Mathematical model of a PCM cold store dedicated to a LAES system

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Abstract:

Electrical energy storage plays a key role in the integration of renewable energy sources with power systems, enabling demand balance and system stabilization. Liquid air energy storage (LAES) offers advantages such as long lifetime, scalability, and the use of environmentally friendly materials. To optimize the performance and round-trip efficiency of these systems, efficient cold thermal energy storage (TES) solutions should be implemented. Various cold TES concepts exist, including packed-bed rock storage, liquid media, and advanced solutions involving phase change materials (PCMs). PCM-based systems offer advantages over conventional cooling methods, such as methanol–propane mixtures or packed-bed configurations, due to their high energy density.

This study presents a mathematical modelling approach for a PCM cold TES designed for LAES applications, using three-dimensional computational fluid dynamics (CFD) simulation. The objective is to develop a predictive framework progressing from simplified analytical approaches to detailed numerical simulations, enabling understanding of thermal behaviour across multiple complexity scales. Simplified one-dimensional models provide semi-analytical solutions for rapid parameter exploration and identification of dominant physical mechanisms, while the 3D CFD model captures multidimensional thermal effects, spatial non-uniformities, and complex flow patterns not represented in reduced-dimensional frameworks. The 3D model incorporates detailed computational geometry, refined mesh structures near thermal gradients, robust solver settings for transient phase change phenomena, and realistic boundary conditions. Model implementation addresses challenges in cryogenic phase change simulations, with individual cases requiring 2–3 weeks of processing time due to fine temporal discretization, three-dimensional complexity, and dense mesh density. Validation is performed against experimental data from cryogenic testing facilities operated with nitrogen, including inlet temperatures of approximately −170 °C and pressures around 6 bar. Results demonstrate that the 3D CFD model provides detailed spatial understanding of complex thermal phenomena. This modelling framework establishes a practical tool for analysing and optimizing PCM cold TES systems dedicated to LAES applications.

Keywords:

Phase Change Materials; Cold Thermal Energy Storage; Liquid Air Energy Storage; Analytical Model; Computational Fluid Dynamics.

1. Introduction

Grid-scale energy storage is a cornerstone of future energy systems dominated by intermittent renewable sources such as solar photovoltaic and wind power [1]. However, its deployment is still not on track with the Net Zero Emissions (NZE) by 2050 Scenario outlined by the International Energy Agency (IEA) [2]. Currently, pumped hydropower and electrochemical batteries account for the largest share of installed grid-scale storage capacity [3]. Despite their widespread deployment, these technologies present several limitations, including high costs, geographical constraints, environmental concerns, and reliance on critical materials. Moreover, they are primarily designed for electricity storage. In contrast, more than half of global final energy consumption is in the form of thermal energy, mainly for heating and cooling [4]. Cooling demand is projected to grow rapidly due to population growth, economic development, and climate change [5]. These trends highlight the need for large-scale energy storage technologies capable of storing and delivering thermal energy alongside electricity.

Thermo-mechanical energy storage technologies integrating thermal energy storage (TES), often referred to as Carnot batteries, represent a promising solution to address this challenge. These technologies—including compressed air energy storage (CAES), pumped thermal energy storage (PTES), and liquid air energy storage (LAES)—store electricity in the form of thermal and mechanical energy and can be integrated with both power and thermal systems. In addition to enabling multi-energy services, they offer advantages such as scalability, long lifetimes, and minimal environmental impact.

Among these technologies, LAES stands out due to its high volumetric energy density (≈200 kWhe/m³) achieved through the storage of air in liquid form [6]. The technology is relatively mature (TRL 7–9), geographically flexible, and based largely on commercially available components with long operational lifetimes [7]. LAES also exhibits strong synergies with cryogenic energy systems, such as liquid natural gas (LNG), liquid nitrogen (LN_2), and liquid hydrogen (LH_2) infrastructures [8,9]. Like CAES, LAES can provide multiple grid services including energy arbitrage, capacity firming, frequency regulation, and black start capability [10]. Additionally, the air purification stage inherently removes CO_2, offering potential integration with carbon capture or direct air capture systems [11].

Despite these advantages, the relatively low round-trip efficiency of LAES (typically 50–70% [12]) remains a key challenge compared with electrochemical storage technologies. One of the main factors limiting system performance is the incomplete recovery and reuse of the cold energy released during liquid air regasification [13]. Efficient cold thermal energy storage (CTES) is therefore critical to improving the overall efficiency of LAES systems and reducing the need for external cooling sources, particularly during start-up and transient operation [14].

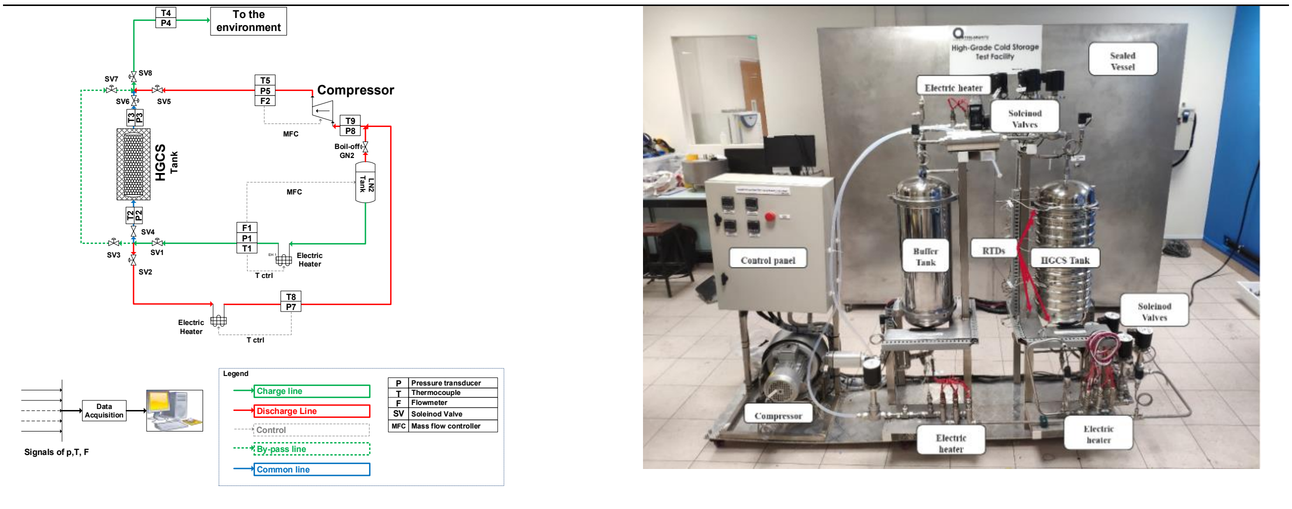
In this case, phase change materials (PCMs) offer significant advantages for CTES in LAES systems due to their ability to store and release large amounts of energy as latent heat at nearly constant temperature. This leads to higher energy storage density and improved thermal buffering compared to sensible heat materials, mitigating thermocline effects and reducing the specific energy consumption of the liquefaction process [15]. However, several challenges limit application of PCM at cryogenic temperatures, including high material costs, limited availability of suitable cryogenic PCMs, and scalability issues for large-scale integration. In addition, many PCMs suffer from low thermal conductivity, which negatively affects heat transfer performance and system efficiency. These drawbacks, along with integration and material development challenges, indicate that PCM based CTES technologies are still at an early stage of development for LAES applications.

The objective of this study is to develop and validate a comprehensive computational fluid dynamics (CFD) model of a cryogenic cold thermal energy storage (TES) system dedicated to liquid air energy storage (LAES) applications. The work focuses on accurately capturing the coupled phenomena of fluid flow, heat transfer, and phase change within a phase change material (PCM)-based storage unit under cryogenic conditions. Building upon simplified analytical approaches, the developed three-dimensional model aims to provide detailed insight into spatial temperature distributions, flow structures, and solid–liquid phase transition dynamics, which are critical for improving system performance and round-trip efficiency. Ultimately, the study seeks to establish a reliable predictive tool supporting the design, optimization, and scale-up of advanced cold TES systems for efficient integration with LAES technology.

2. Methods

2.1 Experimental setup

The experimental data used to validate the model were obtained from the study by Tafone et al. [15], who conducted both numerical and experimental investigations on the thermal behaviour of a novel cryogenic high-grade cold storage (HGCS) packed bed filled with phase change material (PCM) particles. Their work examined how this storage configuration influences the thermodynamic and economic performance of a LAES system compared with a conventional sensible heat storage design. To assess the performance of the PCM-based storage, the authors developed a dedicated experimental setup. The test bench (Figure 1a) was designed to reproduce the operation of an HGCS unit recovering cryogenic energy from the regasification of liquid nitrogen. The facility consists of two open loops representing the charge/discharge and discharge/charge phases of the HGCS/LAES cycle, respectively. Liquid nitrogen (LN_2) and gaseous nitrogen (GN_2) were used as the primary heat transfer fluids during the charging phase instead of liquid air, due to the limited commercial availability of liquid air. The designed test facility allowed for temperature measurement at selected levels of the store, numbered from 1 to 10, starting form the inlet side.



(a) (b)

Figure. 1. Process flow diagram (a) and test rig installation (b) as described in [15].

The main operational parameters of the experimental set-up are provided in Table 1.

Table 1. *Operating conditions of the experimental set-up at TESLALAB@NTU.*

Parameters	**Value**	**Unit**
H, Height	0.678	*m*
D, Internal diameter	0.250	*m*
D_o, Outer diameter	0.254	*m*
t_i, Insulation thickness	0.018	*m*
HTF, Heat transfer fluid	LN_2/GN_2	-
$\dot{V}_f$, volumetric flow rate	6-24	m^3/h
$T_{f,in,ch}$ Charge HTF inlet temperature	-180/-150	°*C*
T_{amb}, Ambient temperature	25	°*C*
d_p, Particles diameter	0.05	*m*

2.2 CFD model

A mathematical model was developed to describe the key physical processes occurring in the investigated cold thermal storage system, including heat transfer, phase change, and fluid flow. The governing conservation equations, together with the k–ω SST turbulence model and the energy equation, were implemented to accurately capture the complex thermo-fluid behavior [16].

Heat and mass transport in the analysed domain should be determined with the help of base flow equations:

continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0 \qquad (1)$$

energy conservation equation

$$\frac{\partial (\rho h_{tot})}{\partial t} - \frac{\partial p}{\partial t} + \nabla \cdot (\rho U h_{tot}) = \nabla \cdot (\lambda \nabla T) \qquad (2)$$

where

$$h_{tot} = h + \frac{1}{2} U^2 \qquad (3)$$

momentum conservation equation

$$\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U \otimes U) = -\nabla p + \nabla \cdot \tau \qquad (4)$$

where

$$\tau = \mu \left(\nabla U + (\nabla U)^T - \frac{2}{3} \delta \nabla \cdot U \right) \qquad (5)$$

Although low velocities occur in the analysed domain, turbulence may develop locally within the packed bed; therefore, a turbulence model was applied [17]. In this study k-ω SST (equations 6-9) was selected like in analogous research [18].

$$\frac{\partial u_i}{\partial t} + u_k \frac{\partial u_i}{\partial x_k} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{1}{\rho}\frac{\partial}{\partial x_k}\left((\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)\right) \quad (6)$$

$$\frac{\partial u_k}{\partial x_k} = 0 \quad (7)$$

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = \hat{G}_k - \beta^* \rho \omega \kappa + \frac{\partial}{\partial x_j}\left((\mu + \sigma_\kappa \mu_t)\frac{\partial k}{\partial x_j}\right) \quad (8)$$

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho \omega u_j)}{\partial x_j} = \frac{\gamma}{\nu}\hat{G}_k - \beta \rho \omega^2 + \frac{\partial}{\partial x_j}\left((\mu + \sigma_\omega \mu_t)\frac{\partial \omega}{\partial x_j}\right) + 2\rho(1 - F_1)\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j} \quad (9)$$

To model the solidification/melting process, the enthalpy–porosity technique was applied, which can be described by Eqs. (10) and (11a-c). This approach is based on assigning each computational cell a parameter called the liquid fraction, which is calculated at each iteration from the enthalpy balance. The semi-solid region (mushy zone), where the phase change occurs, is modelled as a pseudo-porous medium. The liquid fraction in this region varies between 1 and 0, where 1 corresponds to the fully liquid state and 0 to the fully solid state.

The material enthalpy is defined as:

$$H = h + \Delta H \quad (10)$$

where:

h– sensible enthalpy [J/kg];

ΔH– latent heat [J].

The liquid fraction is defined as:

$\beta = 0$ for $T < T_{solidus}$ (11a)

$\beta = 1$ for $T > T_{liquidus}$ (11b)

$\beta = \frac{T - T_{solidus}}{T_{liquidus} - T_{solidus}}$ for $T_{solidus} < T < T_{liquidus}$ (11c)

The developed model was implemented in ANSYS Fluent for numerical simulations. Table 2 presents the materials used in the analysed cold thermal energy storage system, including the structural components and working media. It specifies the materials assigned to the storage tank, encapsulated PCM units, the phase change material itself, and the heat transfer fluid circulating within the system. Main thermophysical properties of the phase change material applied in this study are summarised in Table 3. These include key parameters governing heat storage and transfer processes, such as density, specific heat capacity, thermal conductivity, latent heat, and characteristic phase transition temperatures (solidus and liquidus).

Table 2. *Materials used in the system.*

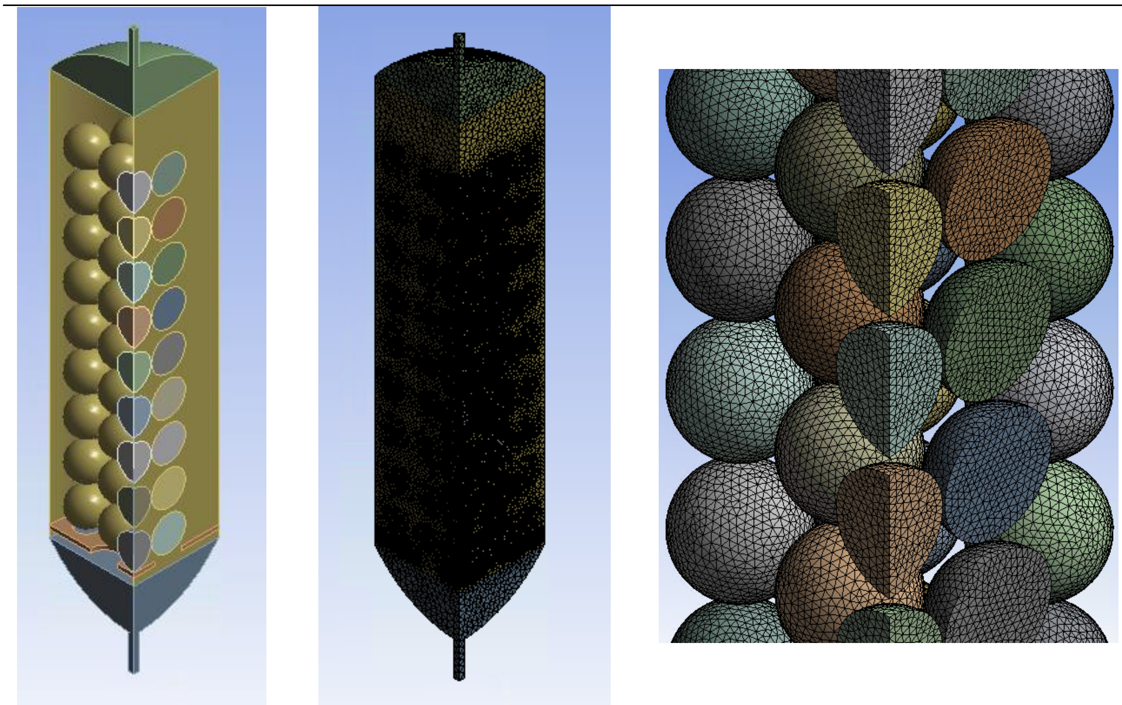
Media	Material
Tank	Stainless steel 304
Capsules	Stainless steel 304
PCM filling	PCM TESLALAB@NTU
Gas	Nitrogen

Table 3*. Main thermophysical properties of PCM used in this study.*

Parameter	Value	Unit
Density	789.3	kg/m^3
Specific heat	1870	*J/kg K*
Thermal conductivity	0.2	*W/m K*
Latent heat	86000	*J/kg*
Solidus temperature	-118	*°C*
Liquidus temperature	-115	*°C*

Based on the experimental studies described above, three-dimensional (3D) simulations were performed within the scope of this work. The entire geometry of the storage tank was reconstructed, including the cylindrical section, end caps, inlet and outlet nozzles, and a diffuser plate located near the bottom end cap of the tank. The supporting lattice structures on which individual rows of capsules are mounted were neglected in the model.

It was assumed that the flow within the storage system is axisymmetric. Therefore, the computational domain of the three-dimensional model represents only one quarter of the actual tank (Figure 2).



A B C

Figure. 2. *Computational domain (A), selected mesh – general view (B) and detailed view (C).*

3. Results

A representative operating case was selected and simulated to validate the developed model. Its main conditions are summarized in Table 4. The analyzed scenario was characterized by a volumetric flow rate of 12 m³/h, an inlet temperature of −170 °C, and an initial storage temperature of 0 °C. The system operated at a pressure of 6 bar, and the outlet boundary condition was defined by a temperature criterion of −50 °C. This set of conditions reflects typical operating parameters of cryogenic cold energy recovery in LAES systems and provides a suitable basis for assessing the thermal performance of the PCM-based storage unit.

Table 4. *Initial conditions for the modelled case.*

Parameter	**Value**	**Unit**
Volumetric flow	12	m^3/h
Inlet temperature	-170	*°C*
Initial store temperature	0	*°C*
Pressure	6	*bar*
Outlet boundary criterion	-50	*°C*

Figure. 3 illustrates the temporal evolution of temperature distribution within the cold thermal energy storage tank during the cooling process. At the initial stage (50 s), the temperature field is nearly uniform, with values close to ambient conditions. As the process progresses, a distinct cooling front develops from the bottom region, corresponding to the inlet of the cryogenic fluid. The lower part of the tank cools significantly faster, leading to strong vertical temperature gradients. At intermediate time steps (2000–4000 s), the cooling front propagates upward through the packed bed of capsules. A clear stratification is observed, with colder regions at the bottom and warmer zones remaining in the upper part of the tank. The phase change region (mushy zone) can be identified by gradual color transitions, indicating simultaneous sensible and latent heat transfer. At later stages (6500–10500 s), the majority of the domain reaches low temperatures, and the temperature field becomes more homogeneous. However, residual gradients persist in the upper section, suggesting slower heat removal due to reduced temperature differences and weaker convective effects. The results highlight the dominant role of buoyancy-driven flow and phase change in shaping the thermal field.

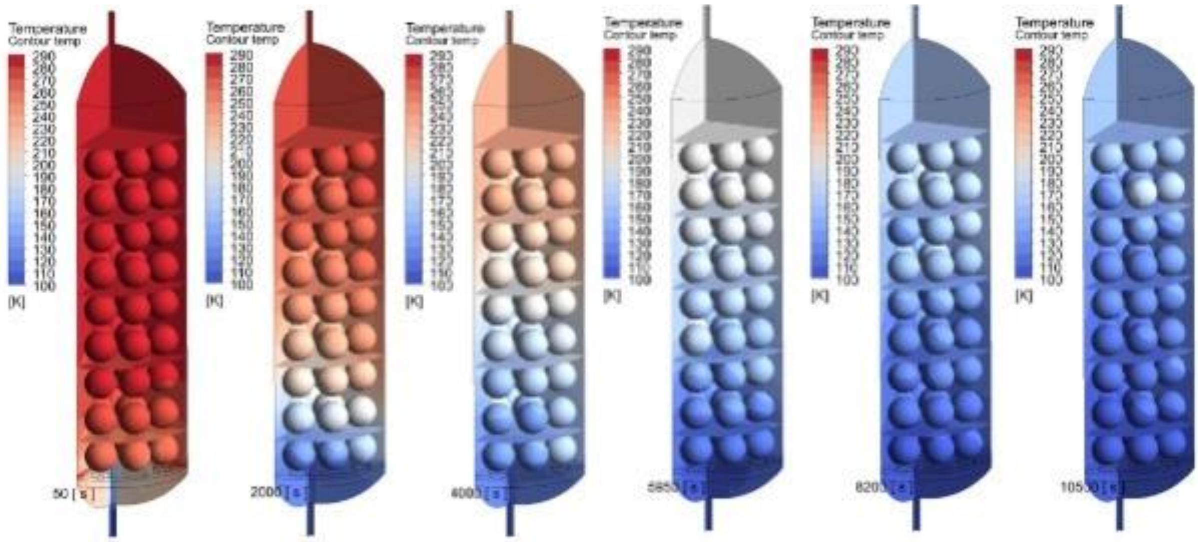


Figure. 3. *Temperature contour for selected time steps.*

A comparison between experimental measurements and CFD model predictions at different axial positions within the tank (T2–T10) are shown in the Figure 4. Overall, good agreement between the numerical and experimental data is observed, confirming the capability of the model to capture the main thermal trends. The temperature decrease is most rapid at lower measurement points (e.g., T2), which are closer to the inlet, while higher locations (T8, T10) exhibit delayed cooling due to the progressive nature of the cooling front. The model successfully reproduces the temporal shift and slope of the temperature curves, particularly in the mid and upper regions of the tank.

Some discrepancies are noticeable at early times and during the phase transition period, where the experimental data show slightly faster cooling or delayed response compared to the model. These differences may be attributed to simplifications in the numerical model, such as idealized geometry, neglect of structural elements, or uncertainties in thermophysical properties, numerical solution instabilities.

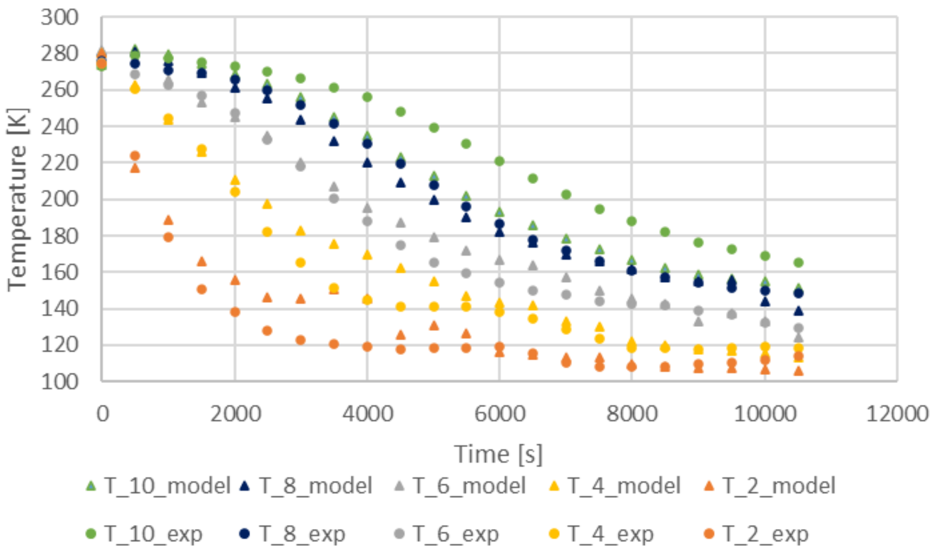


Figure. 4. *Temperature in selected cross sections over time. Modelling results comparison to the experiment.*

The relative error between experimental data and CFD predictions for selected measurement points over time is presented in the Figure 5. The error remains within an acceptable range for most of the simulation period, generally below ±10%. Larger deviations are observed during the transient phase change region, particularly for lower measurement points (e.g., T2 and T4), where the error temporarily reaches values up to approximately −20%. This behaviour is associated with the difficulty of accurately capturing the moving phase boundary and latent heat effects in numerical simulations.

At later stages, the error decreases and stabilizes, indicating improved agreement once the system approaches a quasi-steady thermal state. The results confirm that the developed CFD model provides reliable predictions of the thermal behaviour, with acceptable accuracy for engineering applications.

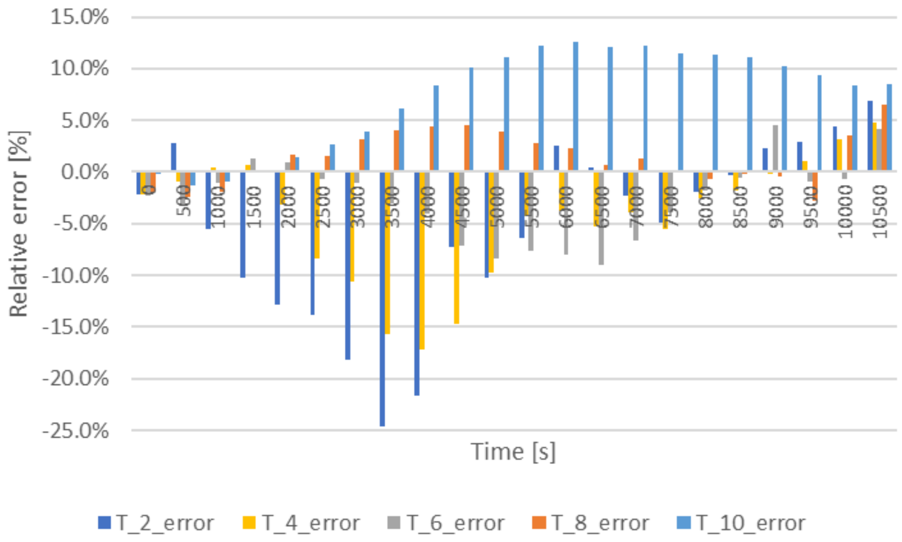


Figure. 5. *Relative error of the model results in reference to experiment.*

4. Outcomes

This study presents a comprehensive modelling framework for a cryogenic PCM-based cold thermal energy storage system dedicated to liquid air energy storage applications. The use of three-dimensional CFD simulations enables a multi-scale understanding of the underlying thermo-fluid processes, including heat transfer, fluid flow, and phase change phenomena.

The results demonstrate that the developed CFD model is capable of accurately reproducing the transient thermal behaviour of the storage system, as confirmed by comparison with experimental data. The model successfully captures the propagation of the cooling front, the formation and movement of the phase change region, and the spatial temperature distribution within the packed bed. The agreement between numerical and experimental results remains within an acceptable range, with relative errors generally below ±10%, validating the reliability of the modelling approach for engineering applications.

The analysis highlights the importance of multidimensional effects, such as flow non-uniformities and thermal stratification, which cannot be fully resolved using simplified one-dimensional models. The study also identifies key challenges associated with modelling cryogenic PCM systems, particularly the accurate representation of phase change dynamics and thermophysical properties. The largest discrepancies between model predictions and experimental data occur during the transient phase transition period, indicating the need for further refinement of phase change models and material characterization.

Overall, the proposed modelling framework provides a robust and practical tool for the design and optimization of PCM-based cold thermal energy storage systems. The findings contribute to improving the performance and round-trip efficiency of LAES systems and support their broader deployment in grid-scale energy storage applications.

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