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Executive Summary of the Thesis

Analysis and Modelling of Latent Thermal Energy Storage for Energy Systems

Laurea Magistrale in Energy Engineering - Ingegneria Energetica

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1. Introduction

Thermal storage represents a crucial technology for the successful integration of renewable sources in the energy mix of modern society. Thermal energy represents a high share of final energy consumption in most European countries, and being able to store it would allow relevant savings both in economical and carbon emission terms. Latent thermal energy storage (LTES) has gained particular attention due to its high energy density. The technology is able to store thermal energy exploiting the phase change from solid to liquid state of the so called phase change materials (PCM) [1]. Furthermore, these materials present phase change temperature ranges close to ambient temperature, which makes them suitable for both residential and industrial applications. The analysis of LTES operation requires its integration in wider energy systems to understand the best control strategies when the system is coupled with the storage. This requires proper modelling of the technology. From literature, LTES has been mainly studied to analyze the physical behavior of the PCM when it undergoes phase transition. These studies have modelled LTES with softwares like ANSYS or COSMOL. These programs are very precise, but not suited for long simulations that complex energy systems coupled with thermal storages require. Accurate models of LTES in dynamic object oriented programs such as Modelica turn out to be suited for this purpose.

2. Objectives

This thesis aims at developing simplified modelling approaches for LTES in the object oriented program Modelica. Among the different storage designs, a slab configuration is considered. This configuration is made of parallel PCM slabs that thermally interact with the heat transfer fluid (HTF) that flows in the channels in between them.
The model is divided in three main heat transfers. The external heat interaction between the HTF and the PCM, the internal PCM heat transfer and the thermal losses through the storage walls. The external heat interaction is determined by conducting a fluid-dynamic analysis on the HTF flow, to determine the convective heat transfer coefficient for heat exchange. The internal PCM heat transfer is solved through the energy equation with an implicit finite difference scheme. The solution is then improved by

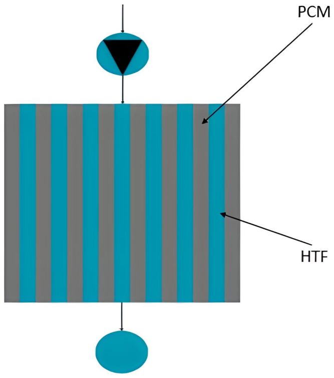

Figure 1: Slab LTES

developing corrective coefficients to account for natural convection. The coefficients are determined by comparing and analyzing the results from the same simulations in Modelica and CFD simulations in ANSYS Fluent. The model accounts for the variability of the material properties with temperature. The thermal losses are modelled in Modelica as conductive + convective heat transfer through the storage walls and ambient boundary conditions.
Finally, the model is inserted in a heat pump system and run for a realistic simulation to investigate typical charging times of the storage. The model is then validated against an experimental study from literature.

3. External Heat Interaction

The heat interaction between the HTF and the PCM represents heat exchange between a liquid and solid interface (PCM slab containment). Forced convection is the main form of heat interaction. The phenomenon is governed by the convective heat transfer coefficient that is determined by the fluid-dynamic state of the HTF in the channel. The model implemented in Modelica calculates the Reynolds number of the flow and, based on whether the flow is laminar or turbulent, applies the correct correlation for the Nusselt number for flat plate geometry. The convective heat transfer coefficient is subsequently determined.

$$\begin{cases} Re = \frac{\rho \cdot u \cdot L}{\mu} \\ h = \frac{Nu \cdot k}{L} \end{cases} \tag{1}$$

and

$$\begin{cases} Nu = 0.664 Re^{0.5} Pr^{1/3} & Re < 5 \cdot 10^5 \\ Nu = 0.0296 Re^{4/5} Pr^{1/3} & Re > 5 \cdot 10^5 \end{cases} \tag{2}$$

where Re is the Reynolds number, ρ is the density of the HTF, u is the velocity of the HTF, L is the length of the slab, μ is the dynamic viscosity of the HTF, k is the thermal conductivity of the HTF, Pr is the Prandtl number, Nu is the Nusselt number and h is the convective heat transfer coefficient.
The model also verifies that no interaction occurs between the boundary layers that develop on the inner face of each slab. To do so, it calculates the thickness of the boundary layers at the length coordinate of the slab and verifies that it is small with respect to half of the thickness of the channel. Sensitivity analysis for the mass flow rate of the HTF in the channel, section of the channel and length of the slab are carried.

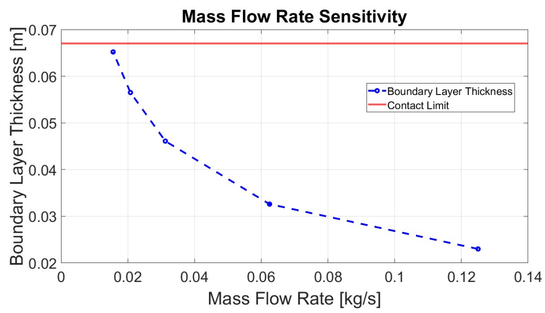

Figure 2: Boundary Layer Thickness: HTF Mass Flow Rate

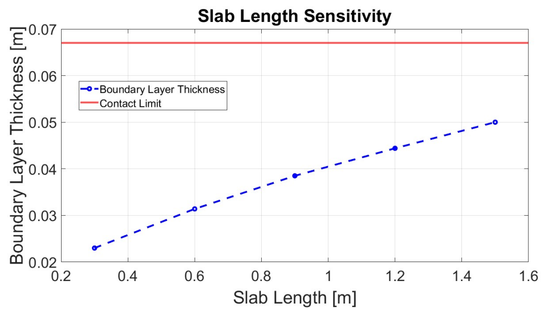

Figure 3: Boundary Layer Thickness: Slab Length

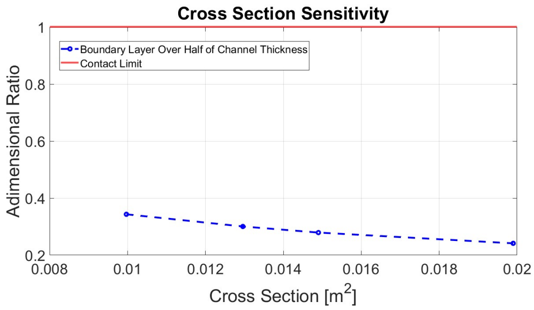

Figure 4: Boundary Layer Thickness: Channel Cross Section

The results show that for typical values of HTF mass flow rate, channel cross section and slab length, the thickness of the boundary layer is well below half of the thickness of the channel. This can be considered as a validation of the usage of the relations reported in (2) to calculate the Nusselt number. It should be noted that there is not a proper definition for the interaction limit of the boundary layers.

4. Internal PCM Heat Transfer

The model implemented in Modelica must account for the thermal propagation inside the PCM slab. Since the focus is on the development of simplified approaches, a first lumped parameter analysis is conducted to verify if the slab can be considered as a single node heat capacitor. The lumped parameter assumption can be accepted only if the Biot number is below 0.1 [2].

$$Bi = \frac{hV}{Ak} < 0.1 \tag{3}$$

where h is the convective heat transfer coefficient of the HTF, V is the volume of the PCM, A is the exchange area and k is the thermal conductivity of the PCM. The results from the analysis show that, because of the extremely low thermal conductivity of the PCM, the temperature gradient inside the material cannot be neglected for typical values of V, A and h. Assuming that the temperature is uniform iside the slab domain is a wrong approach.

The PCM slab is then discretized with a 2D grid, and the heat transfer problem is solved by employing the energy equation.

$$\frac{\partial(\rho\,(T)\,c_P\,(T)\,T)}{\partial t} = \nabla\cdot(k\,(T)\,\nabla T) \tag{4}$$

where ρ is the density and c_P is the specific heat capacity of the PCM. The gradient of the temperature is considered only for the x coordinate, which is the one parallel to the ground, and the y coordinate, perpendicular to the ground. The z coordinate is neglected, because it is assumed that the z dimension of the slab is long enough to not create boundary effects on the edges. The dimensions that are considered are the height of the slab (y axis) and the thickness of the slab (x axis). Since Modelica is not able to solve partial differential equations, the model solves the energy equation through an implicit finite difference scheme. The finite difference scheme solves the conduction model for the 2D grid discretized domain.

The energy equation in (4) does not account for natural convection during the phase change, since it neglects the velocity terms due to motion of the melted material [3]. CFD simulations carried in ANSYS Fluent are employed to verify the assumption of considering only conduction as the heat transfer mode. For many simulations, the results from Modelica and CFD are compared. If varying the height of the slab does not have a significant impact on the deviation between the two models, increasing the thickness does.

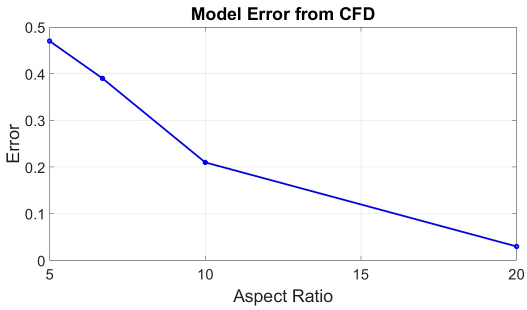

Figure 5: Error between Modelica and CFD: Variable Thickness

In the graph, AR is the aspect ratio and it is defined as the ratio between the height and the thickness of the slab. The error is determined as:

$$e = \frac{t_{Modelica} - t_{CFD}}{t_{Modelica}} \tag{5}$$

where $t_{Modelica}$ is the time that the PCM takes to completely melt in the Modelica model, while t_{CFD} is the time for the CFD simulation. It must be noted that for the analysis in question, the AR was changed by changing only the thickness of the slab and keeping a constant height. Since the error is non negligible, a fictive thermal conductivity model is developed. The idea is to define corrective coefficients to enhance the thermal conductivity of the PCM during phase change, to account for natural convection. The enhancement coefficient is determined as the ratio between the enthalpy of the PCM when natural convection is accounted for and the enthalpy when only conduction is considered.

$$\epsilon = \frac{H_{flow}}{H_{conduction}} \tag{6}$$

where H_{flow} is the enthalpy of the PCM with natural convection and H_{cond} with only conduction.
Several simulations for different slab dimensions are carried. This allows to develop a relation between the enhancement coefficient ϵ and the natural convection intensity, measured with the Rayleigh number.

$$\begin{cases} \epsilon = 1.528e^{1E-05Ra} \\ Ra = \frac{g\beta(T_{wall}-T_m)L^3}{\nu\alpha} \end{cases} \tag{7}$$

where g is the acceleration due to gravity, β is the thermal expansion coefficient of the liquid PCM, T_{wall} is the boundary temperature of the PCM, T_m is the melting temperature of the PCM, ν is the kinematic viscosity and α is the thermal diffusivity.
When the enhancement coefficient is employed, the model is able to properly account for the natural convection effect.

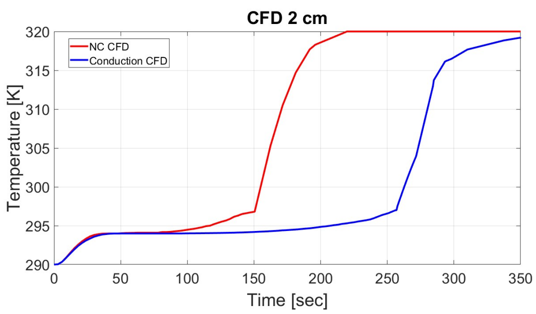

Figure 6: Conduction vs Natural Convection: CFD temperature as a function of time

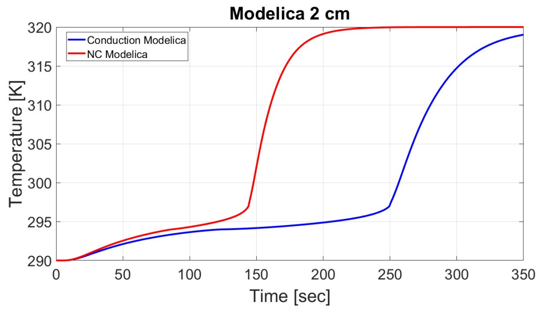

Figure 7: Conduction vs Natural Convection: Modelica temperature as a function of time

The graphs report the case of a slab with a thickness of 2 cm.

5. Modelica Implementation and Model Validation

Modelica is a powerful, object-oriented, equation-based modeling language designed for simulating complex physical systems across various engineering domains [4]. The models previously presented are now implemented in Modelica. Since the LTES incorporates both fluid-dynamic and thermal problems, the model employs components from the Modelica Fluid and Modelica Thermal libraries. The full model is presented in Fig 8.

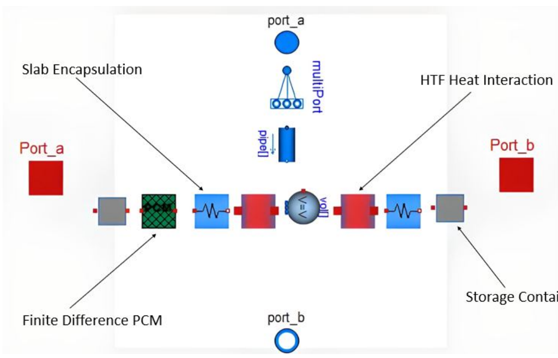

Figure 8: Full LTES Model

The model presents two fluid ports, *port_a* and *port_b*, that serve respectively as the input and output of the HTF in the storage. The *multiPort* component allows the equal division of the inlet HTF mass flow rate in the flow channels present in the storage. Each flow channel is modelled with a pipe that takes into account the fluid resistance to the flow. A control volume models the volume of HTF that is present at each time in the channels that exchange heat with the PCM. The HTF heat interaction block calculates the convective heat transfer coefficient as presented in eq. (1) and (2). The slab encapsulation block is a thermal resistance model that accounts for the slab encapsulation material. The finite difference PCM block models the energy equation for internal heat transfer with the fictive thermal conductivity model, as discussed in paragraph 4. The storage container blocks model the thermal losses to the ambient. These blocks are conductive + convective resistance, accounting for the storage container walls and the ambient air. Finally, $Port\_a$ and $Port\_b$ are heat ports, and are used to specify the ambient temperature boundary conditions for the calculation of the thermal losses. It must be noted that, since in the storage the number of slabs is a degree of freedom, the user can select the number of PCM slabs. Consequently, the number of the discussed components change. In particular, if the storage presents N slabs, the model presents:

- N slabs.
- $N-1$ pipes.
- $N-1$ control volumes.
- $2N-2$ HTF heat interaction blocks.
- $2N-2$ slab encapsulation blocks.
- 2 storage container blocks.

The extreme slabs of the storage exchange heat with the HTF only on the inner face, while the outer face is in direct contact with the storage container, as shown in Fig 1.

The storage is integrated in a heat pump system to simulate a realistic operation. The storage is inserted in a closed loop on the evaporator side of the heat pump. Since no load is connected to the heat pump, the system serves only the storage. To simulate a realistic operation, where the LTES is employed only when needed and the HTF does not always flow in the dedicated loop, a variable signal to the pump is provided to stop the mass flow rate after a certain time. This allows to investigate both the charging time of the storage, as well as the thermal losses to the ambient when the LTES is not used.

The model is run for seven hours, and the charging time of the storage is monitored through the state of charge.

The state of charge is defined as the ratio between the energy stored at a certain time and the maximum storable energy [5].

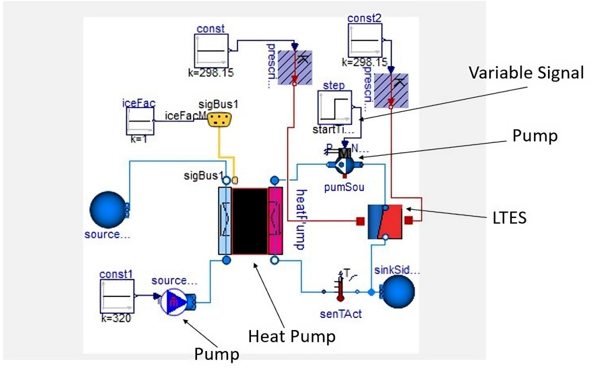

Figure 9: Heat Pump + LTES

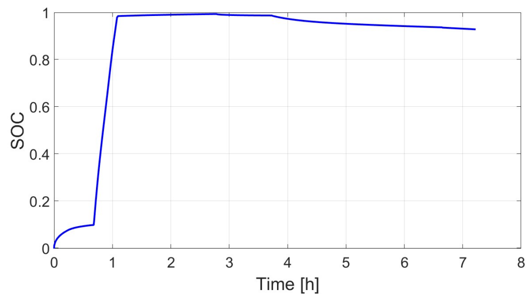

Figure 10: State Of Charge

The results show that it takes one hour to reach 100% of SOC. In the graph, it is possible to see two different trends in the charging process. At first, the PCM is in the solid state, and the energy content is reached through sensible energy. The increase in the slope of the charging process comes from the latent heat of fusion. The highest energy content of the storage, in fact, stands in the enthalpy of phase transition. For this particular case, the charging process stops when the PCM is fully melted. When the circulating pump is stopped, the SOC starts decreasing due to the thermal losses. As expected, due to the very low thermal conductivity of the PCM, and due to the phase change at almost constant temperature, thermal losses are not very relevant. The SOC takes almost four hours to decrease from 100% to 95%.

Finally, the model is validated with an experimental study from literature [6]. The storage design is presented in Fig 11.

The PCM is n-octadecane and its properties [7] are reported in Table 1.

The storage parameters are inserted in the Mod-

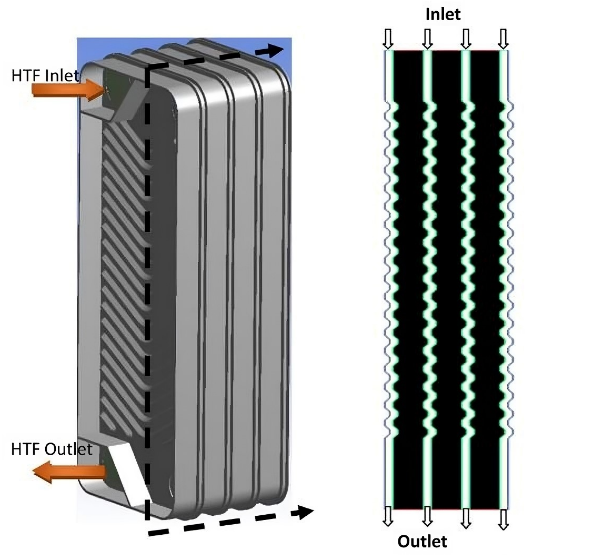

Figure 11: LTES Design

PCM	n-octadecane
ρ_l $[kg/m^3]$	774
ρ_s $[kg/m^3]$	814
T_m $[C]$	28.2
μ $[kg/ms]$	0.0085
$c_{P,s}$ $[kJ/kgK]$	2.150
$c_{P,l}$ $[kJ/kgK]$	2.180
k_l $[W/mK]$	0.1505
k_s $[W/mK]$	0.358
ΔH_m $[kJ/kg]$	189
β $[K^{-1}]$	0.00091

Table 1: PCM specifications

elica model, and the results are compared with the experimental ones. In particular, the authors provided the storage mean temperature as a function of time for three different HTF inlet temperatures. In particular, 62°C, 57°C and 52 °C. The results are reported in Fig 12.
In the graph, the mean non dimensional temperature is the ratio between the mean temperature of the storage and 62°C.
The results show that the temperature trends are very close to the experimental ones. For all cases, the highest difference in the trend is reached in the initial periods of charging. It should be noted that in the study it is not specified how the average temperature of the storage is determined. The average storage temperature for the Modelica model is calculated as the arithmetic mean of the temperature of each node of the 2D grid PCM at each time of the simulation.

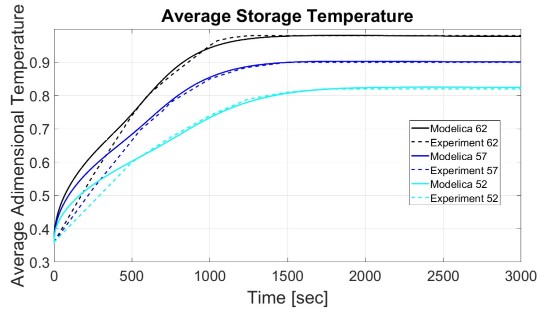

Figure 12: Experimental Validation: Storage temperature as a function of time

The error from the experimental results is computed.

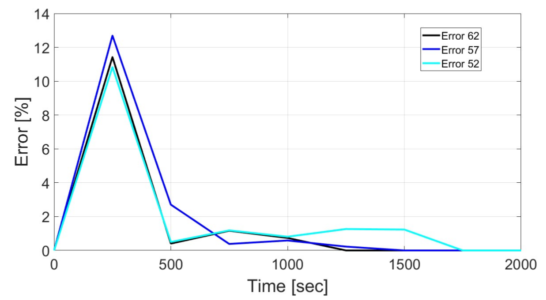

Figure 13: Experimental Validation: Temperature error as a function of time

The error is computed as:

$$e = \left| \frac{T_{model} - T_{experimet}}{T_{experiment}} \right| \cdot 100 \tag{8}$$

The graph shows that the highest error is in the initial times of charging. The error never overcomes 13%. However, it converges quickly to very low values. The very low error is considered as a validation of the Modelica model.

6. Conclusion

This thesis work was able to couple object oriented modelling and CFD simulations to replicate a complex mechanism, such as the one of heat transfer with phase change, with a simplified approach but with an acceptable level of accuracy. CFD turned out to be an extremely powerful tool to be fully aware of the consequences of making particular assumptions when developing simplified modelling approaches.
The integration of the LTES model in a heat pump allowed to investigate the realistic behavior of the system, studying the charging time

and the impact of the thermal losses when the storage is not operated.
The consistency between the Modelica simulation and experimental data not only confirms the robustness of the model, but also provides confidence in its predictive capabilities.
Future work should consider applying the developed guidelines when modelling LTES, to insert it in wider energy systems and develop accurate control strategies and energy management techniques, with an acceptable level of accuracy and computational cost.

7. Bibliography

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