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Sensitivity Analysis of One-Phase and Two-Phase 1D PBTES Models to Thermal Properties Modeling of Copper Slag

Summary

This study investigates the sensitivity of copper slag's thermal properties in a packed-bed thermal energy storage (PBTES) system, focusing on two 1-dimensional models: a one-phase and a two-phase model. Thermal conductivity (k) and specific heat capacity (c_p) were experimentally measured, with temperature-dependent variations considered. Four cases were analyzed, alternating constant and temperature-dependent properties. Key performance indicators (KPIs) such as stored energy, response time, and round-trip efficiency were evaluated. The results show that stored energy is highly sensitive to c_p, with a ~12% reduction when using temperature-dependent values. Thermal conductivity had minimal impact. The findings emphasize the importance of accurate c_p modeling for reliable PBTES system design, particularly for solar energy applications.

Keywords: Thermophysical Properties Modeling, Packed-Bed TES, TES Simulation.

1. Introduction

Packed-bed thermal energy storage (PBTES) systems provide a cost-effective solution for high-temperature storage in applications like Concentrated Solar Power. Using industrial waste materials, such as copper slag—a byproduct of copper smelting—can significantly lower costs due to its favorable thermophysical properties, including high heat capacity and stability at high temperatures (Segovia V., et al. 2025). In a PBTES system, heat is stored by circulating a hot fluid (e.g., air) through a bed of solid particles, charging the bed thermally, and releasing the stored heat during discharge. Accurate modeling of these systems is essential for design and optimization. Two common one-dimensional modeling approaches are: the one-phase model, which assumes local thermal equilibrium with a single energy equation, and the two-phase model, which allows for distinct temperatures for solid and fluid using dual energy equations. This study analyzes how the choice of modeling approach and thermal property assumptions affects performance predictions for a copper slag packed-bed TES. We compare one-phase and two-phase 1D simulations under four scenarios regarding thermal conductivity (k) and specific heat capacity (c_p), considering either constant or temperature-dependent values. Key performance indicators (KPIs) such as stored energy, thermal response time, and round-trip efficiency are assessed to evaluate the impact of model complexity and property variability on system performance.

2. Sensitivity analysis of PBTES models

2.1. Modelling of thermophysical properties

The specific heat capacity $c_p(T)$ was measured via differential scanning calorimetry (DSC) from 100 °C to 450 °C, and the thermal conductivity $k(T)$ was measured at three temperature points (room temperature ~25 °C, 60 °C, and 120 °C) using a transient line source method. The copper slag's specific heat showed a clear increase while its thermal conductivity exhibited a slight decrease (extrapolated from about 1.67 [W/m·K] at 100 °C down to ~1.1 [W/m·K] at 450 °C), as can be seen in Figure 1. This corresponds to a roughly 33% variation in k over the 100–450 °C range, while c_p shows a 20% variation. For cases assuming constant properties, mean values were used, representing the averages over the operating temperature range. In contrast, for temperature-dependent cases, linear fitting was applied to k data, while polynomial fitting was utilized for c_p.

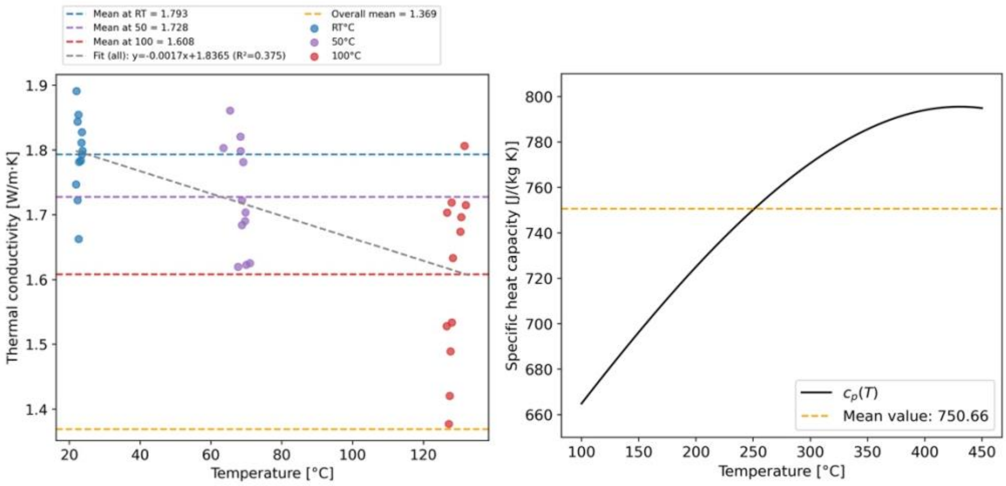

Fig. 1: Experimental thermal conductivity (left) and specific heat capacity (right) of copper slag as functions of temperature (100 °C to 450 °C). The orange dashed lines denote the respective mean values used for constant-property simulations.

2.2. PBTES simulation and Key Performance Indicators analysis

The PBTES system is modeled using 1D simulations of a 67.4 m^3 volume tank (aspect ratio of 1) in two forms: one-phase and two-phase. In the two-phase model, separate energy balance equations were solved for the solid (slag particles) and the fluid (air), with a convective heat transfer coefficient coupling them, as described by Calderón-Vásquez, I., and Cardemil, J.M. (2024). In the one-phase model, a single combined energy equation was used, considering that the thermal front advancement of the solid and fluid is the same as presented in Calderón-Vásquez, I. et al. (2024). All simulations were run considering air entering at 450 °C during charge, while discharge considered air entering at 100 °C. To examine the influence of thermophysical property assumptions, four cases were considered:

- Case 1: Constant k, constant c_p (both properties fixed at their mean values).
- Case 2: Constant k, temperature-dependent $c_p(T)$.
- Case 3: Temperature-dependent $k(T)$, constant c_p.
- Case 4: Temperature-dependent $k(T)$, temperature-dependent $c_p(T)$.

Each case was simulated using both one-phase and two-phase model formulations, resulting in a total of eight results. The following key performance indicators (KPIs) were estimated from each simulation: (1) the energy stored in the packed bed at 1 hour and 2 hours of charging; (2) response time (t_r), which is the duration needed for the outlet fluid temperature to reach, in this case, 200°C; and (3) round-trip efficiency (η_{rt}). As can be seen the KPIs in Table 1, the one-phase model showed higher energy stored with the two-phase model for overall cases. In the first hour of charging, the one-phase model predicted about 8-9% higher stored energy compared to the two-phase model, because the one-phase assumption of instantaneous solid-fluid thermal equilibrium leads to a faster initial heat uptake by the solid. The one-phase model also yielded a slightly shorter response time (t_r ~2.08 h) than the two-phase model (t_r ~2.18 h, ~5% longer), again reflecting the delayed heat transfer in the two-phase approach. Interestingly, the $\boldsymbol{\eta_{rt}}$ of the system was very similar in both models with the two-phase model giving a marginally higher $\boldsymbol{\eta_{rt}}$ (about 0.81–0.82) to that of the one-phase model (0.79–0.80). This small efficiency difference suggests that while the one-phase model slightly overestimates the speed and amount of heat stored initially, it still captures the overall energy balance of the full charge/discharge cycle.

Tab. 1: KPIs results for the PBTES model simulation for each case of thermophysical properties modeling combination.

	Case 1		Case 2		Case 3		Case 4	
KPI	one-phase	two-phase	one-phase	two-phase	one-phase	two-phase	one-phase	two-phase
E_{stored} at 1h (kWh/m^3)	87.21	79.60	76.66	70.49	86.81	79.97	76.42	70.84
E_{stored} at 2h (kWh/m^3)	167.14	160.81	144.87	139.26	166.44	161.04	144.41	139.57
t_r (h)	2.08	2.18	2.15	2.25	2.08	2.17	2.15	2.24
$\boldsymbol{\eta_{rt}}$	0.8047	0.8184	0.7990	0.8123	0.7976	0.8184	0.7920	0.8124

When incorporating temperature-dependent vs. constant thermophysical properties, it is found that variations in c_p have a much more pronounced impact on performance than variations in k as can be seen in Figure 2. Using a temperature-dependent specific heat $c_p(T)$ of copper slag led to significantly lower predicted stored energy at a given time. In the simulations, switching from constant c_p to $c_p(T)$ (Cases 1→2 for constant k, or Cases 3→4 for variable k) reduced the stored energy after 1 hour by roughly 12% in both the one-phase and two-phase models. A similar drop was observed for E_{stored} at 2 hours. In contrast, using temperature-dependent thermal conductivity $k(T)$ in place of a constant k had a negligible effect on the results – the changes in E_{stored} were less than 1% in all cases. The thermal response time t_r was slightly influenced by $c_p(T)$, increasing by about 3% when the variable specific heat was used (i.e. the bed heated a bit more slowly due to the higher heat capacity at elevated temperatures). Again, changing k alone produced virtually no change in t_r (<1% difference). The round-trip efficiency of the storage was largely insensitive to either property variation: incorporating $c_p(T)$ lowered η_{rt} by on the order of 0.5–1%, while different k assumptions changed efficiency by under 0.1%. In all scenarios, η_{rt} remained around 80%.

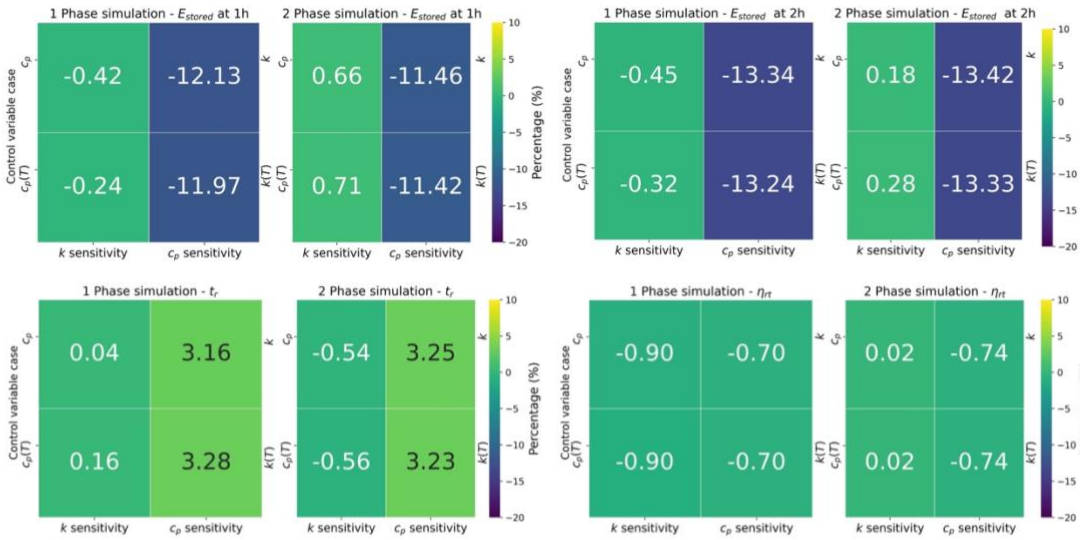

Fig. 2: Sensitivity of performance metrics to thermophysical property variations in one-phase and two-phase simulations.

3. Conclusions

Through 1D simulations, it is found that a simple one-phase model can effectively approximate the performance of a more complex two-phase model, particularly during longer charge times. However, the one-phase model overestimates short-term energy uptake by about 9% in the first hour and slightly underestimates response time and efficiency. These results highlight the importance of accurately characterizing specific heat capacity in the design of PBTES for solar applications. Ignoring the temperature dependence of c_p can lead to a 12% overestimation of stored energy, potentially resulting in undersized designs or ineffective charging strategies. Using an average thermal conductivity (k) is a reasonable simplification that maintains accuracy. In summary, variations in material properties, especially $c_p(T)$, significantly affect packed-bed thermal energy storage behavior. While a one-phase model with constant properties is convenient, incorporating the material's actual heat capacity curve is essential for reliable design. These insights will aid in developing effective modeling strategies for packed-bed thermal energy storage systems using copper slag, enhancing their application in sustainable energy storage, such as solar thermal energy applications.

4. References

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