Numerical Analysis of the Phase Change Behavior of High Power Latent Heat Storages with 3D Wire Structures

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Abstract: Latent heat storage devices use the melting enthalpy of a so-called phase change material (PCM) to store thermal energy. Open porous metals, such as 3D wire structures, allow the design of systems with tailored storage capacity and power. A geometric unit cell was identified, modelled and COMSOL Multiphysics was used to investigate the transient behavior of the PCM melting front within the composite of PCM and 3D wire structure. As a result, the impact of the wire structure's material as well as the influence of brazing the inner connections of the wire structure on storage kinetics were analyzed. In order to scale the model up to the whole storage unit, a simplified geometry was developed. The simplification required an adjustment of the structure's thermal properties to keep the system's characteristics. By comparing the melting front's position over time, the adjustments and also the simplified model were validated.

Keywords: Latent Heat Storage, Phase Change Material, 3D Wire Structure, Transient Melt Front

1. Introduction

One of the main advantages of latent heat storage devices are the high volumetric storage density and the fact that the energy is stored at a nearly constant (melting) temperature. The main drawback of the most common PCMs is their low heat conductivity and, therefore, the storage power is limited. Open porous metals, such as 3D wire structures, are able to improve the effective heat conductivity of the system significantly. This allows the design of systems with tailored storage capacity and power.

PCMs are market available for a wide range of working temperatures between -50 °C up to about 800 °C as shown in Figure 1. Depending on the used PCM the possible storage capacity varies between 150 MJ/m^3 and 900 MJ/m^3. In the work presented, the main consideration were process heat applications with a temperature range of 130 °C to 350 °C. Therefore, nitrate salts like KNO_3, $NaNO_3$, $LiNO_3$ and their eutectic mixtures are used as PCM.

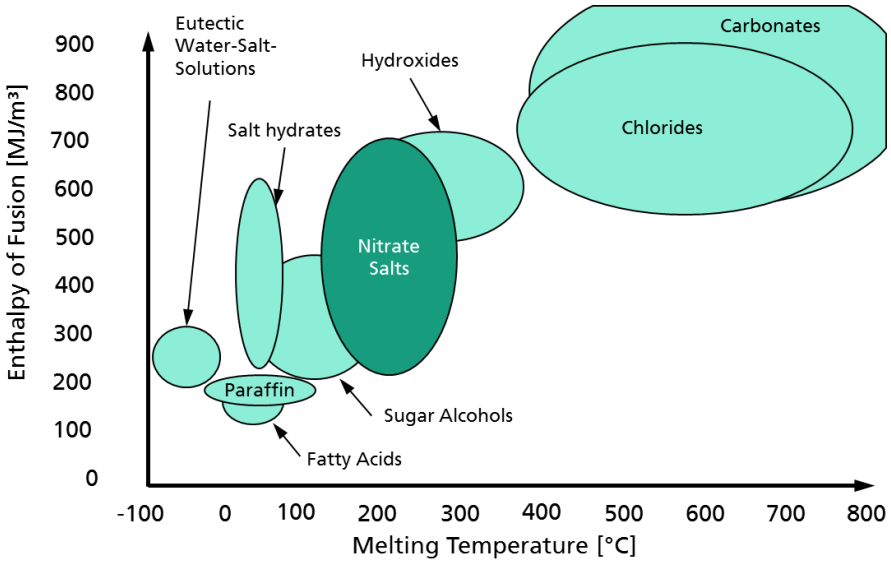

Figure 1: Properties of available phase change materials (PCM)

The aim of the work presented was to develop a simulation model which can be used to design and optimize a latent heat storage in terms of thermal capacity and power. The first step was the definition of a unit cell which was modelled and simulated using COMSOL Multiphysics 5.0.

Thermal properties like density, heat conductivity and heat capacity of the PCM were modeled through temperature dependent equations. The PCM's solid-liquid phase change was included in the heat capacity equation.

Transient simulations were conducted to investigate the influence of non-brazed and brazed wire structures of different materials with corresponding leads on the behavior of the melting front.

2. Geometrical model and simplifications

2.1 Description of the 3D wire structure

The main task was the full geometrical modelling of the 3D wire structure in order to get realistic thermal behavior of the metal-PCM-composite. The modelled 3D wire structure is a size 10 strucwire geometry which consists of regular helices combined in one plane and stacked into a 3D structure. The result is shown in Figure 2 in front and top view.

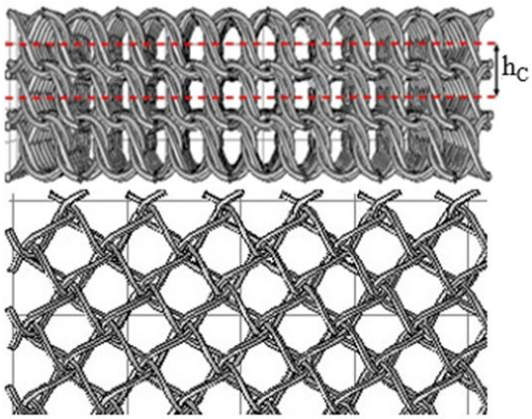

Figure 2: 3D Model of the strucwire structure (top: front view; bottom: top view)

Pipes of the size 8x1 fit in the modelled pores and were used as heat carrier tubes. The tubes are separated by 5 pores in both directions.
Therefore, the model length and width is fixed to that size. The height of the structure is periodic so the unit cell is one cell high as the red dash lines in the front view in Figure 2 indicate. By respecting geometric symmetries, the resulting simulation model contains a quarter of the unit cell including wire, PCM and heater tube, as shown in Figure 3.

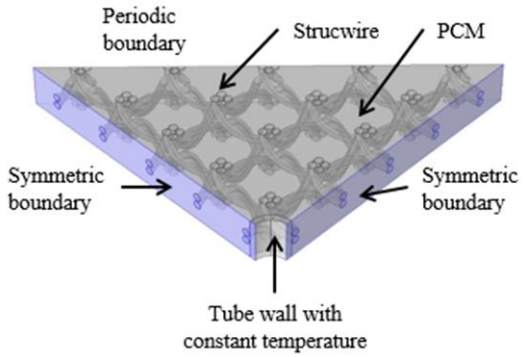

Figure 3: Resulting simulation model with boundary conditions

2.2 Modelling of the brazed wire structure

The effective heat conductivity of the wire structure can be improved by connecting the individual wires by brazing the crossroads. The brazing is done by submerging the structure into a soldering paste and a subsequent heat treatment.

In order to simulate the brazed structure, the lead has to be modelled geometrically. Therefore, a solder body (see Figure 4, left) was developed which fills the gaps between the wires, as the solder does. The wires and the solder body were combined by Boolean operations (Figure 4, right).

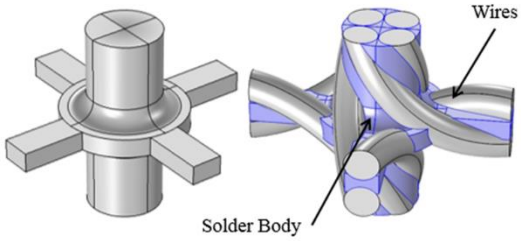

Figure 4: Solder Body (left) and combined with wires in a crossroad (right)

With this modelling approach it is possible to assign different material properties to the wire and the solder, and the influence of brazing can be clearly investigated.

2.3 Boundaries and simplifications

The given boundaries are also visible in Figure 3. Because of the applied periodic

boundaries on top and bottom of the model, the temperature difference inside the fluid flow is neglected and a constant temperature is used as boundary on the inner wall of the heat carrier pipe. Therefore, the temperature field inside the pipe's wall is considered as well as the heat transfer from the outer pipe wall into the wire structure and the PCM.

2.4 The simplified unit cell model

The geometric model has basically two different length scales: the solder knots within the wire crossroads are on a scale of 0.1 mm. The PCM between the wire structures is on a length scale of 10 to 50 mm. Therefore, the simulation mesh is quite fine and the simulated unit cell is not suitable for upscaling to the whole heat storage system. A simplified geometry for the wire crossroads was developed to be used in large-scale simulations and is shown in Figure 6. This simple body-arm construction replaces the complex structure shown in the right side of Figure 4.

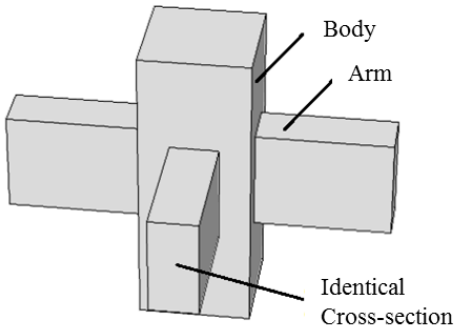

Figure 5: Simplified geometrical model of a wire crossroad including solder body

To maintain a similar behavior of the simplified model, its volume and heat transfer surface to the surrounding PCM has to be the same as in the detailed model. Also the heat conductive area which connects two crossroads has to be the same in both variants.

The thermodynamic properties of the body and the arms were defined separately, based on the composition of solder and wire material in each and every part. To maintain the thermal behavior of the structure, an empirical coefficient was introduced and defined by comparative calculations of the detailed and the simple model.

3. Methods and modelling in COMSOL

3.1 General simulation parameters

The eutectic mixture of $LiNO_3$ – KNO_3 with 33 wt.-% $LiNO_3$ is used as PCM during the simulations. It has a melting temperature of 133 °C and its material properties were taken from [1, 2]. The materials of the wire structure were C50 with nickel and copper based solders and copper with silver based solder. C50 was chosen because of its good corrosive properties in combination with molten nitrate salts. Copper was used because of its high heat conductivity and the expected high storage power.

The transient simulation begins at a system's temperature of 25 K below the melting temperature of the PCM and stops when a monitor probe reaches a temperature of about 5 K above the melting temperature. Within the first time step, the temperature boundary on the inner tube wall increases to 25 K above melting temperature by using a step function.

3.2 Modeling the phase change

The used eutectic mixture has a quite complex melting behavior. As shown in [3], there are two separate phase changes within the simulated temperature range. The first phase change is considered as a solid-solid change at a temperature of about 115 °C ± 1.5 K with a transformation enthalpy of about 18 kJ/kg. The second phase change is the actual melting at about 133 °C ± 4 K with a heat of fusion of 160 kJ/kg.

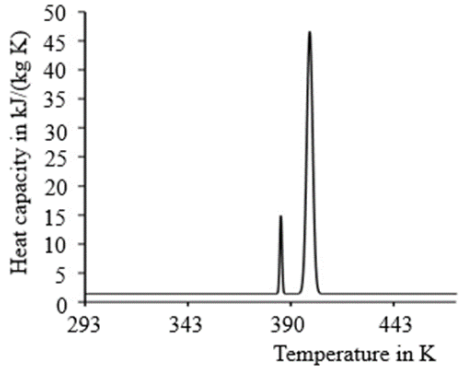

Figure 6: Simulated heat capacity of eutectic $LiNO_3$ – KNO_3 mixture

The heat of fusion is represented by a temperature dependent heat capacity function, which is shown in Figure 6. The function has three

sections: the solid and liquid state heat capacity is set as constant at 2 kJ/(kg K). The melting area is represented by two differently sized peaks considering the heat of fusion of both phase changes.

3.3 Overall melting time analysis

The overall melting time t_m of the unit cell was investigated in order to compare different wire materials and the influence of brazing the wire structure. The melting time was defined when the whole PCM inside the unit cell has changed to liquid phase.

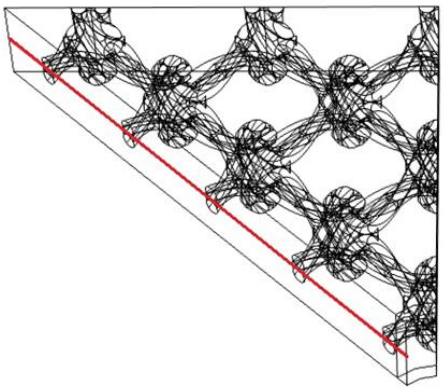

Figure 7: Cut line (red) for evaluating the melting time of the unit cell

Because of the melting area, the PCM's heat capacity was monitored. When its value on the most outer cells reaches the PCM's liquid state, the melting is finished. As shown in Figure 7 a cut line was introduced into the model, where the heat capacity was monitored for every time step calculated.

4. Results and discussion

4.1 Overall melting time

Figure 8 shows isothermal surfaces throughout the unit cell after 100 minutes for a C50 wire structure. The top and lower image represent a non-brazed and a brazed structure, respectively. The dark red isothermal surface is set to the melting temperature of the used PCM mixture, so it represents the melting front.

In the non-brazed case the isothermal surfaces are slightly more advanced around the wires than in the PCM area. This means that the melting takes place around the wires and conduction through the PCM is not the dominant factor. In the brazed case this is even more observable.

The brazed structure results in a clearly more advanced melting front which has almost reached the end of the unit cell. Hence brazed wire structures will result in considerably higher storage power.

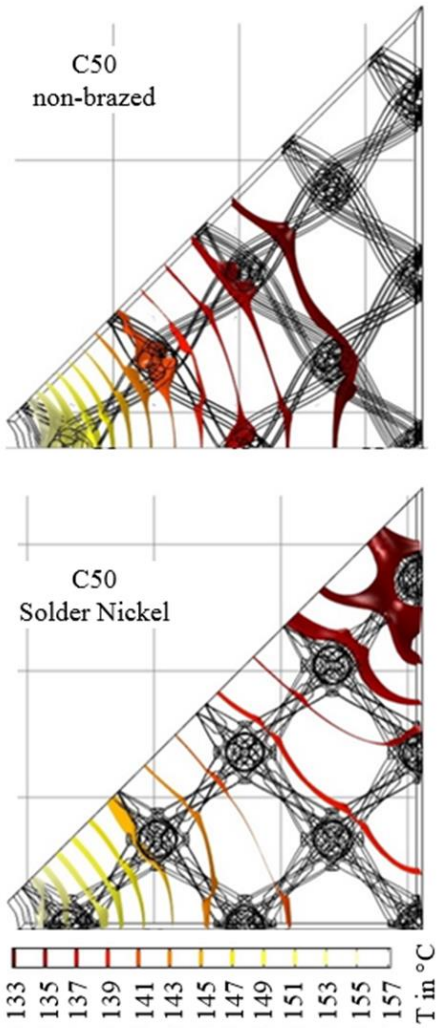

Figure 8: Temperature distribution within the unit cell at a time of 100 minutes

Analog simulations were conducted for the given wire and solder materials for non-brazed and brazed structures. The time needed to melt the whole unit cell for each case is shown in Figure 9. Additionally, the influence of brazing the structure can be seen. Blue bars indicate C50 as wire material, green bars represent a copper structure.

As expected, using copper structures leads to significantly lower melting times and, therefore, a higher storage power can be achieved. A non-brazed copper structure results in an 80 % reduction of melting time compared to a non-brazed C50 structure.

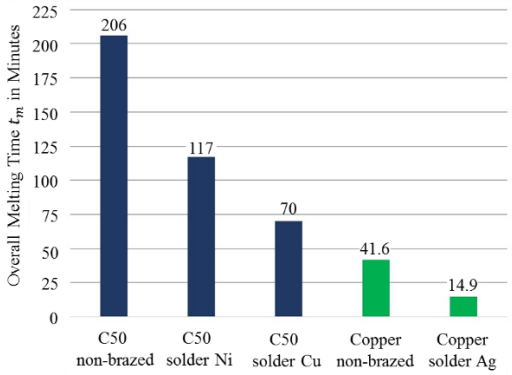

Figure 9: Overall melting times for different materials and brazes

By soldering the wire structure, the melting time can be reduced by about 65 % compared to the corresponding non-brazed structure.

4.2 Results of the simplified model

In order to use the simplified geometrical model to simulate the thermal behavior of a whole heat storage, the thermal properties had to be maintained. The thermal properties of the body and arm sections of the simplified model were designed separately. With this approach, the different composition of solder and wire within both sections was taken into account. The temperature profile over time of both models is given in Figure 10 and both models show nearly the same characteristics. The simplified geometry shows a slightly higher heat conductivity.

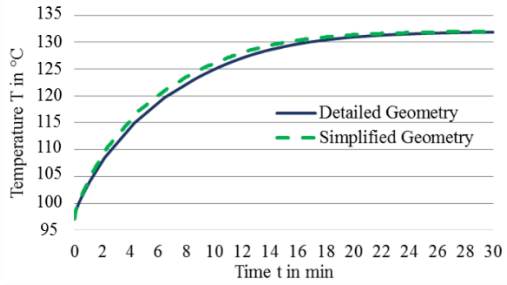

Figure 10: Comparison of crossroads mean temperature of detailed and simplified model

Even this small difference leads to a shorter melting time of up to 10 % of the simplified geometry depending on the used material set. To compensate this, an empirical coefficient was introduced into the heat conductivity of the simplified geometry. This coefficient ranges between 0.90 and 1.05 and depends on the material combination of wire and solder. It was determined through multiple, comparative simulations. For the given case in Figure 11, the factor is 0.91.

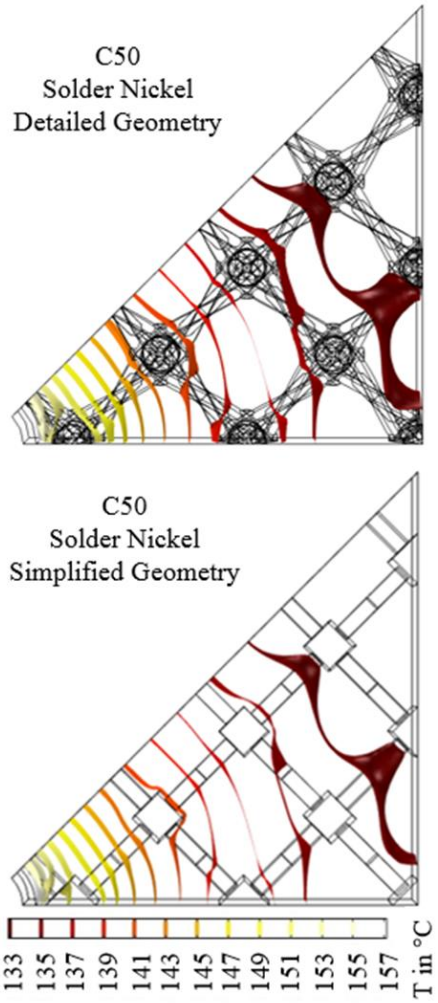

Figure 11: Melting front of detailed and simplified model after 70 minutes (C50, solder Nickel)

By using the simplified model, the calculation time can be reduced by about 25 %. Also the needed time for preprocessing and meshing the model is significantly reduced.

5. Conclusions

With the use of open porous metal structures the storage power of latent heat storages can be improved. The presented simulation model allows the investigation of the transient behavior of the melting process within a unit cell of the storage.

With the presented numerical model it is possible to simulate the transient behavior of the phase change within a latent heat storage with 3D wire structures. The detailed model can be used to investigate different wire and solder materials and alternative PCMs. The wire structure's geometry can be adapted for different mesh and wire sizes. For all material combinations, the empirical coefficients for the simplified model can be acquired.

A simplified model was created to reduce the time needed for preprocessing and meshing as well as the calculation. Therefore, it is possible to analyze a larger part of the latent storage and the influence of system properties (i.e. different heating fluids and temperatures can be evaluated).

Based on the simulation results, it was found that there are two main factors to increase the overall storage power: using high conductive wire materials like copper and connecting the individual wires within the crossroads by brazing the wire structure.

With respect to the costs of the latent heat storage, using a brazed C50 instead of copper as wire structure material deserves a second thought. A soldered C50 structure leads to a reasonable melting time for certain applications.

By using the developed models, it is possible to design a tailored latent heat storage in terms of power and capacity for any given application.

6. References

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7. Acknowledgements

This research has been funded by the Federal Ministry of Economic Affairs and Energy of Germany in the project MoSpeDra (project number 03ESP346C) which is gratefully acknowledged.