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Optimizing Packed Bed Latent Heat Storage Systems: A Machine Learning and Metaheuristic Approach

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ABSTRACT

With the increase in industrial carbon emissions, the efficient recovery of waste heat has become imperative. Thermal Energy Storage (TES) systems utilizing Phase Change Materials (PCMs) present a viable solution, with Packed Bed Latent Heat Storage Systems (PBLHS) being particularly noted for their effectiveness. However, current PBLHS designs face challenges in terms of accuracy and adaptability. This research introduces a Machine Learning (ML) approach to overcome these obstacles. By leveraging data from a validated Computational Fluid Dynamics (CFD) model, a deep ML model was developed and trained, achieving an R^2 value of 0.975 and a MAPE of less than 9.14%. The Harmony Search algorithm emerged as the most effective optimization technique, which, after refinement, enhanced design efficiency by over 40%. The optimized model improved existing experimental setups by up to 84%. This study underscores the potential of ML in advancing TES system designs for efficient waste heat recovery.

Keywords: Waste heat recovery, Thermal Energy Storage, Phase Change Materials, Packed Bed Latent Heat Storage Systems, Machine Learning, Harmony Search.

NONMENCLATURE

Abbreviations	
TES	Thermal Energy Storage
WHR	Waste Heat Recovery
PBLHS	Packed Bed Latent Heat Storage
CPCM	Composite Phase Change Material
LHS	Latin Hypercube Sampling
CFD	Computational Fluid Dynamics
ML	Machine Learning
GA	Genetic Algorithm
ACO	Ant Colony Optimization
HS	Harmony Search
WDO	Wind Driven Optimization
Symbols	
t_charging	Charging Time – [h]
t_discharging	Discharge Time – [h]
T0	Initial Temperature – [K or °C]
T_ext	External Temperature – [K or °C]
T_m1	Melting Point of PCM1 – [K or °C]
T_m2	Melting Point of PCM2 – [K or °C]
T_m3	Melting Point of PCM3 – [K or °C]
T_u	Upstream Temperature – [K or °C]
s_ins	Insulation Thickness – [m]
L1	Length of Storage Tank 1 – [m]
L2	Length of Storage Tank 2 – [m]
L3	Length of Storage Tank 3 – [m]
u	Fluid Velocity – [m/s]
V_in	Inlet Flow Rate – [m^3/s]
ds	Storage Tank Diameter – [m]
Q_charge	Heat Stored – [J]
Q_discharge	Heat Extracted – [J]
dp	Diameter of spherical CPCMs in the packed bed [m]

1. INTRODUCTION

Core industries are essential to the global economy but encounter significant challenges in achieving sustainable decarbonization [1]. The European Union aims to cut industrial carbon emissions by 42% by 2030 [1]. Currently, industries account for 27% of total energy consumption and contribute 30% of heat-related CO2 emissions in the EU [2]. A substantial portion of this energy (70%) is dedicated to thermal processes, representing 18.9% of the EU's total energy demand [3]. Approximately 400 TWh/year of high-quality waste heat is generated, highlighting substantial potential for recovery and reuse [1].

Waste heat recovery (WHR) is particularly crucial for energy-intensive industries [1]. Thermal Energy Storage

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(TES) systems bridge the gap between waste heat generation and consumption, optimizing process parameters and reducing losses during startups and partial operations more cost-effectively than other methods such as Organic Rankine Cycle (ORC) systems or Thermoelectric Generators (TEGs) [1].

TES encompasses sensible, latent, and thermochemical storage methods [3]. Sensible Thermal Energy Storage (STES) provides stability but suffers from drawbacks like temperature decline during discharge and low energy density [3]. Latent Heat Thermal Energy Storage (LHTES) employs Phase Change Materials (PCMs) to absorb and release heat at a constant temperature, addressing temperature variations and offering higher energy density [3]. However, PCMs face challenges, including low thermal conductivity, subcooling, corrosion susceptibility, and volume expansion during phase transitions [3]. Composite PCMs (CPCMs), which integrate PCMs into heat-resistant frameworks, enhance efficiency across various applications, including integrated TES systems [3].

CPCMs improve charging and discharging efficiency, resolve leakage issues, enhance handling, and enable direct heat transfer systems [4]. These direct systems reduce thermal resistance, benefit from favorable thermal stratification, and improve overall exergy, all while being cost-effective due to fewer components [4].

Packed Bed Latent Heat Storage Systems (PBLHS), which incorporate CPCMs, provide effective and flexible solutions for a wide range of temperatures, from Concentrated Solar Power (CSP) systems to low-temperature applications [4]. Their efficiency, cost-effectiveness, and broad applicability have garnered significant attention [4]. Recent studies have explored various advancements in PBLHS design to enhance efficiency and performance. Wu et al. demonstrated that cascaded PCM systems improve charging efficiency [5], while Liu et al. highlighted the significant impact of radial porosity on heat transfer and PCM melting time in 3D models [6]. Wang et al.'s two-dimensional model showed that a radial gradient arrangement enhances heat transfer and reduces pressure drop, achieving an energy efficiency of 84.16% [7]. Dong et al. proposed a biomimetic vein hierarchical structure, improving temperature distribution and thermal response [8]. Nekoonam and Ghasempour used a Genetic Algorithm to optimize PCM thermal conductivity in solar-integrated PBLHS, maximizing stored energy [9]. Other studies, such as those by El Sihy et al. [10] explored various aspects of PBLHS, including PCM configurations, heat recovery, and the effects of inlet velocity and temperature. These studies collectively underscore the potential for ML and optimization techniques to advance TES systems.

Machine Learning (ML) is emerging as a promising and adaptive alternative in TES modeling. ML has demonstrated potential in various TES applications, improving performance prediction and design efficiency compared to traditional Computational Fluid Dynamics (CFD) models [11]. Studies have highlighted the advantages of ML in TES applications, including more accurate performance predictions and design optimizations [11].

Traditionally, PBLHS research has relied on classical finite element models (FEM) and analytical models. While FEM can accurately model heat transfer, it is computationally expensive, time-consuming, and limited to specific scenarios. Analytical models, though more adaptable, often suffer from reduced accuracy due to idealized assumptions.

Recent trends favor ML due to the availability of data, increased computing power, and advancements in algorithms. Unlike FEM and analytical models, ML operates with approximate models, providing near-accurate solutions while managing uncertainty [12]. Additionally, ML requires fewer computational resources without compromising accuracy.

Current research on PBLHS leverages ML for performance prediction. Li and Lv generated training data using Latin Hypercube Sampling (LHS) and numerical simulations, employing LightGBM (LGBM) to analyze the impact of Heat Transfer Fluid (HTF) flow rate, tank dimensions, and PCM phase change temperature on PBLHS performance [12]. Post-optimization with Naive Bayes improved heat metrics, but the study was limited to a 100°C inlet heat stream and did not incorporate cascade systems.

Anand et al. [13] found XGBoost (XGB) yielded the best R^2 (0.982) and lowest error for PBLHS charging/discharging times, but the study was restricted to 25–100°C, without cascade systems. Research gaps remain in expanding temperature ranges, incorporating cascade systems, and enhancing ML model interpretability for PBLHS.

In conclusion, PBLHS with encapsulated PCMs holds significant potential for waste heat recovery. Although ML research in this area shows promise, it requires a broader scope and consideration of cascade systems to realize its full potential.

2. METHODS

2.1 Model Definition

The modeling analysis was conducted using the CFD platform, COMSOL Multiphysics. Several foundational assumptions were incorporated. The computational domain, representing the packed bed with PCM capsules, is treated as a continuous, isotropic porous medium. The tank dimensions and PCM capsule sizes were based on standard industrial parameters. Radiation-driven heat transfer within the tank and intrinsic heat sources were neglected. Fluid dynamics were assumed stable, with no mass deposition or generation, and thermal expansion effects were not considered. For the solid walls interfacing with the fluid domain, a “no-slip” condition was applied, ensuring zero fluid velocity at these boundaries. Similarly, the standard no-slip formulation was adopted within the porous medium. At the inlet, fluid entered perpendicularly, and the total volumetric flow rate was integrated over the inlet boundary. Outlet conditions were regulated to prevent backflow and maintain pressure above ambient.

The “Free and Porous Media Flow” interface was used to compute fluid dynamics within the packed bed, employing the Navier-Stokes equation for compressible flow. Due to high Reynolds number ($Re > 10$) and Knudsen numbers ($Kn > 0.1$), the non-Darcian flow model based on the Ergun equation was utilized. Mass conservation was ensured, with gravity explicitly modeled to oppose the charging flow direction. The Boussinesq approximation was used for thermal convection.

Thermal dynamics were simulated using the “Heat Transfer in Solids and Fluids” interface. Air density was modeled according to the ideal gas equation, and a linear discretization scheme ensured numerical stability and precision. A Local Thermal Nonequilibrium (LTNE) approach accounted for temperature differences between fluid and solid phases.

CPCM properties and phase changes were modeled using average density and specific heat capacity values, considering latent heat and volume fractions of the phases. Thermal conductivity and heat flux, including specific heat flux at the tank's side boundaries, were incorporated.

The problem-solving methodology involved first addressing free porous media flow in a stationary phase, then solving heat transfer dynamics in a time-dependent phase. The Parallel Direct Solver (PARDISO) efficiently handled large sparse matrices, with optimized solver settings and a relative tolerance of 0.0001. A timestep of 0.5 min captured transient behavior.

2.2 Production of the dataset for Machine Learning

To develop an ML model for predicting PBLHS design and performance, we conducted a comprehensive parametric analysis using the previously described model. The parameters examined included structural factors such as aspect ratio and insulation thickness, along with material properties like CPCM particle size and thermal characteristics.

A distinctive aspect of our approach is the treatment of the system as a three-layer cascade with CPCMs. The melting points of these CPCMs were selected progressively from highest to lowest, given the inlet is at the top of the tank, constrained to be compatible with MgO.

To calculate the specific heat capacity (C_p) of each CPCM layer, we used mixing theory and the Cp values of MgO and the respective PCM at its melting point. Latent heat was determined similarly. For thermal conductivity, we utilized the Ratcliffe formula, identified as the best-performing empirical relationship. Each CPCM layer exhibited slightly different properties.

The properties of the CPCMs were defined as functions of their melting points, following an extensive literature review to identify compatible PCMs. The selected PCMs offer a broad range of temperature applications for thermal energy storage. Paraffin RT Series PCM is suitable for lower temperatures (50-100°C), while a quaternary molten salt ($LiNO_3$-$NaNO_3$-KNO_3-$Ca(NO_3)_2$) covers moderate temperatures (98-147°C). The $NaNO_2$-KNO_3 binary molten salt handles higher temperatures (138-220°C), and $NaNO_3$-KNO_3 Solar Salt is ideal for high-temperature applications (220-334°C). These selections accommodate various temperature requirements for thermal energy storage systems.

The prediction model's accuracy relied on consistent data sampling. To ensure this, a large number of diverse parameter combinations covering the entire spectrum were randomly chosen. Among various methods, Latin Hypercube Sampling (LHS) stood out for its ability to uniformly sample multiple parameter combinations, ensuring a robust dataset for the model.

2.3 Deep Learning Model

Deep Learning (DL) offers a superior method for predicting heat storage and extraction in PBLHS compared to traditional regression ML techniques. DL's multi-layered neural networks excel in representing hierarchical features and learning from raw data, enabling better data abstraction and generalization. Additionally, DL supports end-to-end and transfer learning, enhancing cross-task knowledge application.

Table 1. Variables evaluated in the ML model

Symbol	Lower Bound	Upper Bound
ds	0.15	6
din	0.1	2
dp	0.01	0.1
V_in	0.1	6
s_ins	0.01	1
LI	0.1	6
L2	0.1	6
L3	0.1	6
t_charging	1	8
t_discharge	1	28
T0	-5	30
T ext	-5	30
T_m1	0.1	550
T_m2	0.1	500
T_m3	0.1	500
Tu	0.1	650

To characterize PBLHS behavior, a 2D-axisymmetric fluid dynamics and heat transfer set of differential equations for each dataset point was solved, determining heat storage and extraction across scenarios.

Two neural networks were trained: one for heat storage and one for heat extraction. Input variables were categorized into Design Variables (e.g., tank diameter, inlet diameter, particle radius, flow rate, insulation thickness, tank lengths), Time Variables (charging and discharge times), and Temperature Variables (initial, external, CPCM melting points, upstream temperature).

The neural network architecture featured increasing layer sizes for balance and generalization. Starting with a dense layer of 2048 units using ReLU activation, it transitioned through layers of 1024, 256, 64, and 16 units, incorporating dropout layers and L2 regularization to control overfitting. The final single-unit layer outputted continuous values for regression tasks, ensuring effective feature extraction and robust generalization. Input features were standardized using a Standard Scaler, placing variables on a common scale for effective weighting by the neural network.

The coefficient of determination (R^2) and Mean Absolute Percentage Error (MAPE) assessed the neural networks' accuracy. Residuals, the differences between predicted and actual values, were subjected to a Shapiro-Wilk test to check for normal distribution, a crucial assumption in many statistical analyses.

2.4 Optimization with Metaheuristic Algorithms

PBLHS presents complex challenges with numerous variables, requiring extensive optimization to determine optimal configurations. Traditional methods are often computationally intensive. Metaheuristics offer advanced, often stochastic, strategies for navigating large solution spaces efficiently. In this study, several metaheuristic algorithms were integrated with the neural network model to optimize PBLHS, leveraging the neural network's rapid estimation of heat extraction to expedite the process.

1. Harmony Search (HS): Inspired by musical improvisation, HS balances random searches and pitch adjustments to find optimal solutions. It prevents local optima convergence, making it effective for various applications.
2. Genetic Algorithm (GA): Simulates natural selection using mutation, crossover, and selection. GA evolves populations over generations to improve fitness, involving steps like initializing the population, evaluating fitness, selecting candidates, crossover, mutation, and replacement.
3. Ant Colony Optimization (ACO): Inspired by ants' path-finding using pheromones, ACO selects paths based on pheromone levels and heuristic desirability. It updates pheromone trails and balances exploration and exploitation.
4. Wind-Driven Optimization (WDO): Simulates air particle movement, updating velocities considering friction, gravity, mass, and the Coriolis effect. WDO adjusts positions based on updated velocities to simulate wind movements.

Each algorithm was chosen for its strengths in the problem domain and integrated with the neural network for efficient PBLHS optimization.

3. RESULTS AND DISCUSSION

3.1 CFD Validation and Evaluation

The CFD model utilized here was validated using data two validation studies were conducted at high and low temperatures.

In the first study, involving a carbon steel storage tank with 770 capsules, simulations closely matched experimental results, with an average error of 0.46% [15]. The second study, based on Loem et al.'s work, showed a minor discrepancy during the charging phase, with an average error of 2.4% and a maximum deviation of 4.7°C at 18 minutes [16].

Additionally, a grid independence and timestep independence study found negligible variability (<3%).

3.2 Neural Network Evaluation

The model's adaptability and performance are reflected in the R2 values of 0.975 for charge and 0.974 for discharge, capturing over 97% of the variability in both processes. The average MAPE for charging and discharging cycles was ±9.17%, indicating an acceptable level of accuracy that could be enhanced by expanding the dataset.

Residuals analysis using the Shapiro-Wilk test indicated normal distribution for both charge and discharge data, with p-values of 0.2738 and 0.1367, respectively. Effect sizes of 0.084 and 0.098 further suggest minimal deviation from normality, reinforcing the NN model's validity and meeting key regression assumptions. While standardized residuals generally align with a standard normal distribution, minor deviations indicate areas for potential model improvement.

3.3 Optimization through Metaheuristic Algorithms

To find optimal designs for maximizing heat capture and extraction, various metaheuristic algorithms suited to this variable space were employed. Balancing exploration (comprehensive search) and exploitation (optimization in known areas) was crucial. Three scenarios were studied for each algorithm: broad exploration, intensive exploitation, and a balanced approach.

HS algorithms outperformed others in terms of computation time. HS1 achieved the highest heat extraction at 66 MJ in just 86 seconds, while HS3, a more balanced version, reached 79 MJ with about three times the computational demand.

To further enhance performance, a comprehensive grid search tuned key hyperparameters like harmonies, iterations, memory consideration rate, and pitch adjustment rate. This systematic approach yielded an objective function value of 95,930 kJ. In the best scenario, computational time was only 17 seconds.

3.4 Case Studies

This section compares the proposed methodology's results with those from other studies, using data extracted from various literature sources under different setups and temperature conditions. The model consistently outperformed experimental results across all four scenarios, with cases 1 to 3 representing experimentally optimized results.

The fine-tuned optimization algorithm that uses the neural network as the objective function generator showcased significant improvements in stored energy, extracted energy, charging efficiency, and total efficiency. Scenario 4 showed the highest improvements, with a 66.14% increase in stored energy and an 84.26% improvement in extracted energy.

Table 2. Comparative Analysis across Different Scenarios

Reference	**1**(*16*)	**2** (*15*)	**3** (*17*)	**4** (*18*)
Experimental				
Charging Temperature (°C)	465	326	375	65
Flow Rate (m^3/s)	0.0129	0.030 56	0.008 62	0.0075 0
Charging Duration (hours)	1.0	3.33	5.0	3.0
Discharge Temperature (°C)	325	286	50	30
Discharge Duration (hours)	1.33	3.33	3.33	2.0
Stored Energy [MJ]	7.44	3.96	26.41	2.54
Extracted Energy [MJ]	6.48	3.84	25.59	2.16
Charging efficiency [%]	91.5	72.3	76.4	50.5
Total efficiency [%]	79.7	70.1	74	42.9
Modelled				
Stored Energy [MJ]	7.66	5.01	31.11	4.22
Extracted Energy [MJ]	7.12	4.78	28.37	3.98
Charging efficiency [%]	93.6	92.8	90.3	84.4
Total efficiency (%)	87.0	88.5	82.4	79.6

Efficiency metrics also saw substantial gains, with scenario 4 showing a 67.13% increase in charging efficiency and an 85.55% increase in total efficiency. Scenario 2 showed a 28.35% improvement in charging efficiency and a 26.25% increase in total efficiency.

4. CONCLUSIONS

This study introduces an innovative approach in TES. An advanced design and optimization method for PBLHS is presented, leveraging deep learning (DL) coupled with metaheuristics. The key takeaways are:

1. The deep learning model demonstrated adaptability across various scales, with R^2 values of 0.975 for charge and 0.974 for discharge, capturing over 97% of the variability for both processes. Additionally, the model achieved a reasonable MAPE of less than 9.14%.
2. Various algorithms were employed to identify optimal designs that maximize heat capture and extraction. The Harmony Search (HS) algorithm emerged as the most effective, achieving an objective function value of 95.9 MJ, significantly outperforming other algorithms.
3. The model was compared with four experimental scenarios, consistently surpassing experimental benchmarks in terms of energy storage and efficiency, particularly in total efficiency.

In conclusion, this research introduces a novel approach by coupling DL with metaheuristics to optimize PBLHS, advancing TES design. Future work will integrate cost considerations, refine the model for larger energy scales, enhance generalization and interpretability, and validate findings experimentally.

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