEC which works at 800-1000°c instead of 20-100°c for the AEL and PEM (Götz et al. 2016).

1.3.2 Lifetime : Voltage degradation

The lifetime of an electrolyzer is directly linked to its voltage degradation over time. The latter can be seen as an additional electrical resistance decreasing the overall efficiency. As a result, the End-of-Life of an electrolyser is reached when 10% more energy is needed to provide the same quantity of H2 compared to its lifestart. The current lifetimes of each electrolytic technology displays a large gap between AEM - 13 years - and SOEC electrolyzer - up to 2.5 years (Bartuccioli et al. 2014; Hauch et al. 2020).

1.3.3 Dynamic and operation state

According to (Bartuccioli et al. 2014), the dynamic operation of PEM and Alkaline electrolysers is below 1 hour regarding startup time (5-15 min for PEM electrolysers) and below 1min as regard the ramp - down or up - to another regime.

On the contrary, Methanizers suffer from a long heating time up to several hours. Thus, it can be needed to keep them warm to allow dynamic operation. Doing so, three different operating states can be distinguished : * Cold standby : The methanizer is cold, only safety services needs to operate. * Hot standby : The methanizer is kept hot. Thermal losses have to be compensated by a thermal source. Safety services as well as operating ones needs to operate. * Operation : The methanizer is producing SNG. Thermal losses are covered by the SNG exothermal chemical reaction. Safety services as well as operating ones needs to operate.

The table below reproduced from (Gorre, Ortloff, and van Leeuwen 2019) recapitulates assumptions about what could be the thermal and electrical losses from a methanizer plant at year 2050 :

Losses [kWh/(MWel*h)]	Cold Standby	Hot Standby	Operation
Thermal	0	40	0
Electrical	2	20	20

2 Characterization

2.1 Litterature overview

The literature overview is split into 6 different tables where :

- Table **??** displays data about **electrolysis** technologies.
- Table **??** displays data about **methanation** reactors.
- Table **??** displays data about **electrocatalyzers**.

- Table **??** displays data about **H2 storage**.
- Table **??** displays data about **CH4 storage**.
- Table **??** displays data about **Fuel Cells**.

Preliminary comment : (Thema, Bauer, and Sterner 2019) review reported a high variation regarding investment costs with R^2 ratio down to 0.6. One of the reasons cited is the confusion between stack and overall costs fostered by studies which does not indicate clearly what their cost refers to. This is something encountered when collecting the following data.

Tables are hidden for visualisation purpose

2.1.1 Resulting values

The different parameters which were selected are summarized into the 5 following tables :

- Table 2.1 summarizes selected data about **electrolysis** technologies.
- Table 2.2 summarizes selected data about **methanation** reactors.
- Table 2.3 summarizes selected data about **electrocatalyzers**.
- Table 2.4 summarizes selected data about **H2 storage**.
- Table 2.5 summarizes selected data about **CH4 storage**.
- Table 2.6 summarizes selected data about **CH4 storage**.

Table 2.1: Selected parameters about Electrolysis technologies

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comments
Power-to-H2 efficiency	η	76	%	2	3	1	69.930069930069934	Upper value for PEM from (Bartuccioli et al. 2014) was selected. This because the mean value is for the year 2030 and (Gorre, Ortloff, and van Leeuwen 2019) gives an upper-bound of 78% in 2050.
Recoverable heat	η_H	24	%	Irrelevant	Irrelevant	Irrelevant	18.181818181818183	Assumed overall efficiency of 100% without information on non usable heat
Efficiency loss	η_l	0.12	%/1000h	2	3	2	•	Median of the 2 articles values for PEM and AEL

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comments
CAPEX	inv_2	385€/kW for 1MV down to 269.5€/kW for 10MW	€/kWe	1	3	2	1313.9860139860141	Values suggested by (Gorre, Ortloff, and van Leeuwen 2019) are similar to targets set by (Ruf et al. 2020) . Moreover, this fit in the range given by (Bartuccioli et al. 2014)
OPEX - Fixed costs	op_1	3.3	% of capex/year	3	2	2	46.153846153846153	Values for 1MV from (Bartuccioli et al. 2014) on which the 2/3 time decrease factor from (Gorre, Ortloff, and van Leeuwen 2019) was applied
Lifetime	L	10	year	2	3	2	7	NA
Operating temperature	T	70	[°c]	2	3	1	•	(Götz et al. 2016) states ETZ works in the 20-100°c temperature range, it is hence assumed that an ETZ able to cover all heat needs is selected.
GWP	NA	0.11	kg CO2 eq/kgH2	3	3	3	0.21	Only two values with a big gap. Moreover, efficiency normalisation should be applied

As highlighted in the previous sections, electrolysis is a mature process when operating using AEL and in a short time PEM electrolyzers. This is highlighted by the number of articles on the subject found which provides a consistent sets of values on technical aspects. However, cost related values are extremely likely to be substantially with the large scale development of those technologies expected in the next decades (IEA 2021). This explains the great uncertainty - reflected by the large range of values - regarding technology costs.

With respect to the values implemented in EnergyScope, one can notice a higher efficiency and lifetime together with a much lower investment cost, congruent with the expected improvement of electrolysis. The latter is further confirmed by the meta review undertaken by (Thema, Bauer, and Sterner 2019) which expects electrolysis costs from both AEL and PEM to fall below 500€/kWel in 2050.

Table 2.2: Selected parameters about Methanizer technologies

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comments
Conversion efficiency	η	78.00000	%	1	1	1	78.000078000078005	Most of the articles gives the theoretical max efficiency, some of them suggest to remove 1-2% if CO2 is not originally compressed
CAPEX	inv_2	368.50000	€/kW	2	2	2	280	Values from (Gorre, Ortloff, and van Leeuwen 2019), congruent with other ranges. Value for 1MW size.
OPEX - Fixed costs	op_1	3.00000	% of capex/year	3	2	2	5	Value from (Gorre, Ortloff, and van Leeuwen 2019)
Lifetime	L	20.00000	year	3	2	2	20	Value from (Gorre, Ortloff, and van Leeuwen 2019)
Operating temperature	T	400.00000	[°C]	2	3	1	NA	Middle of the temperature range from (Götz et al. 2016)
H2/CO2 ratio	•	0.19800	kgCo2/kWhH2	•	1	1	0.198kgCo2/kWhH2	Stoichiometric ratio
GWP	NA	16.98462	g Co2/kWh	3	?	3	•	Value considering Co2 impact of Co2 capture from exhaust gas.
Thermal losses Hot standby	NA	40.00000	kWh/Mwel*h	3	1	2	•	NA

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comments
Electrical losses Hot standby	NA	20.00000	kWh/Mwel*h	3	1	2	•	NA

As concern methanation technology, (Gorre, Ortloff, and van Leeuwen 2019) is a very exhaustive source and was used both in this study and in EnergyScope to characterise most parameters.

Table 2.3: Selected parameters about Methanizer technologies

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Comments
Power-to-H2 efficiency	η_{in}	77	%	2	2	1	Efficiency considering liquid water entering. Mean of the range
H2-to-Power efficiency	η_{out}	77	%	3	?	1	Assumption this is similar to the P2G efficiency (supported by efficiency values given by (Butera, Jensen, and Clausen 2019)
Power out limitation	$Pmax_{out}$	0.6	kWelout/kWn	3	3	2	Mean of the 2 availables values (considering the output)
Efficiency loss	η_l	0.5	%/1000h	3	3	2	Only one value
CAPEX	inv_2	1500	€/kW	3	3	3	Very important uncertainty, value from (Ruf et al. 2020) taken to have a consistent gap with fuel cell prices
OPEX - Fixed costs	op_1	3	% of capex/year	3	2	2	Same value than methanizer taken
Lifetime	L	10	year	3	3	3	Only one value
Operating temperature	T	70	[°c]	2	3	1	from (Sazali et al. 2020), but the range is high. Does not affect the model as temperature needs are much lower than this range but should be updated when industry needs are to be considered
GWP	NA	1.95E-2	kg/co2 /kWel in	3	3	3	Only two values. The per kW cradle to gate for a SOEC stack was taken over the per kg/h2 as the latter rely on other parameters (as the efficiency)
Elec to heat ratio	NA	1.077/1	kWel/kWth	3	1	1	Only one value
Elect to SNG ratio	NA	1.077/1.742	kWel/kWLHV SNG	3	1	1	Only one value

Table 2.4: Selected parameters about H2 storage technologies

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comment
Compression electrical needs	E_{el}_{comp}	0.12000	kwh_{el}/kwh_{H2}	2	2	2	NA	Value for compress H2 storag efficiency taken (mean of the 85-90 range)
Compression efficiency	η_c	85.00000	%	3	1	2	NA	Need to fi again the references
Expansion efficiency	η_e	93.00000	%	3	1	2	NA	Need to fi again the references
CAPEX	inv_2	13.53459	€/kWh LHV	1	3	3	0.03996	Median of all values from 2030 onwards.
OPEX - Fixed costs	op_1	1.50000	% of capex/year	3	Irrelevant	1	0.00072	Only 1 value
Lifetime	L	60.00000	year	3	Irrelevant	1	25.00000	Only 1 value whic seems qui high
Operating temperature	T	70.00000	[°C]	3	Irrelevant	1	NA	Assumptio it is higher the the SH needs
CAPEX compression	inv_2	1000.00000	€/kW	3	Irrelevant	1	NA	NA
Opex compression	op_1	1.50000	% of capex/year	3	Irrelevant	1	NA	Lower bound taken for consistenc with tank opex

Whereas the selected storage technology is tank storage, the great difference with EnergyScope values comes from the fact it uses cavern storage much cheaper on a power basis. However, this last technology can't be used everywhere and was thus discarded. CH4 was treated similarly even though CH4 networks are already developed and could be used to send CH4 away from the district to be stored in caverns. In EnergyScope, both CH4 and H2 storage lifetime does not correspond to the one cited in the reference (Gorre, Ortloff, and van Leeuwen 2019)

Table 2.5: Litterature about CH4 storage technologies

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comments

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comments
Compression electrical needs	E_{el}_{comp}	0.000000	%	3	Irrelevant	1	•	No value in the literature but must be higher than H2 storage efficiency. Compression losses are considered as negligible
CAPEX	inv_2	4.615385	€/kWh	3	Irrelevant	2	0.01CHF/kWh	Only one reference / Tank storage selected
OPEX - Fixed costs	op_1	1.000000	% of capex/year	3	Irrelevant	1	2	Only one reference
Lifetime	L	60.000000	year	3	Irrelevant	1	25	Only one reference

Table 2.6: Selected parameters about Fuel cell technologies

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comment
Fuel-to-power efficiency	η	65.000	%/LHV basis	1	3	2	58.021978021978029	Upper value of the mid and small scale FC selected
Fuel-to-heat efficiency	η_H	35.000	%/LHV basis	1	2	2	21.978021978021978	Assuming 100% efficiency
Efficiency loss	η_l	1.750	%/year	3	3	2	•	Same value than electrolyser's taken (assumption).
CAPEX	inv_2	1500.000	€/kW	2	3	2	2929.5454545454545	Lower value of the mid-sized range from (Ruf et al. 2020) taken to be consistent with the SOEC selected cost
OPEX - Fixed costs	op_1	3.000	% of capex per year	3	Irrelevant	2	58	Same value than methanizer taken
Lifetime	L	20.000	year	2	3	2	20	NA

Parameter	Symbol	Value	Unit	Literature representation	Range size	Time robustness	Energyscope value	Comment
Operating temperature	T	70.000	[°c]	3	Irrelevant	1	NA	(Sazali et al. 2020) states FC works in the 0-100°c temperature range, it is hence assumed that a FC able to cover all heat needs is selected.
OPEX - Variable costs	NA	0.012	€/kWh	3	Irrelevant	2	•	NA
GWP	NA	0.110	kg CO2 eq/kgH2	3	Irrelevant	3	•	Value of electrolyser taken

One might notice the large uncertainty regarding operational and investment costs of fuel cells (Yao et al. 2017). The lifetime is often expressed in operating hours which could be used as an extra level of liberty by SBD. However, the modelling of such a variable requires integers and would as a result slow down the MILP program.

Sensitivity code :

Literature Representation :

1. *Nearly all papers contain this value,*
2. *About 1 out of 2 papers contain this value,*
3. *Only a few papers contain this value*

Range Size :

1. *Range of values have a variation below 5% around the range midpoint (2.5% for efficiency),*
2. *Same but 10% (5% for efficiency),*
3. *Same but more than 20% (10% for efficiency)*

Time Sensitivity :

1. *There is strong reasons to support that this value won't change with time (the value reached a theoretical plateau, the technology is already mature and deployed at large scale …),*
2. *The value is a priory stable but can't prevent a breakthrough,*
3. *The value belongs to a technology still in R&D and there is large uncertainties about the final value..*

2.2 Modelling formulation

2.2.1 Technology packages

Below are summarized the different pathways which will be modelled into SBD :

- Pathway 1 : An electrolyzer, a H2 storage tank and a CHP unit (non necessary in case of a SOEC/SOFC unit)
- Pathway 3 : Pathway 1 + a methanation reactor
- Pathway 4 : A SOEC + a CH4 storage (no methane upgrade)

The following paths are not modelled yet. First because pathway 2 is out of the boundaries as NG consumption is forbidden. Second, only tank storage is allowed, there is hence no need to upgrade the generated SNG from pathway 4 in 4b. - Pathway 2 : An electrolyzer(+ a CHP unit if the 10% NG consumption threshold is outreached) - Pathway 4b : An additional methanation reactor to pathway 4.

2.2.2 Constraints

In order to use the P2G related technologies in SBD. Several features needs to be modeled as constraints:

Electrolysis

- The negative specific cost - size correlation
- The lifetime
- The entering power limitation
- The efficiency losses over time

Methanation

- The 3 operating states (Hot Standby, Cold Standby, Production) dependent of the previous state
- The lifetime
- The negative specific cost - size correlation
- The offset of the losses during hot standby.
- The entering power limitation
- The mass balance of H2 and Co2

Electrocatalyzers

- The lifetime
- The mass ratio of H2 and Co2
- The entering energy ratio of electricity and heat
- A shared use factor together with the SOFC unit
- The 3 operating states (Hot Standby, Cold Standby, Production) dependent of the previous state

H2 storage

- The storage tank energy balance

CH4 storage

- The storage tank energy balance

Fuel cells

- The negative specific cost - size correlation
- The lifetime
- The entering power limitation
- The efficiency losses over time

2.2.3 Use limitation

Due to the current boundaries of the district under study, the use of the natural gas grid was forbidden. As a result, cavern storage or H2 injection into CH4 grid were not considered.

#Pathway using Co2 from biomass needs to be implemented in a district with a non-zero biomass potential. #Cavern storage won't be modelled but costs will be those taken to consider the SNG storage ?

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Sensible Heat Storage

Author : Jules Mathieu **Last modification date :** January 13, 2022 **Validation status :** Valid

1 Introduction

1.1 Nomenclature

Acronym	Meaning
TES	Thermal Energy Storage
SHS	Sensible Heat Storage
LHS	Latent Heat Storage
TCHS	Thermochemical Heat Storage
PCM	Phase Change Material

1.2 Sensible Heat Storage overview

1.2.1 General principle

Sensible Heat Storage (SHS) rely on the specific heat capacity of the storage medium as it stores heat as a change in the medium temperature. The following equation describe the heat stored or released function of the temperature entering and leaving the SHS component.

$$\Delta h_{SHS} = c_{p,avg}.(T_{in} - T_{out}) \tag{1.1}$$

Compared to LHS and TCHS technologies, SHS storage offers a reduced investment cost as the most used medium is water (Stadler, Hauer, and Bauer 2019) but also because it benefited from scale cost savings as it is the most developed technology (Nazir et al. 2019). The dependency of the previous equation to the temperature regime must be noted as it influences substantially the overall storage capacity of the medium (Flores et al. 2017).

1.2.2 Technology typologies

Tank thermal energy storage

This technology consist of a manmade tank usually made of steel or concrete. The tank has an insulation layer minimizing self-discharge losses and is usually buried. Regarding scale range, it start with a few hundred of litres - as individual housing hot water tanks - up to at least 5700m3 as reported by (Yang et al. 2019).

Pit thermal energy storage

Pit storage is also using a handmade construction, usually a buried reservoir filled with rocks and water. Two different heat exchange options are then available. The first one consist in water directly flowing through the reservoir to discharge the heat. The second in a buried pipe, collecting heat using conduction.

Borehole thermal energy storage

This method uses existing soil as a storage medium. To exploit it, the latter is traversed with 10-15cm wide, 20-150m deep, tubes filled with a water-antifreeze mixture (Stadler, Hauer, and Bauer 2019). This allows to save expensive excavation costs and to exploit volumes larger than 50 000m3.

Aquifer thermal energy storage

This exploit already existing aquifers directly injecting/pumping cold or hot water from it to create a stratified layer storing the provided heat. This is usually a seasonal storage mean and heavily rely upon geological underground characteristics. For hot storage, round trip efficiencies of 67% were measured (Stadler, Hauer, and Bauer 2019).

1.3 Specific key criteria

1.3.1 Capacity cost :

The more the system is energy and ressource intensive, the greater the cost. As a result, borehole storage is the cheapest technology followed by pit storage and then tank storage. (Flores et al. 2017) reports cost from 50 to 500€/m3 depending on the system size (cost of 50€/m3 is for storage larger than 10 000m3)

1.3.2 Charging/discharging time

Systems driven by heat conduction process are likely to display a much lower power to capacity ratio than systems with direct water exchange.

1.3.3 Energy and exergy losses

Energy losses in SHS systems rely on the overall insulation of its boundaries and the different thermal bridges. Regarding exergy, SHS systems rely on stratification to prevent exergy degradation. Stratification is achieved through a gradient where the temperature increase from the bottom to the top of the tank. The latter is then deteriorated by the conduction processes inside water or on the metal-water boundary in case of steel-tanks together with the convection occurring when water is drawn from or added to the tank (**camposceladorImplicationsModellingStratified2011?**; **cruickshankHeatLossCharacteristics2010?**; **rosenExergyStratifiedThermal2001?**).

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2 Characterization

2.1 Litterature overview

The literature overview about SHS is displayed into table 2.1.

Table 2.1: Litterature about SHS technologies

Subtype	Efficiency in	Annual efficiency degradation	CAPEXconv	Year	OPEX - Fixed costs	OPEX - Variable costs	Scale	Lifetime	Global Warming Potential	R
•	η_{in}	L_{RTE}	•	•	C_{Op_fixed}	$C_{Op_variable}$	•	•	GWP	
[-]	[% of elec to LHV (or for Storage simply %)]	[%] of the efficiency	[€/kWn]	[year]	[$/kw-year]	[€/kWh]	[-]	[year]	[Co2e 100years]	0
LT	•	•	•	2011	•	•	0.001-10MW	•	•	(S S 2(
LT	•	•	•	•	•	•	•	•	•	(A 2(

Subtype	Efficiency in	Annual efficiency degradation	CAPEXconv	Year	OPEX - Fixed costs	OPEX - Variable costs	Scale	Lifetime	Global Warming Potential	R
LT	•	•	•	2017	•	•	1000-10000m3	•	•	(F 2(
Seasonnal	•	•	•	1995	•	•	43,5MWh	•	•	(F et
Seasonnal	•	•	•	2003	•	•	638MWh	•	•	(F et
Seasonnal	•	•	•	•	•	•	654,6MWh	•	•	(F et
Vacuum insulated	•	•	•	•	•	•	3020kwh	•	•	(F et
Vacuum insulated	•	•	•	•	•	•	504kWh	•	•	(F et
Water tank	•	•	•	•	•	•	202kWh	•	•	(F et
Water tank	•	•	•	•	•	•	58.7kwh	•	•	(F et
Seasonnal	•	•	•	•	1% of the investment	•	•	14-30 years, median 22.5	•	(Y 2(
Housing use	•	•	•	•	•	•	•	20	•	(N 2(
Housing use	•	•	•	•	•	•	0-60MW	42125	•	(E al

2.1.1 Resulting values

The different parameters which were selected are summarized into the following table :

Table 2.2: Litterature about SHS technologies

Key criteria	Value	Unit	Literature representation	Range size	Time robustness	Comments
Power over capacity ratio	1>	[-]	3	Irrelevant	3	Assumption that the reservoir can be fully discharged in one hour
RTE	70	%	3	Irrelevant	3	Only 1 value. Mean of the range. Includes self-discharge losses and is for long term storage
Self-discharge	0.75	%/day	3	Irrelevant	1	Only 1 value. Mean of the range
CAPEX	9	[€/kWhn]	1	3	3	Median of values with capacity higher than 100kWh taken
Opex	1	% of Capex/year	3	Irrelevant	1	Only 1 value
Lifetime	20	years	3	Irrelevant	1	Only 1 value. (Enescu et al. 2020) was not considered as it groups LHS and SHS which have different lifetime
Energy content of 1m3	40.638888888888879	kWh	Irrelevant	Irrelevant	Irrelevant	Considering dT = 35°c (T min storage =20° and Tmax heat pump =55°c)
CAPEX converted in a m3 basis	365.74999999999989	€/m3	NA	NA	NA	NA

Sensitivity code :

Literature Representation :

1. *Nearly all papers contain this value,*
2. *About 1 out of 2 papers contain this value,*
3. *Only a few papers contain this value*

Range Size :

1. *Range of values have a variation below 5% around the range midpoint (2.5% for efficiency),*
2. *Same but 10% (5% for efficiency),*
3. *Same but more than 20% (10% for efficiency)*

Time Sensitivity :

1. *There is strong reasons to support that this value won't change with time (the value reached a theoretical plateau, the technology is already mature and deployed at large scale …),*
2. *The value is a priory stable but can't prevent a breakthrough,*
3. *The value belongs to a technology still in R&D and there is large uncertainties about the final value..*

2.2 Modelling formulation

The model already in use in SBD can be used for tank storage. A way to model the stratification losses must be explored **first the interest of such modelling**

2.2.1 Use limitation

No use limitation to be applied.

2.2.2 Comparison with values from SBD

SBD considers water tank SHS storage and uses a first-order buffer tank model developed in (Rager 2015). It uses technical values from Viessmann manufacturer for small tanks up to 1000 litres. The model only considers self-discharge through radiative losses and considers stratification as perfect.

Regarding the technology costs, it consist of a fixed cost of 760 CHF and a size-variable cost of 1040CHF/m3. Considering a 40°c

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Latent Heat Storage

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1 Introduction

1.1 Nomenclature

Acronym	Meaning
TES	Thermal Energy Storage
SHS	Sensible Heat Storage
LHS	Latent Heat Storage
TCHS	Thermochemical Heat Storage
PCM	Phase Change Material
SBD	Smart Building Design

1.2 Latent Heat Storage overview

Latent Heat Storage (LHS) refers to Thermal Energy Storage (TES) using the substantial energy density included in phase change to store thermal energy. Phase change occurs at a specific temperature which varies depending on pressure. This dependency is especially relevant when considering the liquid-gas transition as displayed by the Co2 phase diagram in figure 1.1.

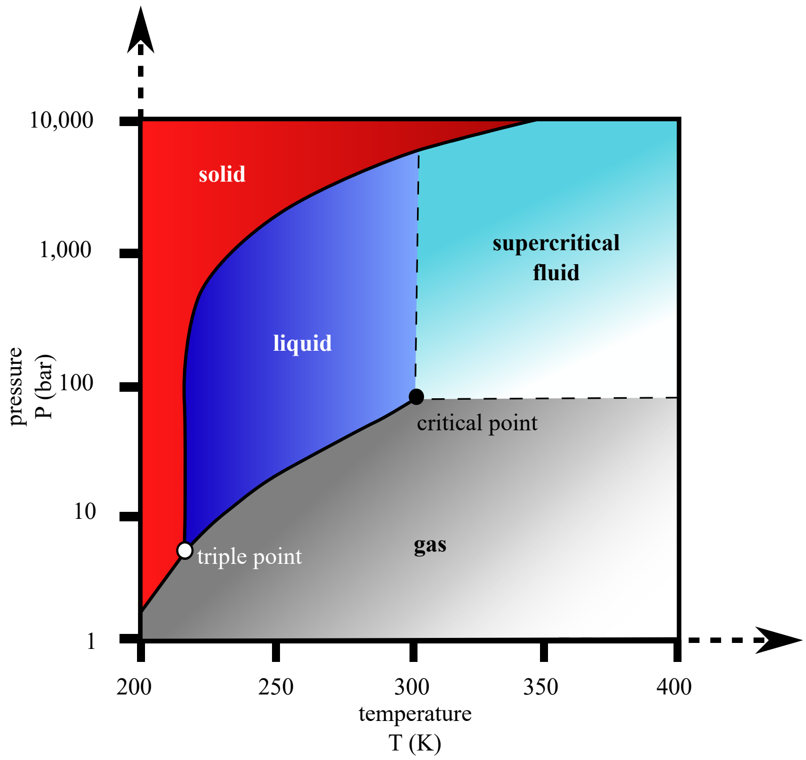

Figure 1.1: Co2 phase diagram from (Jacobs 2010)

As highlighted by (Sarbu and Sebarchievici 2018), the lower volume variation as well as the high melting latent heat of solid-liquids PCMs make them mainly used over the liquid-gas ones.

LHS is usually considered as the most promising technique compared to other TES. Reasons for it are its larger energy storage density - up to 4 times higher than SHS - together with a smaller temperature variation (Sarbu and Sebarchievici 2018). Compared to TCHS, LHS displays better repeatability and controllability. On the contrary, the challenges left to overcome are a low conductivity limiting the power-to-capacity ratio and a low lifetime (Nazir et al. 2019; Tao and He 2018).

The smaller temperature range of LHS prevents temperature stratification considerations present in liquid based SHS systems (Haller et al. 2018). As a result, self discharge losses rely only upon radiative losses determined by the overall insulation of the LHS system. Consequently, LHS displays a better RTE than SHS.

1.2.0.1 PCM

LHS technologies are based on a Phase Change Material (PCM) as the energy storage medium passing from solid to liquid to store energy and inversely to deliver it back. At space heating temperature, paraffin is highly represented among the different PCMs and has the advantage of being available in a large - 5°c to 80°c - fusion temperature range Tao and He (2018). Figure 1.2 presents the different categories depending on the working temperature range in the frame of housing use. LHS can also be used for higher temperature needs, for example in smoothing - during night - solar electricity production as in (Seitz, Johnson, and HÃÂbner 2017).

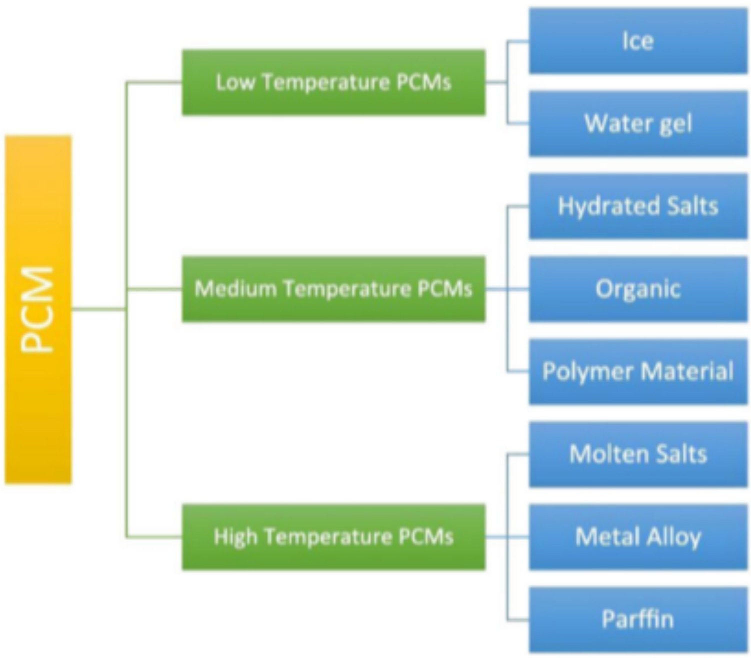

Figure 1.2: Melting point of representative PCMs. Figure from (Ge et al. 2013) itself adapted from (Sarbu and Dorca 2019)

Space heating corresponds to the medium temperature range while low temperature can be used for cooling purpose. High temperature PCMs are mostly used to store energy from solar generation and (Sarbu and Sebarchievici 2018).

Organic PCMs include paraffin, fatty acid, esters, alcohols and glycols. They can endure many cycles and mostly feature non-corrosive behaviour. Paraffin-based PCMs are safer, more predictable and cheaper than other organic PCMs. The latters display high latent fusion heat in exchange for lower conductivity as well as high-temperature instability and flammability risks (Sarbu and Sebarchievici 2018).

Inorganic PCMs as hydrated salts and metal alloys are generally used in high temperature solar application but suffers from a challenging maintenance. Hydrated salts melting phase change consist in a dehydration of the crystalline salt either towards a lower hydrated salt or a completed separation of water and salt. Hydrated salts display a high latent heat density combined with a higher conductivity than organic PCMs as well as a low corrosiveness. Moreover, in contrast with paraffin, they can be used with plastic. Main limitations includes incongruent melting and super cooling As regards metal alloys, they suffer from a low mass latent heat which prevent them to be commonly used disregarding their numerous advantages. They have a high conductivity as well as a high latent heat density(Sarbu and Sebarchievici 2018).

1.3 Specific key criteria

1.3.1 Storage capacity

The following equation describes the enthalpy variation of a PCM particle from one state to another.

$$\Delta h_{LHS} = c_{p,sol}.\,(T_{pc} - T_{low}) + \Delta h_{pc} + c_{p,liq}.\,(T_{high} - T_{pc}) \tag{1.1}$$

with $c_{p,sol}, c_{p,liq}, T_{pc}, T_{low}, T_{high}$ respectively solid and liquid average specific heat, phase change temperature as well as low and high temperature.

Figure 1.3 presents the different PCMs categories function of their melting temperature and energy.

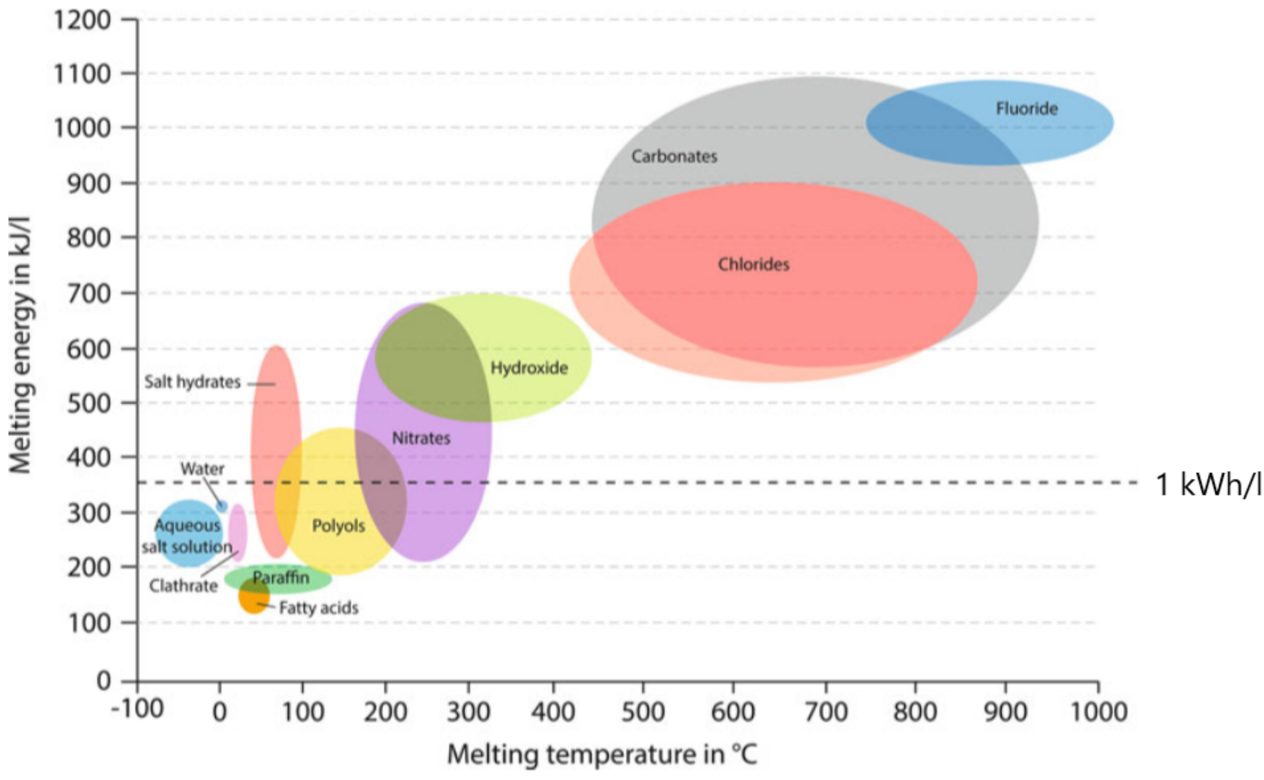

Figure 1.3: PCM categories regarding melting energy and temperature point

1.3.2 Capacity cost :

It heavily depends upon the application type, specific heat of storage media, number of cycles and the thermal insulation technique (Ahmed et al. 2019).

According to (Chiu, Martin, and Setterwall 2009), the broken distribution of costs follows the one in table 1.1.

Table 1.1: Comparison of Cost distribution between SHS and LHS technologies from (Chiu, Martin, and Setterwall 2009)

Technology	SHS	LHS
Tank Cost	45%	17%
Space Cost	3%	1%
Heat medium Cost	0%	43%
Maintenance Cost	3%	3%
Installation Cost	19%	10%
Control System and Utility Cost	29%	24%
Energy Cost	1%	2%
Total	100%	100%

1.3.3 Charging/discharging time

It has been showed that that an 8-hour charge has the ability to reduce the storage cost when compared to the same PCM with a 6-hour charge by about 5% (Jacob et al. 2018).

1.3.4 Exergy Losses

Energy transfers with the PCM composing the LHS system needs a minimal temperature difference between the supply and return sources and the fusion temperature to ensure a certain transfer rate. This results in exergy degradation following carnot efficiency $\eta = (1 - \frac{T_C}{T_H})$ with $T_C \ and \ T_H$ respectively cold and hot reservoir temperature.

2 Characterization

2.1 Litterature overview

The litterature overview is summarized in figure 2.1.

Table 2.1: Litterature about LHS technologies

Subtype	Material	Power in	RTE	CAPEX range	Year	Scale	Lifetime	Gl Wa Pc
•	•	P_{in}	RTE	•	•	•	•	G

Subtype	Material	Power in	RTE	CAPEX range	Year	Scale	Lifetime	Gl Wa Pc
[-]	[-]	[kW/kWhn or kW/kWn]	[%]	[€/kWhn]	[year]	[-]	[year]	[C 10
Housing use	Not precised	•	75-90	10-50	2011	0.001-1MW	•	
Very High Temperature	Molten salt	0.17	•	20-40	2014	Large	•	
Housing use/Non organic	Molten salt	•	•	5.77 - 48.3	2014	Large	•	
Very High Temperature	D-Mannitol	•	•	12-57.3	2013	•	•	
Housing use/Non organic and organic	Non paraffin PCM	•	•	45-293.58	2013-2016	500-10000kWh	•	
Housing use/Organic	Paraffin	•	•	45.58-64.2	2013-2016	500-10000kWh	•	
Housing use/Non organic	NaOAc	•	•	39.6-66	•	1.5-2.5MWh	•	
Housing use/Non organic	Hydrated Salt	•	•	56.6-75.9	•	83kWh	•	
Housing use/Non organic	Salt hydrate + graphite	•	•	•	•	13kWh	•	

Subtype	Material	Power in	RTE	CAPEX range	Year	Scale	Lifetime	Gl Wa Po
Housing use	Not precised	•	75-96	•	•	•	5	
Housing use	Not precised	•	•	•	•	0-60MW	42125	
Housing use	•	•	•	•	•	2MWh/year	10	21 pe he su
NA	NA	NA	NA	NA	NA	NA	NA	NA
NA	NA	NA	NA	NA	NA	NA	NA	NA
NA	NA	NA	NA	20	NA	NA	NA	NA

2.1.1 Resulting values

The different parameters which were selected are summarized into the following table :

Table 2.2: Selected parameters of LHS technologies

Key criteria	Value	Unit	Literature representation	Range size	Time robustness	Comments
Power over capacity ratio	0.17	[-]	3	Irrelevant	3	Only one value
RTE	84.00	%	3	Irrelevant	3	Mean of the mean of each of the 2 ranges
Self-discharge	0.75	%/day	3	Irrelevant	1	Only 1 value. Mean of the range
CAPEX	52.80	[€/kWhn]	1	3	3	Median of the values, themselves mean of their range
Opex	1.00	% of Capex/year	3	Irrelevant	1	No value, same as SHS taken

Key criteria	Value	Unit	Literature representation	Range size	Time robustness	Comments
Lifetime	7.50	years	3	Irrelevant	2	Mean of the 2 values.
GWP	218.00	gCO2/kWh of heat supplied	3	Irrelevant	3	No value

Sensitivity code :

Literature Representation :

1. *Nearly all papers contain this value,*
2. *About 1 out of 2 papers contain this value,*
3. *Only a few papers contain this value*

Range Size :

1. *Range of values have a variation below 5% around the range midpoint (2.5% for efficiency),*
2. *Same but 10% (5% for efficiency),*
3. *Same but more than 20% (10% for efficiency)*

Time Sensitivity :

1. *There is strong reasons to support that this value won't change with time (the value reached a theoretical plateau, the technology is already mature and deployed at large scale …),*
2. *The value is a priory stable but can't prevent a breakthrough,*
3. *The value belongs to a technology still in R&D and there is large uncertainties about the final value..*

2.2 Modelling formulation

First, unlike SHS storage which mostly rely on the temperature difference to set its overall capacity, LHS operates with a low temperature variance. Thus, the functional unit used is the melting latent heat without consideration of the sensible heat. However, the temperature delta needed to ensure a certain conductivity can be reflected using the heat cascade of SBD.

2.2.1 Use limitation

2.2.2 Comparison with values from Energyscope and SBD

This technology is not deployed in Energyscpèe

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