

DYNAMIC MODELING AND SENSITIVITY ANALYSIS OF A STRATIFIED HEAT STORAGE COUPLED WITH A HEAT PUMP AND AN ORGANIC RANKINE CYCLE

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ABSTRACT

The storage of electrical energy is becoming increasingly important to satisfy the demand through renewable energy sources. In this paper, a continuous and discrete simulation of a pumped thermal energy storage system are compared with respect to their computational time and accuracy. The stratified heat storage is modelled using spatial one-dimensional considerations and abstractions. Results show, that the discrete simulation with fixed time step is about 60 times faster and has neglectable deviation in the resolution of heat loss computations and accuracy, compared to the continuous System Dynamics model. The conducted sensitivity analysis shows, that parameters of the storage fluid have little influence on the overall result. The determining factor regarding losses in the storage and possible savings for users, is the insulation of the thermal storage. Increasing the number of temperature layers considered in the simulation shows so called deadlayers, which block the storage if not removed during operation.

1 INTRODUCTION

Worldwide, there is a shift from fossil fuels like coal, oil and natural gas to more sustainable energy resources such as wind and solar in order to limit the global warming to well below two degrees Celsius compared to pre-industrial level and to fulfill the Paris Agreement (Horowitz 2016). For instance, in 2020 renewable energy sources (RES) had a share of 44 % in gross electric power production in Germany (Energiebilanzen 2020) and 21 % in the United States (U.S. Administration 2021), respectively. RES-based energy systems are accompanied by their high dependency on weather and a high degree of decentralization (Quiggin et al. 2012). In order to optimally integrate energy generated from RES into existing energy systems, energy storage devices are becoming increasingly important. They provide the possibility to manage unbalances between fluctuating renewable energy supply and demand. Apart from electrochemical, mechanical and electrical storage systems, thermal energy storage systems are of significant interest for sector coupling mechanisms (Steinmann et al. 2019). Many applications of thermal energy storage systems have been studied in literature including seasonal storage of solar thermal energy (Xu et al. 2014), building cooling demand (Arteconi et al. 2017) or peak shaving (Erdemir and Dincer 2020). In addition, there are other fields of application for thermal energy storage, such as a novel pumped thermal energy storage (PTES) system, consisting of a heat pump (HP), heat storage (HS) and organic rankine cycle (ORC) which we examine more in detail in this paper.

In literature, the modeling and simulation of the HS is of great importance which enables the definition of essential parameters for real operation and the development of realistic control strategies. Computational

Fluid Dynamics (CFD) studies of thermal storages focus on complex phenomena and their differential equations, for example the loss of energy when a stratified storage is fully mixed, and usually take long computational times to solve. For instance, Bouhal et al. (2017) use a CFD simulation to study the thermal stratification in solar hot water storage tanks for domestic applications, whereas Karim et al. (2018) investigate various parameters that significantly influence the thermal performance of stratified thermal storage systems for both heating and cooling applications.

However, to estimate the operating behavior of a thermal storage system over a longer period of time, more abstract models are required that nevertheless reflect the real thermal behavior of the storage system. This includes, for example, the stratification of the storage tank. Kleinbach et al. (1993) did a performance study of spatial one-dimensional models for stratified thermal storage tanks and explained different model approaches. The basic approach for these one-dimensional methods is, that the storage tank is divided in either segments of the same height with variable temperature or segments of constant temperature with variable height. Nash et al. (2017) applied these methods on a simulation of a sensible thermal energy storage with an immersed coil heat exchanger and successfully validated the simulation approach with experimental data.

In this paper, we investigate two different simulation approaches for a PTES with a one-dimensional model for the HS. The first approach is a System Dynamics (SD) model, to simulate the behavior and dependencies of different layers inside the storage according to the simplified differential equations. The second approach is a discrete simulation model with fixed time steps (DS-FT) with a discretization of continuous flows to only calculate balance equations every time step. In general, a DS-FT is faster as the state of the system is not constantly computed like in SD simulations. Both simulations include the same operation logic of the storage system and efficiency curves for the heat engines. We compare these approaches regarding the accuracy of heat losses inside the storage and computational efficiency, to determine if a continuous calculation of heat losses is necessary or if a coarser resolution provides sufficiently accurate results. Finally, a sensitivity analysis is performed for material parameters of the storage fluid and insulation.

The remainder of the paper is organized as follows: In Section 2 we explain the basic idea and the theoretical background of our pumped thermal energy storage system. Section 3 deals with existing modeling approaches for stratified thermal energy storage systems. Our modeling approach and results including a sensitivity analysis are presented in Section 4. Section 5 concludes the paper with a short summary and an outlook on future work.

2 PUMPED THERMAL ENERGY STORAGE SYSTEM

Electricity can be stored both short-term and seasonally with thermal energy storage systems. At the Energie Campus Nürnberg, a PTES system is being set up on a laboratory scale (Steger et al. 2020). The structure of the system is shown in Figure 1. The basic idea of the HP-HS-ORC system is, that surplus electricity is used to operate a HP that exergetically upgrades existing waste heat. This thermal energy can now be stored in a HS until it needs to be converted back to electricity using an ORC. Simulation results from Eppinger et al. (2019) show that power-to-power efficiencies between 50 % and 70 % are achieved with this concept.

Depending on the situation, the system can be flexibly adapted, since the charging and discharging capacity as well as the storage capacity can be increased independently of each other. HP and ORC share a lot of system components as seen in Figure 1 and can therefore be reused, because both engines will not operate at the same time. This not only saves investment costs, but also supports the argument that this PTES is more environmentally friendly than battery systems as shown by (Scharrer et al. 2020).

In general, a HS can be divided into three categories, depending on what happens to the storage medium when heat is supplied or removed. In sensible storage tanks, no phase transition of the storage fluid takes place and only its temperature is changed (Fernandez et al. 2010). If a phase transition takes place, it is

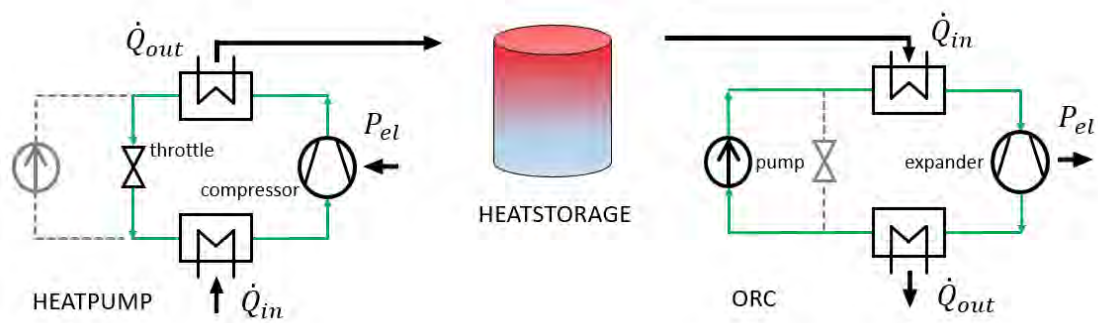


Figure 1: General setup of the HP-HS-ORC system.

considered a latent storage tank (Turchi et al. 2018). Chemical storages represent the last category, where endothermic / exothermic reactions are used to charge / discharge the storage (Zhang et al. 2018).

A sensible hot water storage is a very simple concept but tank design has a huge impact on the stored energy. A perfect separation of hot and cold storage contents, to avoid mixing and therefore destroying exergy, can be achieved with a two-tank setup but might not be economically feasible in different situations. The worst possible design would therefore be a single well-mixed tank (Li et al. 2011). So called thermocline storage systems try to avoid mixing hot and cold storage liquids and make use of their temperature-dependent density (Rosen 2001). Hot water with lower density accumulates in the upper part of the storage tank, while colder water sinks to the bottom. Every layer inside a stratified storage tank is presumed to be evenly distributed horizontally. This temperature distribution over the height of the tank is called a thermocline. Keeping the thermocline and therefore the temperature jump inside the tank as narrow as possible, defines the exergetic efficiency of the tank (Powell and Edgar 2013). To prevent turbulences inside the tank, hot water is leaving or entering the tank at the top, while cold water is taken out or put into the tank at the bottom. Stratification is mainly caused by conduction along the tank walls or by energy extraction/supply and is maintained by operating conditions like flow rate or inlet temperature (Powell and Edgar 2013).

3 STRATIFIED THERMAL ENERGY STORAGE MODELING

Knowledge of the thermoclines that form in a HS is essential for its operation. In order to simulate the HP-HS-ORC system with its storage losses as accurately as needed, a suitable model must be implemented. Depending on the application, different modeling approaches for stratified thermal storages can be found in the literature (Saloux and Candanedo 2019). Mass, energy, and momentum balance equations must be considered in two- and three-dimensional approaches, if a detailed simulation of phenomena within the tank is to be achieved (Savicki et al. 2011; Han et al. 2009). Powell and Edgar (2013) as well as Hafez et al. (2018) show that simpler one-dimensional models with energy or mass balances are sufficient for analyzing the design or operational strategies.

The simulation of the HP-HS-ORC system serves to represent the behavior of the system over one or more years, whereby a one-dimensional representation of the temperature is sufficient. One-dimensional models can be divided into two approaches (Kleinbach et al. 1993). Nodal methods divide the entire volume of the tank into equally sized segments, called nodes (see Figure 2 left). The height of a node stays constant and the temperature is calculated with simple differential equations. In contrast, the plug-flow model considers constant temperatures (see Figure 2 right). The segments assigned to the temperatures vary in size and thus represent a layer over which a constant temperature prevails. Over time, the volume of a layer increases or decreases depending on the current state of the tank.

Plug-flow models are based on geometric considerations and therefore do not require the development of complex differential equations, since the size of the layer depends on flow rates and temperatures (Saloux

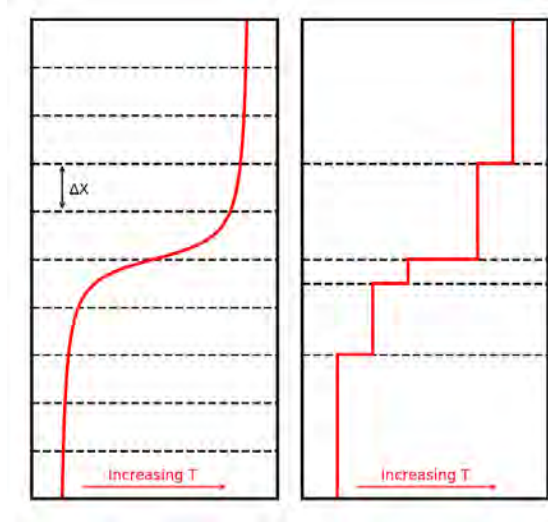


Figure 2: Thermocline Modeling - Node-Method (left) and Plug-Flow (right).

and Candanedo 2019). For example, if the tank is charged and heat energy Q is stored, $Q = mc_p\Delta T$ allows to determine the mass m of storage fluid that is heated. c_p represents the heat capacity of the fluid, whereas ΔT describes the temperature difference.

The temperature difference between the storage and its environment is the driving force for energy losses inside the HS. A heat transfer occurs at the tank wall, which extracts energy from the layers and thus cools it down. According to Roetzel and Spang (2019), this heat flow can be described in the case of a cylindrical storage tank with

$$\dot{Q}_{\text{mantle}} = \frac{2\pi h(T_{\text{layer}} - T_{\text{ambient}})}{\frac{1}{\alpha_{\text{fluid}}r} + \frac{1}{\lambda_{\text{steel}} \ln\left(\frac{r_{\text{steel}}}{r}\right)} + \frac{1}{\lambda_{\text{insulation}} \ln\left(\frac{r_{\text{insulation}}}{r_{\text{steel}}}\right)} + \frac{1}{\alpha_{\text{outside}}r_{\text{insulation}}}}. \quad (1)$$

The thermal conductivity λ and the heat transfer coefficient α , as well as the geometrical quantities such as the different radius r (starting from the middle of the cylinder), do not change over time, which means that the heat flow increases with the height h of the layer. This equation must be considered for all layers in the storage model. Additional heat loss occurs in both the hottest and coldest layers, as they are in contact with the top and bottom wall. Since these are circular plates in a cylinder, the resulting heat flow is also given as

$$\dot{Q}_{\text{top/bottom}} = \frac{r^2 \pi (T_{\text{layer}} - T_{\text{ambient}})}{\frac{1}{\alpha_{\text{fluid}}} + \frac{s_{\text{steel}}}{\lambda_{\text{steel}}} + \frac{s_{\text{insulation}}}{\lambda_{\text{insulation}}} + \frac{1}{\alpha_{\text{outside}}}}. \quad (2)$$

The thickness of the storage wall and insulation are represented with s . In addition to the heat losses due to the outside temperature, there are also heat losses between the individual layers in a stratified storage tank. According to Stephan (2019), a heat flow between the layers is calculated with

$$\dot{Q}_{\text{conduction}} = \frac{r^2 \pi \lambda_{\text{fluid}} (T_{\text{layer}} - T_{\text{colderlayer}})}{\frac{h_{\text{layer}} + h_{\text{colderlayer}}}{2}}. \quad (3)$$

In the denominator, the average height of the two layers is determined to account for an influence of different layer sizes. All heat losses of a layer are added and converted into a mass flow to the colder layer.

In order to apply the model to the HP-HS-ORC system, a few simplifications are made. The inlet ports at the top and bottom of the storage tank are fixed, since it is assumed that water from the coldest existing

layer is always heated to the maximum storage temperature by the HP. At the same time, the flow velocities during charging and discharging are low, which means that mixing of water with different temperatures can be neglected. These assumptions prevent storage losses due to turbulence or temperature inversion. The storage tank itself is a closed system, which means that conservation of mass applies.

4 METHODS

4.1 Simulation Overview

To better compare different simulation approaches, an application on a community level is chosen as the general setup and investigated whether the system can increase the self-sufficiency of a community with PV and reduce the electricity costs for residents. During the day, PV produces electricity, which covers the community's demand. If the electricity production exceeds the demand, this surplus can either be sold or stored via the HP. When the demand can no longer be satisfied during the evening/night, the ORC is put into operation. The electricity generated from stored heat supports the community which means that less electricity has to be purchased. The savings for residents can be determined by the difference between the lost profit from not selling PV electricity (feed-in tariff of 10 ct/kWh) and the savings from not buying electricity from the grid (electricity price of 30 ct/kWh). The proposed PTES is still in development and therefore no reference values of possible savings are available, but the savings for the community serve as a value to compare and evaluate the simulation approaches to each other. The PTES is not meant as a long-term storage system but aims at daily charge and discharge cycles. The calculated savings do not include any investment costs and only refer to the operation of the PTES. A first glimpse at the necessary reduction of investment costs based on the laboratory plant can be found in (Scharrer et al. 2020).

The analysis focuses on a community of 40 houses with a total PV area of 1000 m². The load profiles of houses are from Tjaden et al. (2015) and the electricity produced by the PV is calculated through weather data from Kaspar and Mächel (2016). The HS has a maximum storage capacity of 1000 kWh and is designed as a cylinder with an inner radius of 1.45 m and a height of 4.35 m. The charging temperature of the storage is 120 °C and discharge is 90 °C, while a constant ambient temperature of 10 °C is assumed. The maximum electrical input for the HP is 20 kW and the maximum electrical output of the ORC 10 kW. With this fixed setup, this study specifically evaluates the influence of different model approaches, as well as the sensitivity of different parameters.

4.2 Model Creation and Comparison

Simulations are a cost-effective solution to investigate the behavior of processes or systems. Bazan (2017) develops the "i7-AnyEnergy" software library for AnyLogic 8, which allows users to create models of complex energy systems. The library provides modular components, for example photovoltaics (PV), demand or battery storage systems, to develop holistic simulations. In order to represent the mentioned HP-HS-ORC system, thermal components such as thermal engines or thermal storages have been developed for the library.

Different efficiency curves based on the results of Eppinger et al. (2020) are implemented in the modules of the HP and ORC. Furthermore, start-up and shut-down times as well as power thresholds, below which the HP or ORC can not operate, are taken into account, to better represent the part load behavior. The HS is modeled according to the presented principles. The charging, discharging and ambient temperatures can be freely selected. The number of intermediate layers, which represent the cooldown process, can be selected dynamically and thus allow flexibility in the resolution of the HS.

Dynamic systems can be simulated in different ways. For the HP-HS-ORC system, two models are created using different simulation approaches in order to compare their influence. The aforementioned restrictions and implementations are the same for both simulations, only the methodologies are different. The plug-flow model is applied with only 5 layers in total, to keep the simulation time to a minimum for the comparison. In addition to the charging, discharging and ambient temperature layers (in case the storage

is cooled down completely), additional layers are added at 105 °C and 50 °C to represent intermediate cooldown layers.

As mentioned before, the detailed behavior in thermal storages is simulated in CFD simulations, which is explicitly not done here. Nevertheless, in order to consider the influence of the one-dimensional equations as accurately as possible, the first model is built as SD and considered as baseline for comparison. SD simulations represent complex systems over time using stocks, flows and feedback loops with differential equations to calculate system variables. Heat losses as in equation 1, which are calculated as a function of the layer height, determine the content of stocks via flows, which represent the system (Bala et al. 2017). In SD simulations, the fixed time step for differential equations influences the accuracy of the result. The equations might be continuously calculated, but rely on different results throughout their iteration depending on the size of the timestep. The SD simulation is run with different timesteps and the resulting savings for the community, as well as the necessary computing time to simulate one whole year, are displayed in Table 1.

Table 1: Comparison of simulation types.

Simulation Type	Timestep	Computing Time (s)	Savings (€)
SD	360 ms	~ 1700	1817
SD	1 s	~ 900	1817
SD	30 s	~ 600	1802
SD	1 min	~ 600	1779
DS-FT	1 min	~ 10	1777

Simulating with a timestep of 360 millisecond or 1 second does not change the savings, it only influences the computing time by almost cutting it in half. A timestep of 1 second might be a good enough accuracy for the simulation, but in reality neither the HP nor the ORC can react within a second to changing parameters. As these engines need time to react, a more realistic representation is with a timestep somewhere between several seconds and a minute. Simulations with a 30 second and a 1 minute timestep take about the same time to simulate a whole year, but the savings differ slightly due to the different accuracy of the calculations.

The second implemented methodology is DS-FT. The main difference to SD is, that no continuous calculations are performed to update stocks and flows. The simulation advances in time depending on the set timestep and calculates the results of the equations for each timestep, which allows the simulation to run faster than with SD. For comparison, DS-FT with a timestep of 1 minute is also available in Table 1. The calculated savings with DS-FT change almost not at all, but the difference in computing time is enormous. While the SD simulation with a 1 minute timestep took about 10 minutes, the DS-FT is already finished after 10 seconds.

However, the minimal difference in the savings shows that a more detailed analysis of the simulation curves is necessary. In Figure 3, the curves for the content of the 120 °C layer in liters over 3 days (left) and one month (right) are shown. The simulation period for each analysis is one year, always starting on January 1st and ending on December 31st. The shape of the curves is essentially the same, although there may be small differences in the valleys and peaks. Since these differences are only a few liters and the system has already been used daily for eight months, it is safe to assume that these are only minimal deviations that result from the different calculation methods over time.

In the SD model, 0.4 % more electrical energy is stored than in the DS-FT model, but only 0.3 % more energy discharged. With identical profiles for demand and PV production, this means that the losses within the storage are more detailed in the SD model, since more energy would have been discharged. Among other factors, this slightly lesser performance of DS-FT might also be due to the fact that the comparison was only carried out for models with a total of 5 temperature layers. It is obvious, that a SD simulation with, for example, 100 layers does not make sense, since the simulation runtime for only one single use case

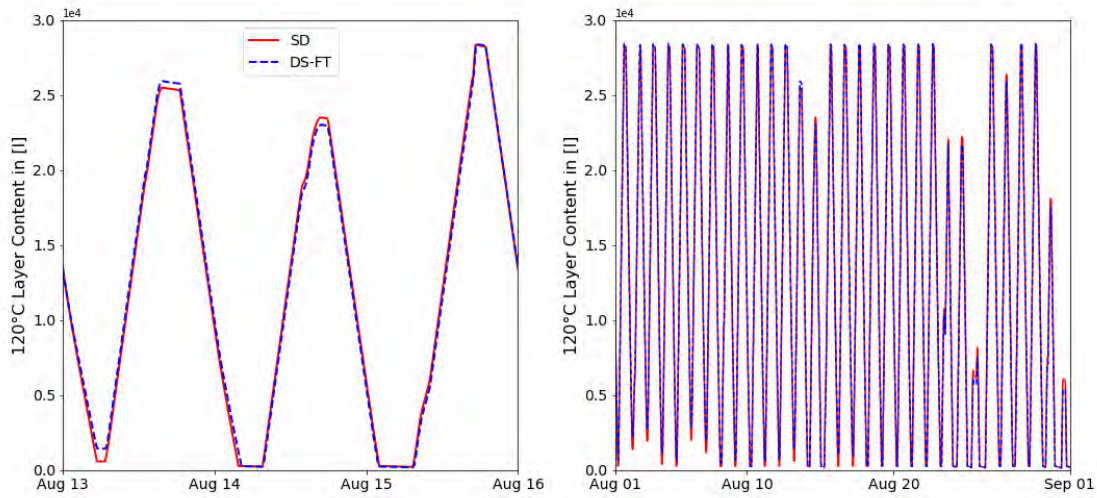


Figure 3: Content of 120 °C Layer over time for both simulation models.

would take a disproportionately long time. In general, all results point to the fact that a DS-FT simulation of the HP-HS-ORC system with 1 minute timestep is sufficient enough to analyze long-term effects.

4.3 Sensitivity Analysis

Simulations offer many advantages in the investigation of PTES, but a wrong choice of simulation parameters can strongly influence the results. Thermal stratification is a complex process in itself, which can be influenced by factors like geometrical structure or operation conditions (Han et al. 2009). To show which material parameters in the underlying model have the biggest influences, we perform a sensitivity analysis with the DS-FT model.

Applying the plug-flow model with a small number of temperature layers is essentially not wrong, as long as the energy or mass balance is maintained. The problem is, that a small number of layers simplifies the cooldown process inside the tank and results are therefore distorted. In order to represent the HS as detailed as possible, the number of layers plays an important role. Figure 4 shows the simulated thermoclines for the cooldown behavior over the height of the tank for a different number of layers. 5 layers represent the previously mentioned 120, 105, 90, 50, and 10 °C layers. 12 layers reflect a resolution of 10 °C temperature steps, while 111 layers reflect 1 °C steps between 120 °C and 10 °C. At the beginning of the cooldown simulation, the storage is always fully charged, the 120 °C layer therefore occupies the entire volume of the tank. An insulation thickness of 20 cm with a thermal conductivity of 0.04 W/mK, $\alpha_{fluid} = 450 \text{ W/m}^2\text{K}$ and $\lambda_{fluid} = 0.55 \text{ W/mK}$ is assumed.

A general look at the four snapshots shows, that all three resolutions depict the cooldown behavior in a largely similar way. On closer inspection however, there are differences which can strongly affect the operation. After just one day, differences can be seen in the bottom of the tank. The 5- and 12-layer models indicate that a temperature of 120 °C still prevails for the most part in the storage tank, whereas the 111-layer model shows that the 120 °C layer only fills the storage tank for about 50 %. It can also be seen that, depending on the resolution, the models indicate that after one week and also after one month the 120 °C layer still exists. However, in the 111-layer model, the maximum temperature in the tank has already dropped to 117 °C after one week. After two months, the maximum temperature in the storage tank has already fallen below the discharge temperature for 111 layers, while the other two resolutions are still above it.

Ideally, the storage should not remain unused for weeks or months when it is designed for a daily operation. In reality, depending on the weather conditions, the system may not be operated for several days.

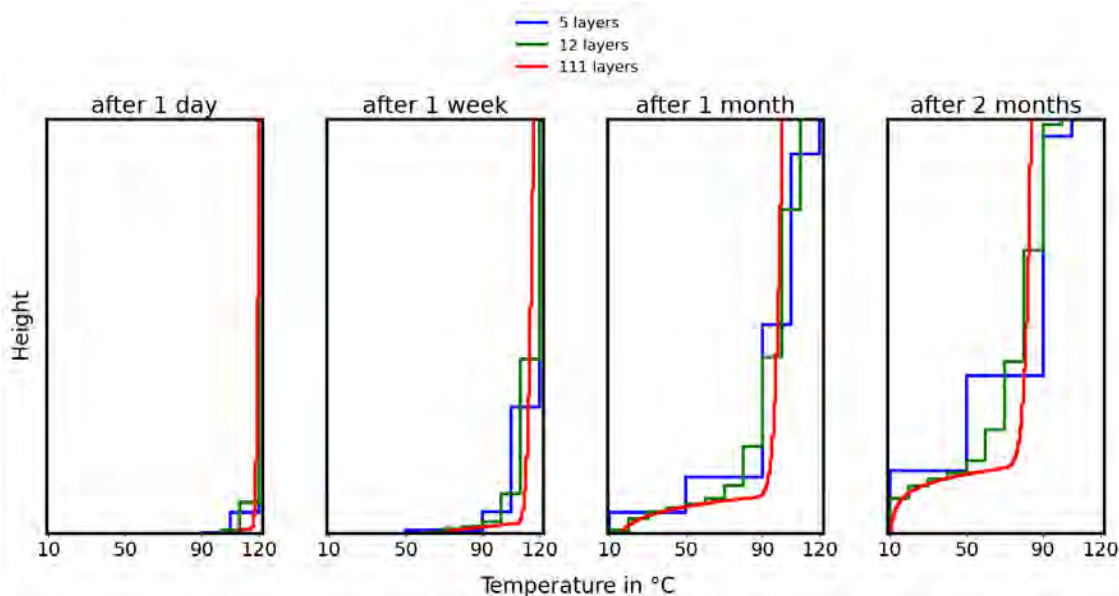


Figure 4: Cooldown behaviour over time with different numbers of layers considered.

Therefore, a more detailed cooling behavior is important, as this can influence the operation. If surplus electricity is available, the HP is operated and always heats the coldest available layer to the maximum temperature of 120 °C. However, the HP has limits up to which temperature it can operate. It is designed for a temperature of 90 °C but can also go into a kind of "overdrive" mode. Temperatures below 90 °C are no problem, but there is an upper limit for temperatures above 90 °C. Depending on the HP, this temperature varies and can affect the PTES in the long run. For the thermoclines in regular operation shown in Figure 5, the maximum overdrive temperature of the HP is set to 105 °C.

A day in summer is shown on which it would theoretically be possible to operate the HP all day and thus store energy. If we first follow the course of the 5-layer model, the desired behavior is clearly visible. At 6 a.m. the storage tank is still charged to about 25 %, afterwards charged and full at 2 p.m. With this resolution the only layer between charging and discharging is a 105 °C layer, which corresponds to the maximum possible overdrive temperature for the HP. The second model with 12 layers shows a similar behavior at first, but already at 10 a.m. no further charging is possible. The 100 °C layer can still be heated to 120 °C in overdrive, but this is no longer possible for the 110 °C layer. In this case, so-called "dead layers" take up almost half of the storage volume, which therefore reduce the effective storage capacity of the system by half.

An extreme case can be seen with the 111-layer model. Already at the beginning, the minimum temperature in the tank is above 105 °C, which means that no more energy can be stored during the entire day. Since the storage system has already been in operation for several months at this point, the finer resolution of the temperature layers means that the dead layers have grown over time to such an extent, that they fill the entire storage. Operation of the storage system has thus become impossible. To prevent this, the maximum temperature of the ORC can be reduced, in order to draw energy from colder layers as well.

Not only the number of layers can have an influence on the simulation result, but also the selected material properties in equations (1) to (3) affect the heat transfer and thus the losses of the system. For the heat transfer coefficient α and the thermal conductivity λ of the storage fluid, as well as the thermal conductivity and the thickness of the insulation, a sensitivity analysis is performed. For this analysis, the 12 layer model was removed, to focus on the extreme differences between a high and low layer resolution. The results are shown in Figure 6.

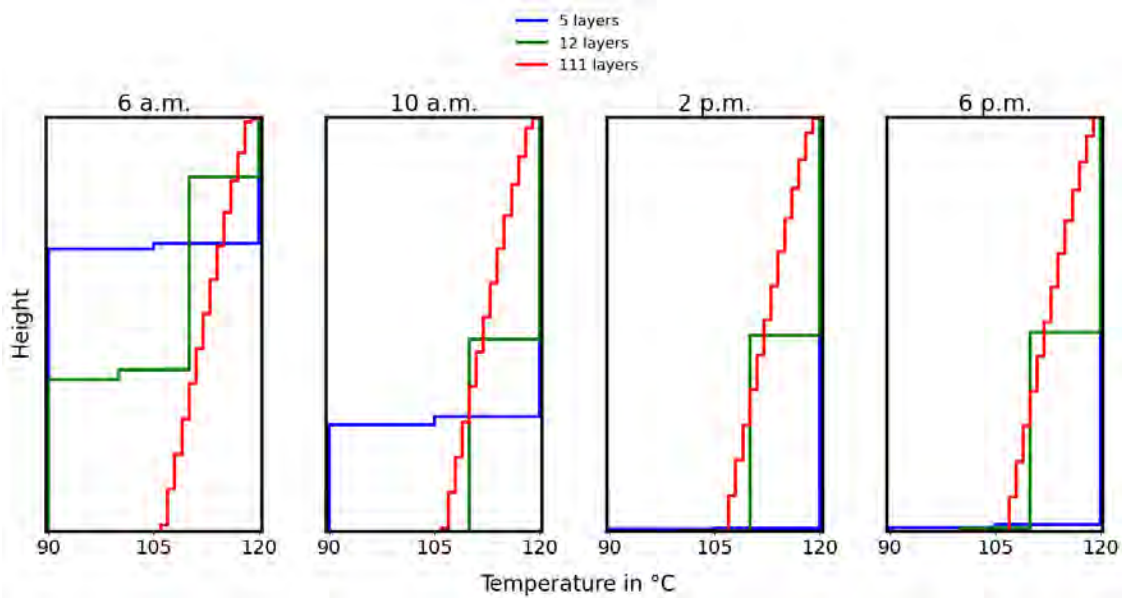


Figure 5: Development of deadlayers in the storage with increasing number of layers considered.

In the case of heat transfer by free convection, α can normally be calculated from the Nusselt number $Nu = \frac{\alpha L}{\lambda}$. L is the so-called characteristic length and represents the primary dimension of the flow. Defining this length for a layer is extremely complex with decreasing layer height in the tank. For the simulation, the value of α is therefore varied between 10 and 1000 in small steps. The detailed model with more layers predicts about 200 € less savings than the simple model, but also no dependence on α can be seen. An elaborate determination of α can thus be neglected, since simulations of well above a value of 1000 did not yield any different results.

According to Kretzschmar and Wagner (2019), the value of thermal conductivity of water is about 0.6, so the analysis is done in a range from 0.5 to 0.7. Again, the influence of the number of layers can be seen, but a change in thermal conductivity changes the result only a little bit. In reality, both α and λ are temperature dependent, but differ only slightly for small temperature differences. Since the temperatures in the storage under normal operating conditions are in a temperature range of approx. 30 °C, the temperature dependence of α and λ is neglected.

Fantucci et al. (2015) analyze insulation materials for thermal energy storages. The commonly used Mineral Wool has a value of 0.04, but materials with as low as 0.005 are available. A sensitivity analysis in the range of 0 to 0.05 shows, that the insulation material alone can make a difference of up to 300 € in savings for the community. Another important parameter is the thickness of the insulation around the storage. No insulation at all results in tremendous losses for the community, as the stored energy is simply lost too quickly to the environment. An insulation of a few cm is already enough to produce some savings for the community, even though they are relatively small. Varying the thickness between 5 and 25 cm has the biggest changes in the savings, whereas anything bigger than 25 cm has only a small influence.

5 CONCLUSION

For the novel storage system, which is a combination of a HP, HS and ORC, two simulations were built and compared. The SD model and the DS-FT model deliver approximately the same results depending on the timestep, but differ greatly in the necessary computing time. The integrated plug-flow model gives different results depending on how detailed the HS is represented. A variation of the total number of considered layers shows that a too coarse resolution of the storage distorts the possible savings. The sensitivity analysis

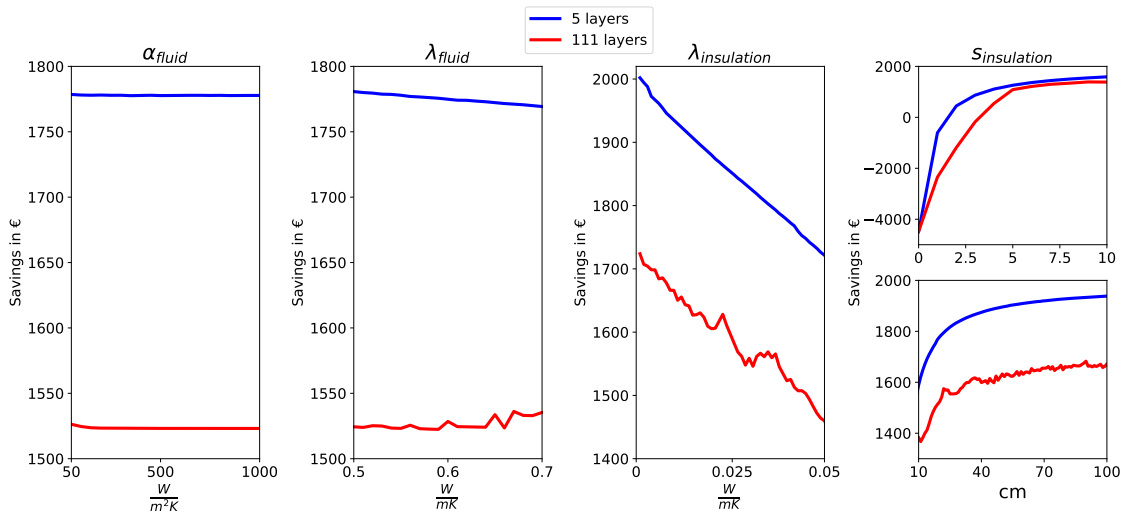


Figure 6: Sensitivity analysis for different material parameters that influence the heat equations.

showed that the influence of material properties of the storage fluid can be neglected, since the insulation is the determining factor. Both the thickness applied and the insulation material itself have the greatest influence on possible savings with the system.

The number of layers has also shown that so-called dead layers block the storage and need to be eliminated. For future research it is planned to further investigate this phenomenon combined with which resolution of the layers is sufficient enough. An international application will also be investigated, as the weather data used so far is related to Germany.

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