CFD modeling of heat charging process in a direct-contact container for mobilized thermal energy storage

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Spring 2011

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Abstract:

Thermal energy storage and phase change materials become increasingly important topics during the last 20 years for heating and cooling purpose in buildings. When there is time delay or mismatch between producing energy and energy demand, thermal energy storage provides a great solution. Furthermore, in the case of space differences between supplier and end user, the mobilized thermal energy storage can be introduced. In this solution the waste and excess heat, which is released from a factory, is recycled by storing in the PCM through heat transfer fluid and transported by a mobilized container to a consumer. In charging process the PCM is initially solid; it becomes melt while the heat transfer fluid flows inside the container. In order to achieve the highest efficiency of transferring energy in charging and discharging process, the melting and solidification times should be considered. In this paper the heat transfer behavior of the phase change material during the charging process has been simulated by CFD modeling of the previous work on Mobilized Thermal Energy Storage. Transient two dimensional heat transfer problems are solved by simulating in the Fluent software while heat is stored in PCM. In order to simulate the phase change in PCM, the Volume-Of-Fluid (VOF) method is extended by the energy conservation to solve for the temperature in the material. The validation of the computational model has been conducted by comparison between experimental data and CFD results; the agreements between the results are convincing. The liquid fraction as functions of time is achieved and the total melting time is estimated. Presented results in this paper lay the groundwork for a future investigation to get more accurate prediction of thermal performance of mobilized thermal energy storage system.
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1. Introduction:

1.1. Background:

Due to the exhaustion of natural energy resources and heavy environmental impacts such as climate change, global warming, ozone layer depletion etc. thermal energy storage (TES) is becoming increasingly important topic for heating and cooling purpose in buildings. There are various materials that can be used for thermal storage, selecting the proper material is very important. Among these materials the phase change materials (PCM) receives a great attention. Waste heat from the factory has a potential to supply thermal energy for space heating. With the application of the PCMs, waste heat can be delivered to a distributed end user, instead of being released to the atmosphere, which can be harmful to the environment. In order to deliver the waste heat a new concept of mobilized thermal energy storage (M-TES) system was proposed, which consists of a thermal energy storage container, a heat exchanger for charging and discharging heat, thermal storage (TES) material, a pump and a lorry.

Some companies in Germany such as LSG Sky Chefs and TransHeat were among the earliest companies which introduced and used a commercial M-TES system. In Japan, three M-TES systems have been implemented, in the first one heat is transported between two factories by using the excess heat produced by electric company and supply preheat feed water for a boiler in another company. In the second and third system the higher temperature heat is supplied for industrial and residential users by transporting waste gas from furnace.

To make a systematic study of the M-TES system, a compact lab-scale system was designed and built by Weilong Wang in laboratory of Mälardalen University. Also, Characteristics of PCM were studied, and the performance of the direct-contact TES container was investigated. However, some approaches such as designing different structures for M-TES container in order to decrease the charging process and speeding the melting time were not investigated. The CFD modeling of heat transfer in charging process has been done in the presented work. In future work in order to enhance the thermal performance of M-TES, different structures for container will be investigated.
Because of their broad potential applications, thermal energy storage technology is a promising technology for heating and cooling purpose in energy efficient buildings.

1.2. Scope of the Thesis

In this work the heat transfer for a system with direct-contact was investigated using Fluent version 12.1. The study is focused on the transient heat transfer during melting PCM, in the M-TES system.

1.3. Objective

The objectives of this work are:

- Setup the CFD modeling of heat transfer during the melting phase change of material
- Validation of model by comparing the results with experimental data
- Heat transfer enhancement in order to provide guidelines to the design of M-TES container

1.4. Input and Assumptions:

The initial temperature of the whole system is uniform, 26°C i.e. the PCM is in solid phase. The process starts with a flowing of the HTF through the inlet. According to the experimental data in the charging process in order to provide the PCM change of phase, the temperature of the HTF within the mass flow rate of 21.01 l/min is 141 °C. The PCM becomes melt after storing the released heat from HTF. The computational model has been validated with experimental data. As a result of the simulation for observing the evolution of the heat transfer in the system while PCM is being melted, PCM melt fraction contours has been presented.
2. Literature Review of Mobilized Thermal Energy Technology:

A literature review including reviews on TES technologies, TES materials, and TES applications has been conducted as the following text.

2.1. Thermal Energy Storage technology:

2.1.1. Thermal Energy Storage Methods

Thermal energy can be stored in different methods; the most common of them are sensible heat, latent heat and chemical energy.

2.1.1.1. Sensible heat

When adding heat affects the temperature of material it would be classified as sensible type. Similarly, it would be sensible heat when the temperature of materials falls while heat is removed from an object.

2.1.1.2. Latent Heat

The difference between sensible heat and latent heat is related to changing the temperature of materials by adding heat, if the temperature stays constant by heating and just the phase is changed it would be classified as latent heat. By comparison, latent heat storage can store more heat due to large thermal energy storage density and phase changing of storage material; these materials are called Phase Change Material (PCM). Since the large amount of energy can be stored at a nearly constant temperature in relatively small volume, the latent thermal energy storage method received a great consideration.

2.1.1.3. Chemical Reaction

When by adding heat the compound is broken into its initial components or vice versa, the system of storing heat is based on chemical reaction.
2.1.2. Thermal Energy Storage Container

Thermal energy storage (TES) container can be designed in two ways which are direct contact and indirect contact.

2.1.2.1. Direct Contact

In TES direct contact container, TES materials, PCM, are directly mixed with the Heat Transfer Fluid (HTF). So, in this method the chosen PCM should not be able to soluble in HTF and for separating from each other it is necessary to have a large density difference between the PCM and HTF. In this method HTF is pumped into the container to heat the PCM and cause melting, the result is a great heat transfer performance due to a direct contact. After this dynamic charging process, due to the density difference HTF rises and exists from the container.

2.1.2.2. Indirect Contact

Another kind of TES container is indirect contact method, in this way HTF passes through the heat exchanger that located in the container, the heat transfer performance depends on the PCM thermal conductivity and contact surface area between PCM and HTF.

2.2. Thermal energy storage material:

2.2.1. Phase Change Material (PCM) for Energy Storage:

Phase change materials (PCMs) have been widely used to store thermal energy as latent heat. PCM can absorb a great amount of heat when it reaches the melting point while its phase changes without increasing the temperature. The PCM changes its phase to solid and release heat when the nearby ambient temperature of it falls. Hence, PCM changes its phase and absorb or release heat approximately in a constant temperature. The low thermal conductivity of PCM, which is usually below 0.5 W/(m*K), affects considerably the heat transfer enhancement and performance of the TES system. Hence, in order to compensate the low thermal conductivity of PCM the appropriate techniques for heat transfer should be developed.
2.2.2. Classification:

Phase change material (PCM) can be divided into two major groups which are organic or inorganic compounds.

2.2.2.1. Inorganic Compounds:

The inorganic PCM has poor stability in two aspects which are during repeated thermal cycling and corrosion between PCM and container. Also, in liquid phase they have sub-cooling effect and they show corrosive behavior to many metals, the most important advantage of inorganic material is their high thermal conductivity as well as high heat storage capacity that sometimes is two times bigger than the organic compounds.

2.2.2.2. Organic Compounds:

The organic compounds show great stability during thermal cycling; they are non-corrosive and nontoxic. In addition, during solidification they have no sub-cooling effect; the main disadvantage of the organic compounds is low thermal conductivity.

Figure 1 Classification of energy storage materials.
2.3. Thermal Energy Storage Application:

2.3.1. PCM Application:

PCM application has been growing widely during the last few years; followings are some applications of PCM:

2.3.1.1. Buildings Applications:

PCMs can be used in building envelopes such as wall, floor, windows or ceiling for heating or cooling purpose, they contribute to decrease the active heating demand i.e. in winter time they store solar energy during the day and release it to indoor air at night when the temperature falls, also during summer time cool from ambient air at night can be stored by natural or forced convection and released during day time to the indoor air. By smoothing the temperature variation, the main PCM application in building envelope is in light weight buildings when high heating and cooling is demanded. Due to their low thermal inertia the light building face great temperature fluctuation, so by adding PCM into building materials thermal capacity of building envelope can be increased.

2.3.1.2. Waste Heat Recovery Application:

PCM can be used to store waste heat available from industry, furnace, company etc. and recover it when there is heating demand. PCM can be placed in the container and change its phase by passing heat transfer fluid (HTF), which is heated by waste heat, through the container.

2.3.1.2.1. Mobilized Energy Storage:

Meeting heating demand in sparse area and detached houses that are not connected to the district heating (DH) need a large capital investment to extend the existing DH to these areas, this solution is not economical since there is low heating demand and high enterprise. Mobilized thermal energy storage (M-TES) can be a good solution to meet the heating demand in sparse and detached area by recovering waste industrial heat. A heat transfer medium such as oil or water should be used for transferring heat from supply to demand. By using M-TES a balance can be generated between the heat source and an end user, no matter how far they are from each other.
M-TES Components:

M-TES system consists of TES container, heat exchangers in a charging or discharging station, circulated pumps, lorry, TES material and heat transfer medium (HTM). TES material plays an important role in storing and releasing heat in charging and discharging process respectively. HTM can be oil or water which is used in delivering heat from supply to demand.

2.3.1.3. Other Applications:

PCM can be used in the air conditioning, chiller, heat pump, solar collector or even in computer cooling. Also, another application could be in transporting food, medication or other sensitive materials that must be preserved above the specific temperature since the PCM can store heat or cold in a range of very limited degrees.

3. Definition of problems and methodology:

3.1. Definition of problems:

The CFD simulation of the PCM chamber has been done to investigate the heat transfer mechanism, the melting time and the influence of the structure in charging process using Fluent 12.1.

3.1.1. Charging Process

In the charging process, the PCM which is in solid phase is melted by getting heat from the hot oil; the oil is pumped into the container and the heat is transferred by direct contact between HTF and PCM. The mass flow rate of HTF with the temperature of 141 °C is 21 l/min.

3.2. Methodology:

For simplifying the model, only the PCM chamber is considered with five inlets in bottom edge and outlet in the upper edge. The VOF method is used for introducing the multiphase model. The
HTF comes to the PCM chamber through the inlets and goes out from outlet. The heating transfer by direct contact between PCM and HTF is achieved.

4. CFD Modeling of Mobilized Thermal Energy Storage:

4.1. Model:

A simplified 2-dimentional pressure-based CFD model was developed in Fluent to simulate the heat charging process. Due to the time dependency the unsteady condition is used in this calculation.

In order to simulate the phase change in PCM, the Volume-Of-Fluid (VOF) method is extended by the energy conservation to solve for the temperature in the material.

![Figure 2 Geometry of the Model](image)

The solidification and melting option is enable in this model within retaining the default value of mushy zone constant which is 100000 and is acceptable for most cases. Since we have the heat transfer problem, the energy equation should be active.

During the charging process, the main heat transfer mode in the TES system is transient conjugate phase change convection, and heat is transferred from the HTF to the PCM. In order to
reduce the heat transfer to the environment, the outside tube was thermally well insulated. Therefore adiabatic conditions are assumed during charging process.

4.1.1. Governing equations

For transient 2-D heat transfer problem in latent thermal energy storage unit the governing equations are energy, momentum and continuity equation. The segregated solver is only available for solving the equations in solidification/melting model. In this method each discrete governing equation is linearized implicitly considering dependent variable of equation.

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta$</td>
<td>liquid fraction</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Heat Capacity (j / kg.°C)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density (kg/m3)</td>
</tr>
<tr>
<td>$H$</td>
<td>the total enthalpy (j/kg)</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>latent heat enthalpy (j/kg)</td>
</tr>
<tr>
<td>$h$</td>
<td>sensible heat enthalpy (j/kg)</td>
</tr>
<tr>
<td>$h_{ref}$</td>
<td>the reference enthalpy (j/kg)</td>
</tr>
<tr>
<td>$k$</td>
<td>thermal conductivity(w/m. k)</td>
</tr>
<tr>
<td>$L$</td>
<td>latent heat of the material (J/kg)</td>
</tr>
<tr>
<td>$P$</td>
<td>pressure (pa)</td>
</tr>
<tr>
<td>$S_n$</td>
<td>Energy source/sink term (W/m3)</td>
</tr>
<tr>
<td>$S$</td>
<td>Momentum source/sink term ( N/m3)</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature (°C)</td>
</tr>
<tr>
<td>$T_{ref}$</td>
<td>reference temperature (°C)</td>
</tr>
<tr>
<td>$V$</td>
<td>fluid velocity (m/s)</td>
</tr>
<tr>
<td>$v_p$</td>
<td>solid pull velocity (m/s)</td>
</tr>
<tr>
<td>$\mu$</td>
<td>dynamic viscosity (kg/m.s)</td>
</tr>
</tbody>
</table>
4.1.1.1. **Energy Equation:**

\[
\frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\rho v H) = \nabla \cdot (k \nabla T) + S_n
\]

where:

\[
H = h + \Delta H
\]

\[
h = h_{\text{ref}} + \int_{T_{\text{ref}}}^{T} C_p \, dT
\]

\[
\Delta H = \beta L
\]

\[
\begin{cases}
\beta = 0 & \text{if } T < T_{\text{solidus}} \\
\beta = 1 & \text{if } T > T_{\text{liquidus}} \\
\beta = \frac{T - T_{\text{solidus}}}{T_{\text{liquidus}} - T_{\text{solidus}}} & \text{if } T_{\text{solidus}} < T < T_{\text{liquidus}}
\end{cases}
\]

The source term, \( S_n \), contains contributions from convection, latent heat transfer due to phase change and any other volumetric heat sources.

As it can be seen from above equation, the linear relationship between temperature and liquid fraction is used in Fluent; other relationships are not currently available in Fluent\(^2\).

4.1.1.2. **Momentum Equation:**

A single momentum equation is solved throughout the domain, and the resulting velocity field is shared among the phases. The momentum equation, shown below, is dependent on the volume fractions of all phases through the properties \( \rho \) and \( \mu \):

\[
\frac{\partial}{\partial t} (\rho v) + \nabla \cdot (\rho vv) = \nabla [\mu (vv + vv^T)] - \nabla P + \rho g + S
\]
Where

\[ S = \frac{(1-\beta)^2}{(\beta^3 + \varepsilon)} A_{mush} (v - v_p) \]

The momentum source term, \( S \), contains contributions from the porosity of the mushy zone, the surface tension along the interface between the two phases, and any other external forces per unit volume\(^4\). Momentum sink terms are added to the momentum equations to account for the pressure drop caused by the presence of solid material\(^4\).

\subsection*{4.1.1.3. Continuity:}

\[ \frac{\partial p}{\partial t} + \nabla \cdot (\rho v) = 0 \]

\section*{4.2. Mesh:}

A structured quadrilateral mesh for the system was created. A boundary layer was applied to all wall surfaces during meshing. CFD modeling has been studied for a grid size of 943 nodes.

![Figure 3 meshing of the model](image-url)
4.3. **Assumption:**

The modeling is based on the following assumptions:

- the PCM is homogeneous and isotropic
- the HTF is incompressible
- flow of the HTF is laminar
- inlet mass flow rate of HTF is constant
- inlet temperature of HTF is constant
- initial temperature of the system is uniform and the PCM is in the solid phase for melting
- adiabatic wall is assumed
- the problem is two-dimensional
- thermo physical properties of the HTF and the PCM are constant

4.4. **Boundary condition:**

The boundary condition is divided into four parts which are: walls, inlet, outlet, and PCM chamber.

The temperature of HTF within the mass flow rate of 21.01 l/min in charging (melting) process for inlet is 141 °C (according to the experimental data).

**Table 3: Boundary Condition**

<table>
<thead>
<tr>
<th>Boundary/ zone name</th>
<th>setting</th>
</tr>
</thead>
<tbody>
<tr>
<td>outlet</td>
<td>Pressure outlet</td>
</tr>
<tr>
<td>inlet</td>
<td>Mass-flow inlet</td>
</tr>
<tr>
<td>Outer wall</td>
<td>wall</td>
</tr>
<tr>
<td>PCM</td>
<td>interior</td>
</tr>
</tbody>
</table>
4.5.  **Input data:**

4.5.1.  **Materials:**

The properties of materials, including the melting heat, solidus temperature, and liquidus temperature, according to the following tables are given to the program. The material properties used in the simulations are based upon the experimental chosen materials i.e. Erythritol as PCM and thermia oil as HTF.

4.5.1.1.  **Erythritol:**

Erythritol (molecular formula: $C_4H_10O_4$) is a natural sugar alcohol (a type of sugar substitute) which has been approved for use in the United States and throughout much of the world.

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting point (°C)</td>
<td>118~121</td>
</tr>
<tr>
<td>Enthalpy (kJ/kg)</td>
<td>339</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>1450 (at 20°C)</td>
</tr>
<tr>
<td>Specific heat (kJ/kg. °C)</td>
<td>1.35 (at 20°C); 2.74 (at 140°C)</td>
</tr>
<tr>
<td>Viscosity (kg/m s)</td>
<td>0.02895 (at 20°C); 0.01602 (at 150°C)</td>
</tr>
</tbody>
</table>

4.5.1.2.  **Thermia Oil C:**

There is no detailed Information on Thermal oil C, but Shell company offer the Information of Thermia Oil B, which is based on carefully selected highly refined mineral oils chosen for its ability to provide superior performance in indirect closed fluid heat transfer systems. It is said by Shell Company that Thermia oil C has better characters of heat transfer with a lower viscosity.
Table 2 Properties of Thermia oil B

<table>
<thead>
<tr>
<th>Temperature</th>
<th>°C</th>
<th>0</th>
<th>20</th>
<th>40</th>
<th>100</th>
<th>150</th>
<th>200</th>
<th>250</th>
<th>300</th>
<th>340</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>kg/m³</td>
<td>876</td>
<td>863</td>
<td>850</td>
<td>811</td>
<td>778</td>
<td>746</td>
<td>713</td>
<td>681</td>
<td>655</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>kJ/kg*K</td>
<td>1.809</td>
<td>1.882</td>
<td>1.954</td>
<td>2.173</td>
<td>2.355</td>
<td>2.538</td>
<td>2.72</td>
<td>2.902</td>
<td>3.048</td>
</tr>
<tr>
<td>Conductivity</td>
<td>W/m*K</td>
<td>0.136</td>
<td>0.134</td>
<td>0.133</td>
<td>0.128</td>
<td>0.125</td>
<td>0.121</td>
<td>0.118</td>
<td>0.114</td>
<td>0.111</td>
</tr>
</tbody>
</table>

4.6. Solution:

Since the liquid-solid mushy zone is treated as a porous zone in Fluent the enthalpy–porosity approach is used as a solution for solving the problem. In this attitude the porosity for each cell is equal to the liquid fraction of that cell. According to the enthalpy equation the liquid fraction \( \beta \), which indicates the fraction of the cell volume that is in liquid, is computed at each iteration. In the liquid phase \( \beta \) takes the value 1, in the solid \( \beta = 0 \) and \( 0 < \beta < 1 \) in the mushy zone. The mushy zone is modeled as a “pseudo” porous medium in which the porosity decreases from 1 to 0 as the material solidifies; the velocities also drop to zero. The fluid flow was assumed to be laminar due to the small velocities applied in the present investigation. The CFD model developed under normal atmospheric pressure.

The modeling parameters are as following items:

- Double-precision with pressure-based solver
- Energy under-relaxation factor of 0.8, default values for all other components
- First Order Upwind discretization of Momentum and Energy equations.
- SIMPLE Pressure-Velocity coupling
- Polynomial correlation used to define temperature dependent material properties (i.e. density, Specific Heat and thermal Conductivity)
- The residual value for solution convergence criteria for the energy equation is set to \( 1 \times 10^{-6} \), default values for all other components.
5. Results and Discussion:

5.1. Results:

As a result, the melting of the PCM has been observed, at initial condition the PCM was solidified in the room temperature. With respect to the low HTF inlet velocity of 0.9 m s\(^{-1}\), the laminar flow has been considered for modeling. The simulations provided detailed phase distributions as the following figures.

![Figure 4: Phase distribution](image)

The temperature distributions are non-uniform in PCM due to very low thermal conductivity. The conduction heat transfer is predominated in the system from the beginning of the process till starting the phase change of the PCM. After starting the melting phase, both heat conduction and natural convection are taking place in the system. The more progress in melting process, the more enhancement of natural convection is occurred. The temperature of the system reaches the steady state condition when all of the PCM is melted and heated to the inlet HTF temperature. The total melting time is about 1 hour.

5.2. Discussion:

In the experiment the mass of the PCM was 72.8 kg with 0.27 kg.s\(^{-1}\) oil flow rate through the inlet; however the figure of 11.8 kg for PCM’s mass and 0.27 kg.s\(^{-1}\) for oil flow rate in inlet was considered in the simulation. The required time for melting the 11.8 kg PCM in simulation is about 1 hour, it is obvious that it should be lower than experimental results which were 4 hours
for melting 72 kg PCM. But if the linear proportion between melting time and mass of the PCM was considered, the figure of 40 minutes should be achieved. This disagreement between the numerical and experimental can be attributed to uncertainties of measurements, simplifications of model and using cubic shape for container rather than cylindrical shape.

By comparison between the melting shape of PCM in experiment and simulation it can be observed that the central part of PCM is melted easily and quickly but much time is required to melt those PCM that are closed to the container wall. The Agreement of heat transfer mechanism provides guidelines to design more efficient M-TES container by CFD simulation since experimental approaches require much laboratory work and money.

6. Conclusion:

In the present study, the literature review regarding the TES technologies, TES materials, and TES applications as well as the 2-D CFD modeling of heat transfer during charging process in M-TES system with a direct contact container have been conducted. Simulation predictions in charging process showed quite well agreement with the experimental data. The achieved numerical results provide a good estimation of the phase change material melting processes. It can be concluded that the presented study could be guidelines for thermal performance of the mobilized thermal energy storage system.

7. Future outlook:

In future work the author is going to conduct the 3-D model simulation for different structures of container with heat transfer enhancement in order to optimize the heating performance in the system. Also, some experiments will be done for model validation.

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