State of charge estimation using regression models in a novel photovoltaic thermal storage system with macro-encapsulated phase change material

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Abstract

Photovoltaic heat pump systems (PV-WP Systems) are becoming a standard for low-carbon building heating. In this framework, this work aims to optimize photovoltaic (PV) systems coupled with heat pumps (WP) by integrating a novel high-density thermal storage unit to address the mismatch between solar energy production and heating demands. Through a pilot setup featuring an 800 L storage tank equipped with multiple sensors, comprehensive data was collected over the 2022/2023 heating seasons in Switzerland. This dataset formed the base for the development and validation of state of charge (SoC) estimation models for latent thermal energy storage (LTES) systems. Challenges in defining SoC due to temperature differentials within the storage were addressed using both energy balance and machine learning approaches. The machine learning approach, leveraging regression techniques and ensemble algorithms, proved particularly effective, achieving a prediction accuracy with a deviation of less than 2.06 kWh for 95% of data points with a total storage capacity of 45 kWh. This approach enabled adaptive SoC predictions, enhancing the operational efficiency of the storage system without additional hardware. Further work will focus on redefining of these models to improve accuracy, explore scalability across different system configurations, and reduce computational demands to facilitate integration into existing energy management systems. This research indicates significant potential for advancing thermal energy storage technology in PV-WP systems, contributing to more sustainable building heating solutions.

Keywords: Photovoltaic systems, thermal energy storage, state of charge, latent heat, machine learning, energy efficiency

10.18086/eurosun.2024.06.06 Available at http://proceedings.ises.org

1. Introduction

Thermal energy storage systems (TES) are key-enabling technologies when it comes to enhancing the efficiency of renewable energy systems, particularly photovoltaic (PV) systems in building applications (Dong and Xu, 2023). TES systems work by storing excess thermal energy generated during periods of low demand and releasing it when energy demand is high, thereby balancing supply and demand. A traditional way of storing heat for the residential and commercial building sector has been hot water storage tanks, which are currently used in conventional building systems in Switzerland and Europe (Renz, 2020). An upcoming approach to storing large amounts of thermal energy is phase change materials (PCM), where the phase change of a material is utilized to absorb or release heat at a constant temperature. As a result, a larger amount of energy is stored with the same storage volume compared to conventional water storage tanks. There are different approaches to implementing PCM into heating systems to facilitate the heat exchange between water and PCM. A popular approach is through the macro-encapsulation of the PCM (Vérez *et al.*, 2021), where existing boiler systems in buildings are filled with capsules to increase the energy density in the storage tank and the building's consumption is increased (Jaradat *et al.*, 2024).

In this work, a new type of pilot system in the form of a hot water buffer storage is developed and integrated into the heating system of a single-family home. The buffer storage tank of the heating system is filled with PCM45 capsules from COWA Thermal Solutions (Maranda and Waser, 2024). These are incorporated into the storage tank as a bulk material, where the entire system is analyzed over two full heating periods (2022-2023). For comparison purposes, the 2022 heating period without the use of COWA capsules and the 2023 heating period with the use of the capsules.

One of the challenges in operating a storage tank with PCM is determining the state of charge (SoC). Unlike with water storage tanks (Kachalla and Ghiaus, 2024; Ritchie and Engelbrecht, 2022; Nemitallah *et al.*, 2023), in latent thermal energy storage (LTES) systems with encapsulated PCM the SoC cannot be determined directly from the pre-installed measurement equipment, as the progress of the phase change inside the capsules is unknown and takes place at a constant temperature. For LTES systems different approaches using additional equipment have been discussed in the literature. Energy balance approaches use an energy meter at the inlet and the outlet of the storage to constantly monitor the SoC and have been successfully used for systems with finned heat exchangers (HEX) (Zsembinszki *et al.*, 2020). However, the literature states that a reference state must be approached at certain intervals during the determination process to prevent the result from drifting. To overcome the challenge of drift, it has been shown that by inserting a small number of temperature sensors into the PCM and using mathematical models, the SoC, the state of the PCM and the temperature distribution can be reliably determined (Barz *et al.*, 2018). Another approach is to use regression models, which are used to fit a model that best describes the relationship between one or more predictor variables and a response variable (Maulud and Abdulazeez, 2020). The advantage is that once the model has been trained, no further measurement equipment is required and it can be applied directly to new systems. Bastida *et al.*, 2024 successfully demonstrated the determination of the SoC of a LTES module with internal counter-flow HEX by using a regression model. The model, built using MATLAB's deep learning toolbox (Hudson *et al.*, 2024) requires the current mass flow and temperature at the inlet of the storage tank and the past SoC. Jančík *et al.*, 2021 developed a simulation model using the mean liquid phase fraction method to determine the SoC of a LTES system filled with cylindrical capsules. Accurate results could be achieved using only the temperature and mass flow rate at the inlet of the LTES as input.

In residential buildings there is usually pre-installed measurement equipment available to monitor temperature and mass flow on the primary (charge) side. As the additional installation of measurement equipment on the secondary (discharge) side is a challenge, the aim of this work is to train a regression model that allows the SoC to be determined with the existing measurement equipment.

2. Filler Capsules and PCM Material

Capsules developed by COWA Thermal Solutions are used for the LTES system (Figure 1). The capsules achieve an approximate packing density of 62% in cylindrical boilers. The outer shell is made of polyethylene (PE) and each is filled with 0.109 L of PCM45 from COWA. The PCM45 is based on a sodium acetate mixture (Wang *et al.*, 2022). Figure 2 illustrates the thermal behavior of the PCM45 during charging and discharging, as determined by differential scanning calorimetry (DSC) (Fatahi and Claverie, 2022). The PCM45 has an approximate heat capacity when discharging of 190J/g in the temperature range of 47°C to 44°C.

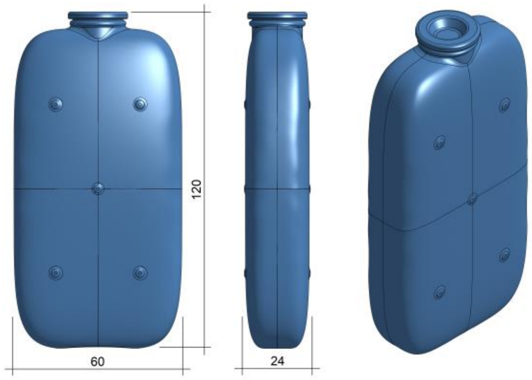

Figure 1: Geometry of the COWA Capsule, dimensions in millimeters.

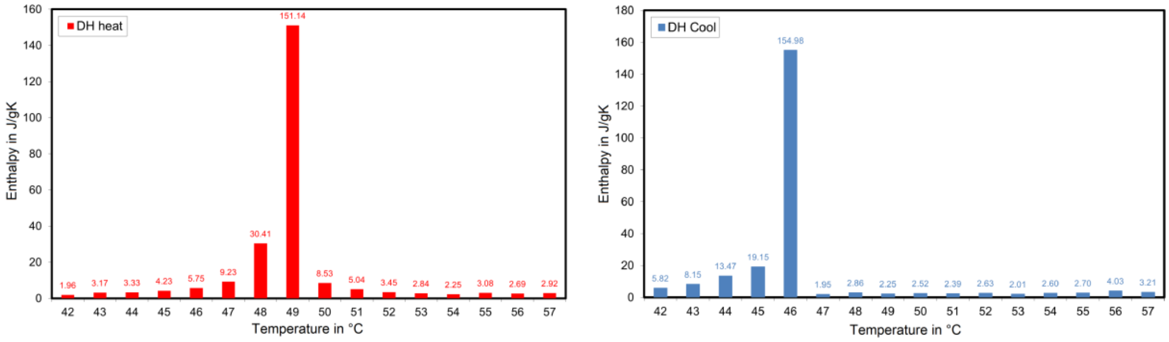

Figure 2: Charging (left) and discharging (right) behavior of the PCM45 measured by DSC.

3. Pilot Setup

The pilot setup is located in a single-family house with a rental apartment located on a sunny terrace in Pany (GR) in Switzerland (Figure 3) at an altitude of 1,178 meters. The house, built in 1988, has a photovoltaic (PV) system with 26 west-facing and 24 east-facing modules, covering a total area of 84.4 m² and providing 17 kWp of power. Surplus solar energy is used to charge a 7.7 kWh electrical battery to support off-grid operation. The heating system comprises an air-to-water heat pump (Oertli LSI 140 SHW-SG) with a thermal output of 5.7 - 15.8 kW, connected to an 800 L buffer tank and a 500 L hot water tank, both fitted with heating elements. The buffer tank is filled with 3550 COWA PCM45 Capsules (Figure 4) Key indicators of the pilot are:

- PV system: 17 kWp, 84.4 m², 26 modules west, 24 modules east.
- Estimated heat demand: 100 kWh/m²/year, energy reference area: 200 m².
- Electricity consumption: 4000 kWh/year.
- Hot water consumption: 180 Liters/day, heated from 16°C to 55°C.
- Heat pump efficiency with a seasonal performance factor (SPF) of 3.2.
- Heat pump output: 5.7 kWth to 15.8 kWth.
- Buffer tank (800 Liters) operating between 40°C and 52°C (up to 60°C with heating rod), providing a capacity of 11.2 kWh to 14 kWh (39.1 kWh with 3550 COWA Capsules, without heating rod)

Figure 3: Pilot building in Pany (GR), Switzerland.

Figure 4: Left 800L buffer boiler. Right: Inside-view of the buffer boiler 30% filled with COWA Capsules.

Figure 5 shows the comparison of the buffer boiler in heating period 1 (HP1) without the capsules and in heating period 2 (HP2) including the capsules. Two days were selected with comparable PV production, outside temperatures and heating requirements. By installing the capsules, it was possible to increase the building's heating self-sufficiency from 26% to 41.4% and the PV yield from 6679.4 kWh to 11050.8 kWh.

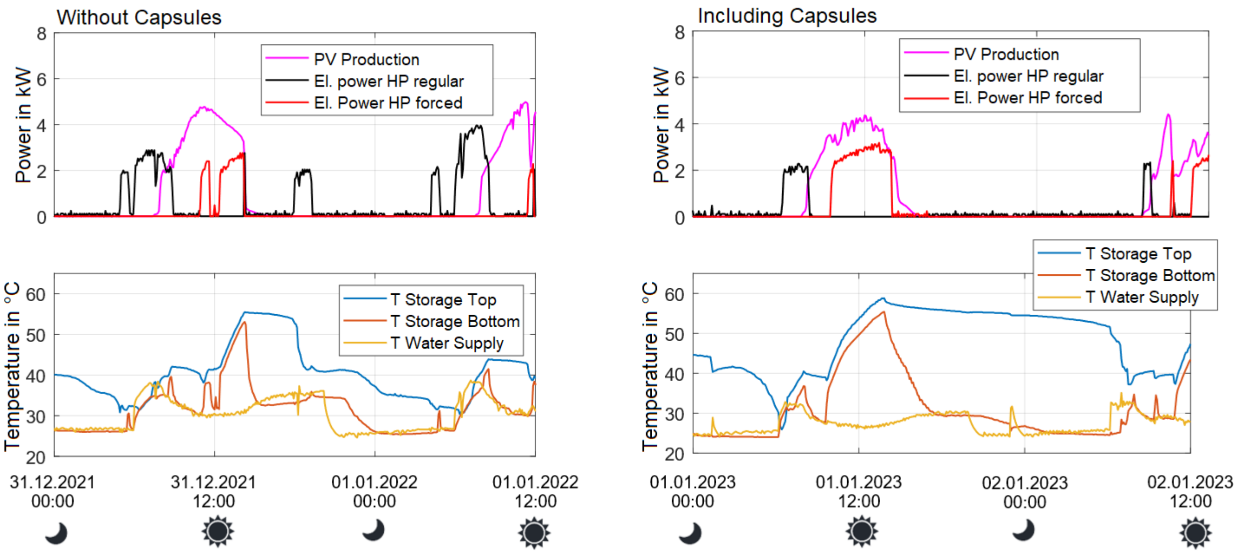

Figure 5: Comparison of two days of the HP1 and HP2 with similar PV production, heating loads and similar average outside temperature. Left: HP1 (2022) without capsules; Right: HP2 (2023) with COWA capsules.

4. State of Charge Determination

To overcome the limitations of direct measurements, a machine learning model was developed using MATLAB's Deep Learning Toolbox (Hudson *et al.*, 2024). The ensemble learning model, coupled with a Bayesian optimizer that varies the hyperparameters for each iteration, is used to estimate the SoC based on indirect measurements such as inlet and outlet temperatures and flow rates from the heat pump. The model was trained using data collected from the pilot installation (Figure 6), which included different operating scenarios over a heating season. The use of ensemble learning algorithms improved the model's ability to generalize across different operating conditions, significantly reducing prediction errors.

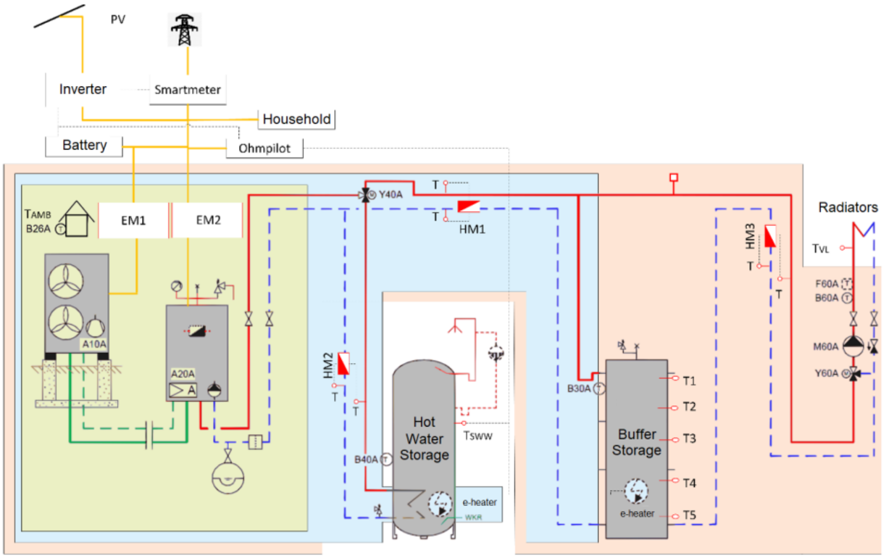

Figure 6: Diagram of the pilot plant with measuring equipment for determining the training data.

The experimental data was collected from COWA's pilot installation in Pany during the 2022/2023 heating season. Measurements were taken using two energy meters positioned at the inlet and outlet of the LTES, allowing for the calculation of an approximate SoC via an energy balance approach. Initially, storage losses were estimated based on the mean temperature of the LTES, a constant external temperature, and the thermal resistance of the insulation.
Despite subtracting the estimated losses from the measured energy difference between the inlet and outlet, the resulting SoC values exhibited an increasing trend, indicating additional unaccounted losses (Figure 7, blue curve). To address this, a baseline correction was applied by smoothing the energy balance curve using a 24-hour moving average, resulting in the adjusted baseline (Figure 7, red curve).

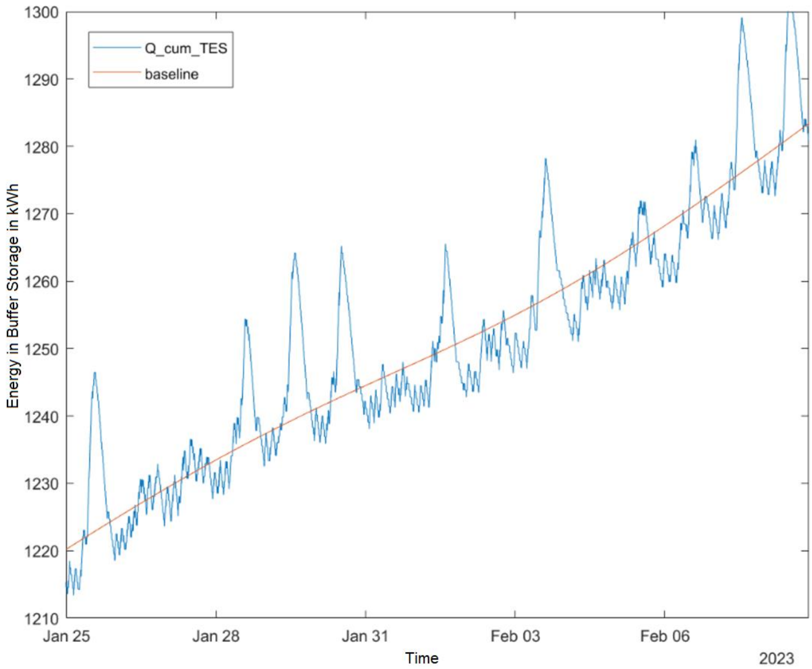

Figure 7: Trend of energy in buffer storage and baseline correction.

To mitigate errors introduced by averaging SoC over several days, four distinct periods of 3-4 days each were manually selected. Since only the change in accumulated energy was measured, the SoC values needed appropriate offsets relative to a reference state. Due to the LTES not reaching the reference state in two of the four periods, some uncertainty in the offsets was inevitable.
The dataset for model training and testing was expanded by incorporating storage history information. Using logical criteria, the end times of charging cycles were identified, leading to the creation of two additional variables: The temperature inside the storage tank at the end of the last charging cycle, and the time elapsed since the last charging cycle ended. These variables are viable for use in practical applications as well.

The complete dataset comprised the following variables:

True Response:

- Thermal energy stored in the LTES.

Predictors:

- Temperature measured at a fixed point inside the LTES.
- Mass flow of the heat pump.
- LTES charging inlet and outlet temperatures.
- Temperature inside the LTES at the end of the last charging cycle.
- Time elapsed since the end of the last charging cycle.

5. Results

The results (see Figure 8) demonstrate that the machine learning approach not only predicts the SoC with a high degree of accuracy but also adapts to various system behaviors without the need for additional hardware. The model achieved a prediction deviation of less than 2.06 kWh for 95% of the data points, with a root mean square error close to 1 kWh. These results indicate a promising direction for optimizing the management of thermal energy storage systems.
Furthermore, the integration of machine learning into the system's operational framework can allow real-time adjustments and optimizations, enhancing the overall efficiency of the thermal storage system. The increased autonomy from improved SoC predictions can enable more effective use of solar energy, reducing reliance on external energy sources and optimizing operational costs.

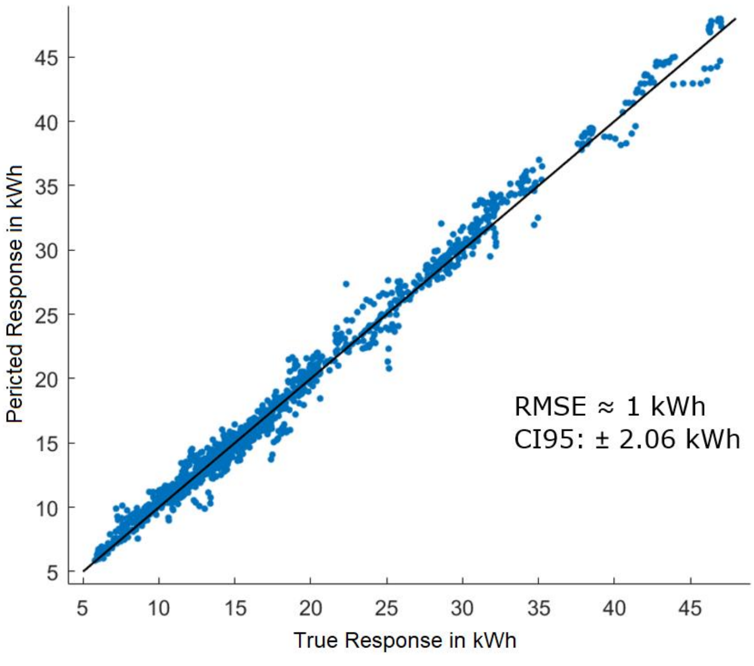

Figure 8: Comparison of Predicted Response and True Response of the SoC of the LTES using ¼ of the datapoints of HP2 as separated test data.

6. Conclusions

The model successfully demonstrated the potential of integrating advanced state of charge estimation techniques with photovoltaic thermal storage systems to enhance their efficiency and autonomy. The innovative use of machine learning for SoC estimation has proven to be a viable solution to the challenges traditionally associated with thermal energy storage systems, offering significant improvements in energy management and system performance. The work presented leads to the following conclusions:

- Improved Energy Efficiency: Incorporating PCM capsules into the thermal storage system significantly enhances the energy density and storage capacity, as demonstrated by the increased heating self-sufficiency from 26% to 41.4%.
- Enhanced PV Utilization: The integration of PCM capsules also improves photovoltaic yield, increasing from 6679.4 kWh to 11050.8 kWh, illustrating the potential for better utilization of solar energy in residential settings.
- Machine Learning for SoC Estimation: The developed machine learning model, leveraging MATLAB's Deep Learning Toolbox, effectively predicts the SoC with high accuracy, achieving a prediction deviation of less than 2.06 kWh for 95% of data points. Reducing the error in determining the true state of charge in the training data can potentially lead to an even greater reduction in the error in the actual prediction.
- Minimized Hardware Requirements: The model provides accurate SoC predictions using existing measurement equipment, avoiding the need for additional costly and complex sensors, making it a practical solution for residential applications.
- Scalability and Applicability: The methodology and findings from this study can be scaled and applied to similar residential setups, potentially leading to widespread improvements in energy efficiency and renewable energy utilization in buildings. However, it is very likely that a different model will need to be trained for different configurations of the system.

Future efforts will focus on refining the estimation models to further enhance their accuracy and reliability. Additional research will explore the scalability of the developed techniques to larger systems and different configurations, potentially broadening their applicability across various residential and commercial settings. Moreover, ongoing efforts will aim to reduce the computational demands of the models to facilitate their integration into existing energy management systems, making sustainable technology more accessible and practical for widespread adoption.

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