# Multiscale thermo-fluid modelling of macro-encapsulated latent heat thermal energy storage systems

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# 1 Introduction

The Paris agreement was approved by approximately 170 countries, which establish goals to reduce global temperature by 1.5 to 2 °C [1]. To meet these demands, reducing exhaust gas emissions from conventional energy forms is also equally important alongside moving to renewable energy forms. According to REN21, renewable energy production contributed only up to 20 % of the global energy supply in 2016 [2]. Due to the growing infrastructure and increasing energy demand, conventional energy forms cannot be terminated very soon without sufficient contribution from alternative energy forms. Therefore, reusing energy losses from conventional energy processes is a wise solution, which supports emission reduction alongside increasing system efficiency.

In many industrial processes heat is produced as a bi-product, which is generally gone ”wasted” when released into environment. This heat can actually be stored as thermal energy in different forms. Thermal energy storage units in this aspect play an efficient role to store this energy and deliver it back when needed. Thermal energy can stored in the form of sensible heat, latent heat and thermo-chemical heat [3]. Thermo-chemical energy storage (TCES) units involve chemical reactions to store thermal energy, which is influenced on the chemical stability and operating conditions. Sensible heat thermal energy storage (SHTES) units are relevant in processes where waste heat can be instantly required, because they exhibit larger heat losses compared to latent heat thermal energy storage (LHTES) units. In addition, SHTES units also have a lower storage density compared to latent heat thermal energy storage (LHTES) units. Whereas, LHTES units which employ phase change materials (PCM) show high storage density compared to SHTES units.

LHTES units with PCM showcase a high storage capacity but also low charging and discharging powers. The low charging and discharging of LHTES units is triggered by poor thermal conductivity of PCM. In this case, macro-encapsulation of PCM is an effective way to treat the low charging and discharging powers through an enhanced heat transfer area [4]. Meanwhile, macro-encapsulation of PCM offers a wide range of encapsulation forms alongside different layout possibilities. Heat transfer fluid (HTF) used to charge and discharge the storage unit also plays an important role on the heat transfer around the PCM capsule. Therefore, to develop an efficient LHTES unit, different parameters need to be studied. Practical construction of LHTES units with such different configurations is expensive and time consuming. Here, numerical modelling and simulation of macro-encapsulated LHTES unit at different scales provide a detailed overview of the parametric influence on efficiency. Therefore, a detailed study of macro-encapsulated LHTES unit at multiple scales is presented in the present work. Different length scales are defined, where PCM capsule size is considered as the smallest scale and LHTES unit as large scale. The row of multiple PCM capsules in a LHTES unit is defined as an intermediate scale.

To store thermal energy below 100 °C, water is generally affordable. But, to store thermal energy at higher temperatures, PCM are more appropriate. Alongside storing thermal energy at high temperatures, PCM also offer a high storage capacity. This high storage capacity when combined with macro-encapsulation offers a wide range of applications ranging from stationary to mobile storage units. Transport of waste heat with mobile storage units has a great potential to serve energy demands [5]. Thereby, in the present work a laboratory scale macro-encapsulated LHTES unit for mobile applications is developed. For the developed laboratory scale macro-encapsulated LHTES unit, salt-hydrate $MgCl_2 \cdot 6H_2O$ is employed as PCM and aluminium is used as an encapsulation material. Therefore, a great demand to study the behaviour of LHTES unit exists at a large scale. But, due an opaque liquid phase of $MgCl_2 \cdot 6H_2O$, it is difficult to employ optical measurement technique to study phase change in a PCM capsule. Therefore for small and intermediate scales, paraffin RT35HC from Rubitherm is employed to validate numerical models for solid-liquid phase change.

During the charging and discharging of a LHTES unit, melting and solidification of PCM in the PCM capsule is observed respectively. Due to the presence of liquid natural convection and close contact melting, melting of PCM is relatively more complex than solidification process. These effects in a melting process can accelerate and deteriorate the melting rate of PCM. Whereas, PCM solidification in a macro capsule can be represented by a simple Fourier conduction equation. Therefore in the present work, numerical model is employed to investigate and validate a melting process inside a PCM capsule. Whereas, using the complete numerical model for a large scale LHTES unit both charging and discharging processes are studied. Description of numerical models along with the structure of this work is described in chapter 4.

# 2 Motivation for the present work

In order to meet the increasing energy demands and reducing emissions, installation of latent heat thermal storage units in different industrial applications need to be intensified. For better thermal charging and discharging with large heat transfer surface, macro-encapsulation of PCM is relevant. Moreover, to achieve better storage configurations studying heat transfer and fluid flow inside macro-encapsulated LHTES unit at different scales is also very important. But, due to large choice of PCM and capsule forms it is difficult to investigate various storage parameters of a macro-encapsulated LHTES unit through prototyping. In this case, analytical models are not sufficient to represent the detailed physical occurrence of fluid flow and heat transfer in a LHTES unit accurately. Therefore, numerical modelling and simulation plays a vital role here to understand and optimize the behaviour of thermal storage unit at different length scales.

The goal of this work is to bridge the gaps between detailed modelling of PCM capsule and system simulation of storage units, which supports an effortless parametric study of the thermal storage units. Therefore, in the present work a multi-scale numerical modelling is introduced to represent latent heat thermal storage units at different scales. Its focus answers the following questions:

1. How evolved is the field of numerical simulation to substantially study the behaviour of LHTES units at different length scales?
2. How can physical process in a small scale PCM capsule be represented in a large scale macro-encapsulated LHTES unit?
3. What is the role of natural convection and close contact melting in a macro-capsule?
4. Which factors need to be taken into account to develop an efficient macro-encapsulated LHTES unit?

In this work, these questions are answered using a systematic approach. The methodology developed to study LHTES units at different scales is structured in the form of different numerical models. Experiments are employed to validate these numerical models at multiple scales. The structure of the present work is depicted as:

- The detailed description of state of the art in chapter 4 draws the motivation for this work.
- The core of work lies in multiscale modelling of LHTES systems, which is described in chapter 5. The distinctive numerical models presented in the chapter 5 illustrate the governing equations required to model the latent heat thermal storage units at different scales.
- Experimental set-up adapted to validate the numerical models is described in chapter 6. The experiments range from studying the solid-liquid phase change in a small scale cavity

to investigating the thermal charging and discharging of laboratory scale thermal storage unit.

- The boundary conditions and material properties of the experiments are adapted into computations with developed numerical models. These computed results from numerical models are compared with experiments in chapter 7. Deviations of numerical results from experiments is also discussed in chapter 7. In chapters 5 and 7, the methodology to compute the charging and discharging of a LHTES unit from a small scale capsule is presented.
- In chapter 8, the influence of capsule material and capsule wall thickness are studied with the developed large scale storage model.

The systematic approach developed to establish an efficient storage configuration is shown in Fig. 2.1.

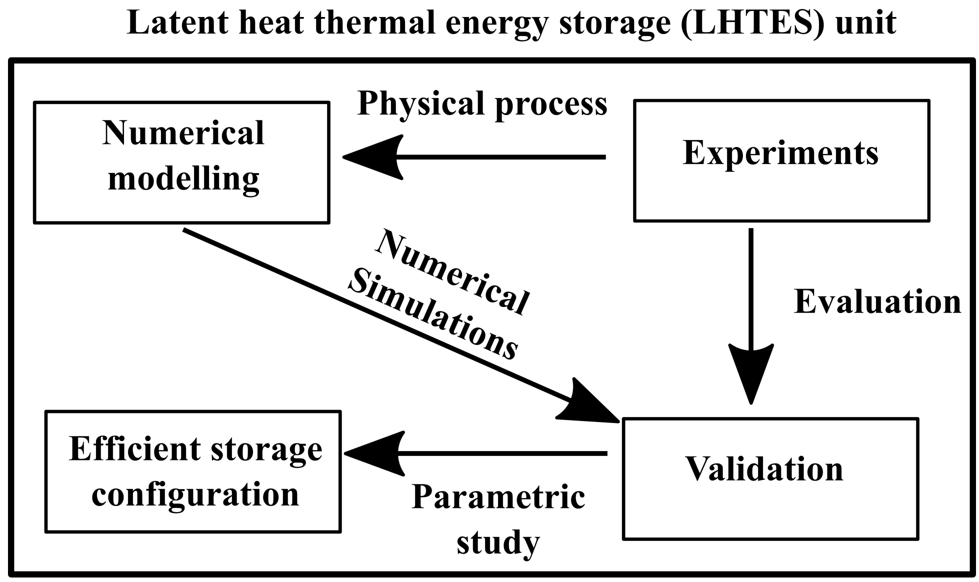

Figure 2.1: Overview of steps involved to develop an efficient storage configuration.

# 3 Computational Thermo-Fluid Dynamics

Physical phenomena involving heat transfer and fluid flow are found in different industrial and natural processes. Scientific understanding of such processes can be improved by studying them in detail. Different physical and operating conditions need to be investigated for a detailed understanding of such processes. Therefore, a conclusive study of any physical process demands a huge investment of time and resources. At the same time it is also difficult to understand complex physical phenomena without having a concrete understanding of each parameter. Numerical modelling in this context may reduce the effort needed to investigate a physical process in detail. Here, a physical process can be represented in the form of numerical model using governing equations. The work-flow involved to find a physical solution for an existing physical process using a numerical model is shown in Fig. 3.1.

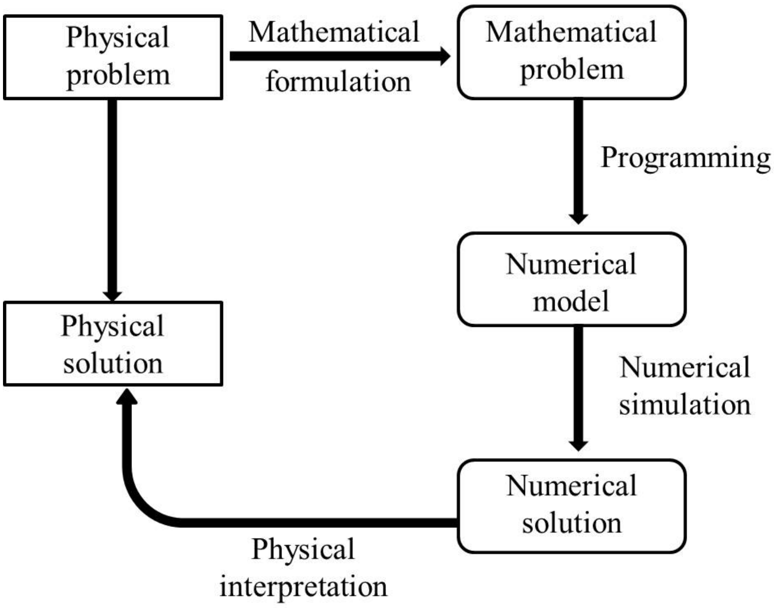

Figure 3.1: Work flow chart depicting the steps to represent a physical process in the form of a numerical model.

The reality is formulated as a mathematical problem, which is implemented in the form of a numerical model using computer programming. A numerical model employs mathematical equations to obtain solutions with defined boundary conditions of a physical problem. In general, a numerical model can be solved to obtain strong or weak solutions, which depends on the mathematical formulation. For a weak formulation, the accuracy of the numerical model depends on its problem definition and solution methodology. In computational thermo-fluid dynamics, physical phenomena are represented in the form of governing equations, which are solved to conserve basic governing laws in a computational domain [6].