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## Numerical modelling of wetting phenomena during melting of PCM

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### Abstract

Latent heat thermal energy storage (LHTES) units using phase change material (PCM) exhibit a high thermal capacity, but also a low charging and discharging power. Macro-encapsulation of PCM is one way of enhancing the heat transfer rate in thermal storage units. During encapsulation, the cavity left to reduce mechanical stresses in the macro capsule, locks air. This makes the capsule a multiphase system consisting of immiscible phases namely PCM and air.

Numerical modelling of a PCM capsule enables a detailed understanding of the phase change process of the PCM under the influence of air. In this article, two immiscible fluids PCM and air have been modeled using a continuum surface force (CSF) model in the open source computational fluid dynamics (CFD) software, OpenFOAM. The wetting of the melted PCM on the capsule wall is taken into account by implementing a contact angle boundary condition. The surface tension of the PCM with air is just contributed to the liquid phase of the PCM. The nonlinear enthalpy-temperature relation during the phase change is taken into consideration by a source-based fictitious method. The flow in the solid phase of the PCM is ramped down by considering a high solid viscosity. Experimental results are employed to validate the overall model.

The results obtained from the complete numerical model have shown a great acceptance when compared with experiments. Despite several small deviations in the results, the numerical modelling is a potential tool to optimize the efficiency of thermal storage units.

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## 1. Introduction

Providing sustainable and clean energy is one of the major contemporary challenges in the field of energy science. Thermal energy storage plays a key role to attain these goals by storing e.g. waste heat released from industries and residential areas. The stored heat can be transported using different mobile carriers or can be stored for later purposes. PCMs can store a comparable high amount of energy per kilogram and are therefore a favorable storage material for mobile applications. Thermal energy storage units containing encapsulated PCM are suitable for mobile applications due to the large heat transfer area leading to a high charging and discharging power. Numerical modelling and simulation of the phase change process of PCM helps to understand the thermal response of the encapsulated storage material. This helps to improve the efficiency of a complete thermal storage.

Numerical modelling of the solid-liquid phase change phenomenon for metallurgical and industrial applications is found empirical. Different techniques exist to model the moving solid-liquid interface in melting and solidification problems. Crank [1] proposed the initial detailed idea to model the moving solid-liquid boundary by solving a diffusion equation. Later, Voller [3] proposed the famous enthalpy method to model convection as well as diffusion during the phase change and also solid velocity ramp down, using the Darcy-Forchheimer equation as a source term in the momentum equation [14]. Gartling [4] proposed a solid viscosity ramp down by implementing a temperature dependent viscosity. This method is called the variable viscosity method (VVM). The first model taking into account the settling of solid PCM and close contact melting was introduced by Asako et al. [5].

Assis et al. [7] modeled the melting of a PCM in a spherical shell using the enthalpy-porosity approach by applying an arbitrary small Darcy constant. Later Rösler [8] extended this method by simulating the more exact melting phenomenon using an enhanced settling method. In this article, a source based enthalpy approach proposed by Swaminathan and Voller [9] is implemented to model the melting of PCM in a capsule. Ramping down the velocity in the solid phase is implemented by the VVM. To account for the two immiscible fluids PCM and air the volume of fluid (VOF) approach is implemented [10]. The surface tension is a material property leading to the elasticity tendency obtained from molecular adhesion of the fluid. Brackbill et al. [6] proposed a continuum approach to model the surface tension between two immiscible fluid phases or fluid-gas phases. In this work the surface tension is modeled using the same CSF approach and the wetting of the PCM fluid is implemented with a contact angle boundary condition. The surface force between the fluid and the gas phase is modeled as a source term in the momentum equation.

The detailed numerical model of a PCM capsule which accounts for phase change, settling of solid PCM, heat transfer and surface tension between PCM and air is modelled in OpenFOAM 2.2.2. Finally the achieved numerical results are compared to experimental results.

### Nomenclature

H	Enthalpy, J
F	Force, N
g	Gravitational acceleration, m/s <sup>2</sup>
L	Latent heat, J/kg
Q	Heat rate, W
$c_p$	Specific heat capacity, J/(kg·K)
h	Heat transfer coefficient, W/(m <sup>2</sup> ·K)
k	Thermal conductivity, W/(m·K)
p	Pressure, Pa
S	Source term
T	Temperature, K
t	Time, s
u	Velocity, m/s
V	Volume, m <sup>3</sup>

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