International Journal of Heat and Mass Transfer 119 (2018) 523–532

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Theoretical and numerical analysis on phase change materials (PCM): A case study of the solidification process of erythritol in spheres

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ARTICLE INFO

Article history:
Received 5 September 2017
Received in revised form 22 November 2017
Accepted 24 November 2017

Keywords:
Phase change materials (PCM)
Computational fluid dynamics (CFD)
Solidification process
Erythritol in spheres
Convective motions
Heat Flux
S-curve

ABSTRACT

Phase change materials (PCM) present great potential for energy efficiency gains in thermal systems by storing solar energy or waste heat in industrial processes. This is due to the great amount of energy stored per mass unit within a small temperature range. In this paper we focus, by means of the numerical investigation, on the solidification process of the PCM erythritol in spheres, having 10, 20, 30 and 40 mm diameter, under wall temperatures of 10, 15, 20, 25, 30 and 40 K below the phase change temperature of the material. The problem is considered two-dimensional in geometry and transient in time. The numerical model here adopted consists of mass, momentum, energy and volume fraction equations. The results have been initially validated by comparison with data found in literature. Afterwards, analysis of the convective streams on the liquid PCM, liquid fraction, heat flux in the sphere wall and total solidification times have been widely illustrated. The liquid fraction suffers a sharp reduction at the beginning of the solidification process due to the high heat flux at the initial times. As the solid layer adjacent to the shell increases, it causes an augmentation of thermal resistance, significantly reducing the heat flux. The shape of the curve representing the solid fraction shows similarity with the S-curve pattern of solidification. The total solidification time proved to be dependent on both the diameter length and the temperature difference ΔT (between phase change material and wall temperature), being its influence reduced for lower temperature values. Finally, the liquid fraction results, as a function of Fourier and Stefan numbers, have been employed to amend a dimensionless correlation found in literature.

1. Introduction

Thermal energy storage has great importance for energy peak attenuation and energy supply during low availability periods. The main forms of thermal energy storage currently used are sensible and latent heat. The latter presents a greater advantage as it has the possibility of storing large amounts of energy per mass unit within a small temperature range. Materials that store latent heat, i.e. phase change materials (PCM) can be applied to many fields [1], i.e. solar thermal energy, refrigeration, food temperature conservation, medical applications, storage in concentrating solar power plants and heat recovery in industrial processes. Thus, PCM demonstrated great potential for use, mainly from the point of view of energy efficiency, which has also obvious economic benefits.

The choice of a PCM for a specific application is defined, mainly, for its phase change temperature; most of the PCM actually studied have temperatures between 0 and 60 °C [2]. In this range of temperatures, heating ventilation air conditioning (HVAC) and solar energy are the main applications. Among the above mentioned studies of PCM with phase change temperature below 60 °C, particular emphasis can be ascribed to the works of Assis et al. [3,4] with RT27, Tan et al. [5] and Chan et al. [6] with n-octadecane. It is worth to mention that all these studies analyzed spherical domains.

Regarding different geometries than spherical domain, even in the field of low phase change temperature, the works of Katsman et al. [7], Schmueli et al. [8] and Dubovsky et al. [9] with vertical cylinders, and the works of Ye et al. [10] and Shatikian et al. [11] with rectangular cavities are fully noteworthy. The numerical study highlighted in Ref. [12] covers the melting of 5 PCMs whose phase change temperatures vary from 4 °C (RT4) to 82 °C (RT82), in vertical cylinder. Al-Abidi et al. [13] analyzed experimentally a tubular configuration with RT82, both in solidification and in melting processes. Hosseinizadeh et al. in Ref. [14] investigated experimentally and numerically the melting of RT80 in rectangular cavities.

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https://doi.org/10.1016/j.ijheatmasstransfer.2017.11.124
0017-9310/

Nomenclature

c_p	specific heat at constant pressure (J/kg K)
C	mushy zone constant (kg/m^3 s)
D	sphere diameter (m)
Fo	Fourier number
g	gravity acceleration (m/s^2)
h	specific enthalpy (J/kg)
k	thermal conductivity (W/mK)
L	latent heat (J/kg)
p	pressure (Pa)
q″	superficial heat transfer rate (W/m^2)
S	momentum source term (Pa/m)
Ste	Stefan number
t	time (s)
T	temperature (K or °C)
$\vec{V}$	velocity vector (m/s)
x, y	coordinates (m)

Greek symbols

α_n	volume fraction
β	liquid fraction
ε	numerical value (to avoid division by 0 in Eq. (4))
μ	dynamic viscosity (kg/ms)
ρ	density (kg/m^3)

Subscripts

a	average
l	liquidus
le	latent enthalpy
ref	reference value
s	solidus
se	sensible enthalpy
w	wall

As for PCMs with phase change temperature between 100 and 200 °C, very few reports have been published [15,16] and even more rare are the studies on PCMs with phase change temperature exceeding 200 °C. Archibold et al. for example analyzed the melting [17] and solidification [18] processes of sodium nitrate ($NaNO_3$), whose phase change temperature is 306.8 °C, in spherical geometry.

Nevertheless, the majority of the researches conducted so far is concentrated on phase change temperatures below 100 °C. Thus, this work's aim is to study the solidification process of erythritol, whose phase change temperature (118 °C) is in the above mentioned "rarely explored zone" (100–200 °C). The solidification process in spheres has been analyzed regarding the convective motions in the liquid, the liquid fraction, the heat flux and the total solidification time. The geometrical domain here explored is not dissimilar from the one illustrated in Ref. [19] (please see Fig. 6) in which constructal design [20–23] has been employed. The difference is that in the present work the solidification process is constrained into the spherical shell while Constructal theory manifests itself when the shape is free to morph, so that the final geometry associated to solidification springs out as dendritic.

2. Problem statement

A packed bed system used for thermal energy storage with PCM consists in a reservoir filled with spheres containing PCM. The heat transfer fluid flows around the spheres, transferring heat to or from the spheres. As the PCM density changes between the solid and liquid phases, a certain amount of air is needed inside the spheres in order to absorb the volume variation and maintain the shell's integrity. The fluid between the spheres flows with a temperature gradient through the entire domain, and the temperature at a certain point slowly changes over time [24].

It is important to mention that some studies consider the whole packed bed or a section with several spheres in the domain (which better represents real applications of a PCM packed bed) using simplifications such as considering the packed bed as porous media [25–27]. In these studies, as the focus is the flow around the spheres, the main simplifications are made on the PCM spheres instead of the fluid flow between the spheres. In the present work, as the focus is the PCM inside the sphere, we consider constant temperature around a single sphere, in order to simplify the model in the external flow. Both approaches in the model simplification (external flow or in the PCM) are usually done to reduce computation time.

2.1. Physical model

The studied geometry, depicted in Fig. 1, is spherical; it is filled with 98.5% of PCM and 1.5% of air. In order to keep constant pressure, the upper part of the sphere is opened, allowing air to enter. The geometry is symmetrical in the vertical axis, making possible to model half of the sphere in two dimensions. The diameters (D) here analyzed are: 10, 20, 30 and 40 mm. The PCM contained in the spheres is erythritol, whose phase change temperature is 391 K (118 °C). The other properties, deduced from literature [15,28,29], are shown in Table 1.

With reference to all the tested cases, air that enters the domain has the same temperature of spheres wall and atmospheric pressure (101.3 kPa), with density (ρ) varying with temperature the following dependence: $\rho = 1.2 \times 10^{-5}T^2 - 0.001134T + 3.4978$ [3].

2.2. Governing equations and boundary conditions

The mathematical model consists of the mass (1), momentum (2) and energy (3) equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0 \tag{1}$$

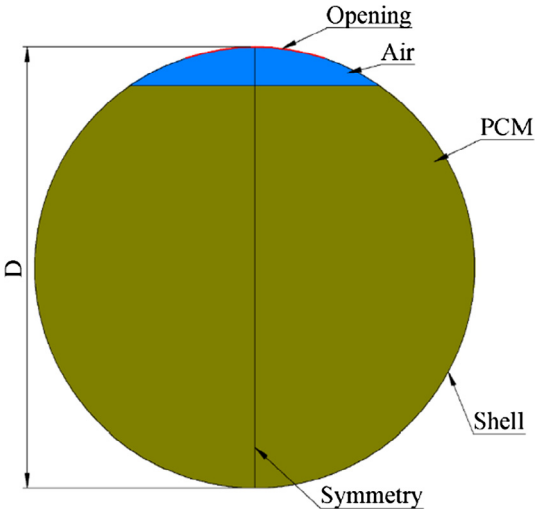

Fig. 1. Physical model.