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MODELING AND SIMULATION OF HEAT STORAGE IN PHASE-CHANGE MATERIALS BASED ON COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT
A process for simulation of heat storage in phase-change materials (PCM) based on computational fluid dynamics (CFD) approach is presented. Cylindrical shape of PCM heated by an inner tube is analysed, in which two different heat-transfer mechanisms are considered: (i) conduction only, and (ii) combined natural convection and conduction. The physical properties of a PCM from literature are adopted for testing, and describe a typically used, commercial paraffin-based material. This preliminary study indicates successful use of CFD simulations in investigation and analysis of thermal energy storage in PCMs.
Keywords: energy storage, PCM, modeling, simulation, CFD

1. INTRODUCTION
In the recent years, energy storage has become a very significant engineering topic, due to growing demand in two possible areas of application: (a) storage of fluctuating energy in the process of energy conversion from renewable sources, such as in solar or wind power plants, or (b) storage of energy obtained through waste-heat recovery, so that the stored energy might be applied at remote places, or in later periods of time. In order to store relatively large amounts of energy at narrower temperature ranges, it is convenient to use the latent heat during the phase change of a storage material.

2. THERMAL ENERGY STORAGE IN PCM
Typically, phase-change processes occur at nearly constant temperatures. This makes them attractive for use in a variety of technical applications. Theoretically, all phase-change processes might be employed for storage and release of energy: solid-liquid (melting and solidification), liquid-gas (evaporation and condensation), solid-gas (sublimation and re-sublimation), as well as solid-solid transformations. Processes including gas involve considerable volume changes of the working material, or changes of the operating pressure also affecting the phase-change temperature, which implies specific design issues, while solid-solid transformations usually mean relatively low latent-heat values. Thus, *solid-liquid transitions* seem to be the most attractive choice.

There is a wide variety of the PCM-based thermal energy storage design concepts. Beside simple shapes like flat plates, cylinders or annular tubes, also macro- and micro-encapsulations with containers of different shape are used (e.g. spheres as the simplest one), or slurries containing PCM as well. Integral, quasi-1D calculations, such as presented by Retterstøl [1], may be used for quick overall analysis of storage design, and can be applied to conduction-dominated problems. On the other hand, numerical simulation such as done by Roesler and Brueggemann [2] allows detailed tracking of

phase-change process within PCM with its accompanying phenomena including, among others, combined conductive and convective heat transfer.

3. COMPUTATIONAL METHOD

The phase-change process is described by balance equations of continuum mechanics, governing conservation of mass, momentum and energy [3]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho \,\mathrm{d}V + \oint_S \rho \vec{v}\,\mathrm{d}\vec{S} = 0\,, \qquad \text{... (1)}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho \vec{v}\,\mathrm{d}V + \oint_S \rho \vec{v} \otimes \vec{v}\,\mathrm{d}\vec{S} = -\oint_S p\,\mathrm{d}\vec{S} + \oint_S \boldsymbol{\tau}\,\mathrm{d}\vec{S} + \int_V \vec{f}_V\,\mathrm{d}V\,, \qquad \text{... (2)}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho h\,\mathrm{d}V + \oint_S \rho h \vec{v}\,\mathrm{d}\vec{S} = \oint_S \lambda\,\mathrm{grad}\,T\,\mathrm{d}\vec{S} + \int_V q\,\mathrm{d}V\,, \qquad \text{... (3)}$$

where ρ is the density of the material, $\vec{v}$ is the velocity vector, $\vec{S}$ is the control surface, V is the volume, t is the time, p is the pressure, $\boldsymbol{\tau}$ is the stress tensor related to the strain rate through a suitable constitutive relation, $\vec{f}_V$ is the vector of body forces, h is the specific enthalpy, λ is the thermal conductivity, T is the temperature, and q is the heat source or sink. The specific enthalpy can be described as:

$$h = \int_{T_0}^{T} c_\mathrm{p}\,\mathrm{d}T + f\,H_\mathrm{L}\,, \qquad \text{... (4)}$$

with c_p being the specific heat capacity, H_L the latent heat of phase change, and f the volume fraction of the liquid phase, which varies linearly with temperature between solidus and liquidus state, from 0 in the solid to 1 in the liquid. After imposing eq. (4) to eq. (3), the latter is solved for temperature, with latent heat becoming a part of the heat source/sink q.

The body forces in the momentum equation, eq. (2), contain the buoyancy force caused by temperature-triggered density variation and gravity, as well as the resistance force to the flow of the liquid phase caused by the solid fraction in the mushy region. In this study, the resistance obeying Darcy law is assumed to be constant with sufficiently large values obtained from numerical experiments (with order of magnitude 10^6-10^{10} Pa·s/m^2). For more detailed investigation, a solid volume-fraction dependent resistance can be derived from Carman-Kozeny relation, as used, for example, by Voller and Prakash [4].

Discretization of eqs. (1-3) with appropriate constitutive relation for Newtonian, incompressible, viscous fluid is performed using the finite-volume method, as described by Demirdžić and Muzaferija [5] and Teskeredžić et al. [3]. All simulations in this work are done using commercial CFD software *STAR-CCM+* version *8.02*.

4. TEST EXAMPLE

Heat transfer with phase change in a shell-and-tube PCM storage tank is considered. Assuming sufficiently long PCM-shell and inner tube, variation of the quantities in axial direction can be neglected, so that a 2D approximation can be adopted. The data used in this example are mostly taken from the case investigated by Roesler and Brueggemann [2].

The cross-section of the PCM storage with its dimensions is illustrated in Fig. 1. In this work, the thickness in axial direction is 1 cm. The boundary-fitted, trimmed Cartesian computational mesh, automatically generated in the region occupied by PCM, is also shown. The PCM is placed between the inner tube filled with heat-transfer fluid (HTF) whose temperature is 70°C, and the outer adiabatic wall. Physical properties of the PCM are given in Tab. 1. Energy storage process, i.e. heating along

with melting is observed. The initial temperature of PCM is 25°C, sufficiently below the solidus temperature, implying that the entire material is in the solid state at the initial instant of time. Laminar flow is assumed since small liquid velocities are expected, and the Rayleigh number based on the temperature difference between the wall and the melting point turns out to be small.

Two cases are calculated: (a) neglecting gravity effects, which could be applicable to an annulus placed in horizontal plane, between two parallel, thermally insulated slip-walls, i.e. inner tube is arranged vertically, and (b) considering gravity acceleration directed downwards (negative y-direction, Fig. 1), which represents a section of a long, horizontally placed tube. In the first case, the heat transfer occurs through conduction only since the buoyancy is neglected, and there are no other driving forces causing the motion of the liquid phase (walls are assumed to be fixed). In the second case, both heat conduction and convection are arising.

Table 1. Physical properties of the PCM used in simulation. The properties correspond to RT 42 *Rubitherm*® [2].

Density, solid	860	kg/m^3
Density, liquid	780	kg/m^3
Dynamic viscosity of liquid	0.02534	Pa s
Specific heat, solid	1800	J/kgK
Specific heat, liquid	2400	J/kgK
Thermal conductivity	0.2	W/mK
Thermal expansion coefficient	0.001	K^{-1}
Latent heat	141600	J/kg
Solidus temperature	39	°C
Liquidus temperature	43	°C

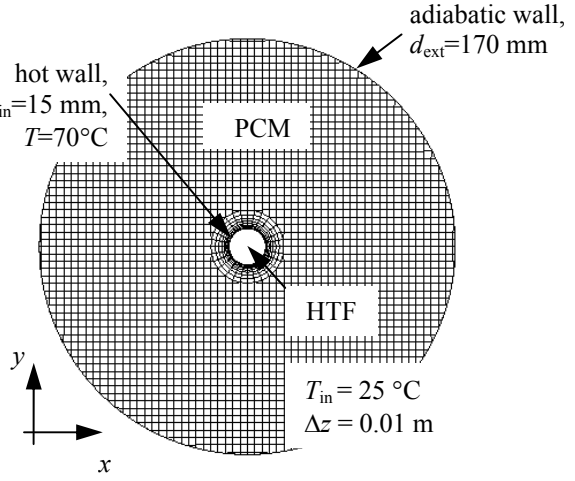

Figure 1. The geometric definition of the cross-section of the PCM storage, with initial and boundary conditions, as well as computational mesh displayed.

5. RESULTS

Fig. 2 shows the distribution of the solid and liquid phase after 90 min of heating in the case with gravity ignored. The heat, and herewith the melted region, remain concentrated around the inner tube, as indicated by black-colored annulus around the inner tube with HTF. The liquid-solid interface is relatively sharp, i.e. the transitional, mushy region (a mixture of solid and fluid) is narrow.

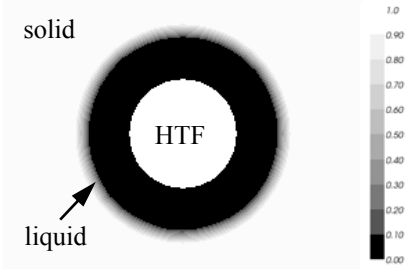

Figure 2. Conductive heat transfer: instantaneous volume fraction of solid.

In Fig. 3, results at four different instants of time for the buoyancy-including case are shown. Even at the early stage of melting, some amount of heat is transferred by convection through the liquid phase away from the tube. Hence, a considerable part of the solid becomes mushy (lightgrey-shaded region). The density of the liquid is smaller than that of the solid, thus the liquid transport occurs primarily in the vertical direction upwards, while the solid fraction within the mushy region moves downwards.

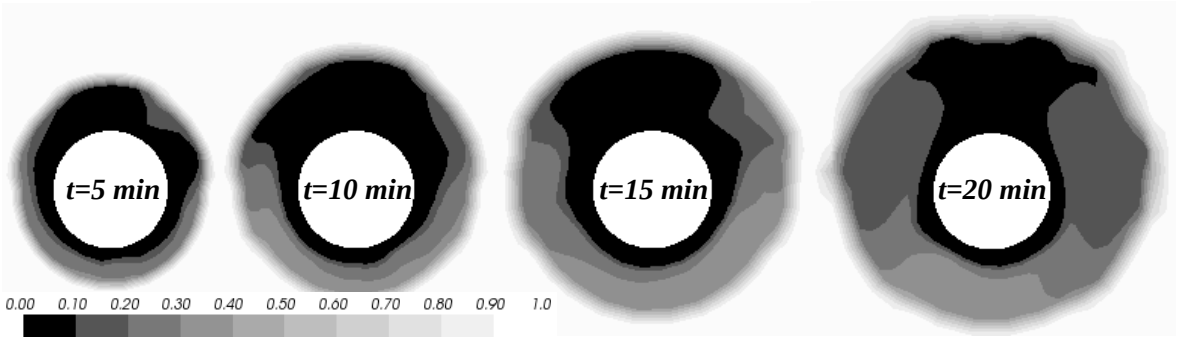

Figure 3. Gravity-induced natural convection: volume fraction of the solid phase at four different instants of time.

Consequently, the melting rate in the case of convective heat transfer is considerably higher. This is clearly seen from Fig. 4, where the history of the solid volume-fraction in the entire PCM is depicted (left), as well as the maximum distance of the melted region (the liquid-phase volume fraction not smaller than 50%) measured in *y*-direction from the center of the inner tube (right). Advancing of the melting front is noticeably faster with natural convection, than with the conductive transfer only.

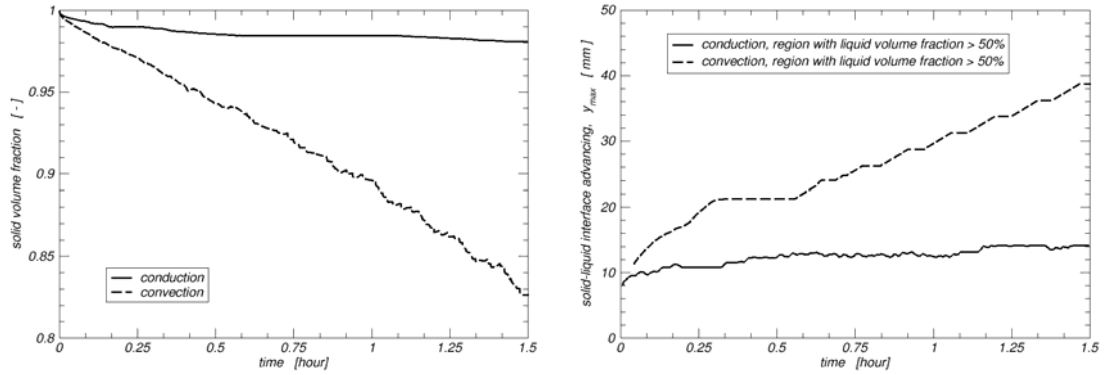

Figure 4. History of the solid-phase volume fraction in the entire PCM (left), and advancement of the liquid phase through the time (right).

As long as heat conduction only is considered, and buoyancy is ignored, the simulations turn out to be time-efficient. Natural convection triggered by buoyancy in PCM, which becomes particularly important when large temperature differences arise, makes the coupling of momentum and energy equation stronger, leading to potential instabilities and longer computing times. In addition, numerical testing showed dependence of the results on flow resistance in mushy regions, which requires detailed modeling.

6. CONCLUSIONS

CFD-analysis of phase-change materials for thermal energy storage enables detailed insight into their physical behavior. The CFD simulations confirm that the heat transfer by conduction results in a slow phase-change process keeping the solid-liquid interface relatively sharp, while convection-dominated phase change transfers the heat further into the PCM, promoting the advance of the liquid phase.

7. REFERENCES

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