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A review on phase-change materials: Mathematical modeling and simulations

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ABSTRACT

Energy storage components improve the energy efficiency of systems by reducing the mismatch between supply and demand. For this purpose, phase-change materials are particularly attractive since they provide a high-energy storage density at a constant temperature which corresponds to the phase transition temperature of the material. Nevertheless, the incorporation of phase-change materials (PCMs) in a particular application calls for an analysis that will enable the researcher to optimize performances of systems. Due to the non-linear nature of the problem, numerical analysis is generally required to obtain appropriate solutions for the thermal behavior of systems. Therefore, a large amount of research has been carried out on PCMs behavior predictions. The review will present models based on the first law and on the second law of thermodynamics. It shows selected results for several configurations, from numerous authors so as to enable one to start his/her research with an exhaustive overview of the subject. This overview stresses the need to match experimental investigations with recent numerical analyses since in recent years, models mostly rely on other models in their validation stages.

Contents

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1. Introduction

The ever increasing level of greenhouse gas emissions combined with the overall rise in fuel prices (although fluctuations occur) are the main reasons behind efforts devoted to improve the use of various sources of energy. Economists, scientists, and engineers throughout the world are in search of (1) strategies to reduce the demand; (2) methods to ensure the security of the supplies; (3) technologies to increase the energy efficiency of power systems; (4) new and renewable sources of energy to replace the limited and harmful fossil fuels.

One of the options to improve energy efficiency is to develop energy storage devices and systems in order to reduce the mismatch between supply and demand. Such devices and systems also improve the performance and reliability by reducing peak loads and allowing systems to work within an optimal range. Thus, they play a preponderant role in conserving energy. The different forms of energy that can be stored are mechanical, electrical, and thermal. Here, mechanical (gravitational, compressed air, flywheels) and electrical (batteries) storages are not considered while thermal energy storage is discussed in the context of latent heat (sensible heat and thermochemical heat are not considered).

Latent heat storage is based on the capture/release of energy when a material undergoes a phase change from solid to liquid, liquid to gas, or vice versa. Latent heat storage is particularly attractive since it provides a high-energy storage density and has the capacity to store energy at a constant temperature – or over a limited range of temperature variation – which is the temperature that corresponds to the phase transition temperature of the material. For instance, it takes 80 times as much energy to melt a given mass of water (ice) than to raise the same amount of water by 1 °C. Table 1 provides a typical comparison between properties of different thermal storage materials used at room temperature. For the interested reader, excellent global reviews that pertain to phase-change materials and their various applications were proposed by Farid et al. [1], Sharma et al. [2], Zhang et al. [3], Regin et al. [4], Tyagi and Buddhi [5], Mondal [6], Sethi and Sharma [7], and especially the recent one by Verma et al. [8].

Nevertheless, the incorporation of phase-change materials (PCMs) in a particular application calls for an analysis that will enable the researcher to determine whether or not PCMs will improve performances sufficiently to justify extra costs for additional systems and/or controls needed. Mathematical modeling of latent heat energy storage materials and/or systems is needed for optimal design and material selection. Therefore, a large amount of research has been carried out on PCMs behavior predictions whether they are considered separately or within specific systems.

Table 1 shows the main differences, on average basis, between sensible heat storage materials and latent heat storage classes of materials. The table indicates that generally, PCMs require much less mass or volume to store the same amount of energy at a more or less constant temperature.

This paper is building on previous reviews [1–8] to update the available references that pertain to mathematical modeling and simulation of thermal energy storage with phase-change materials. First, it presents the fundamental mathematical description of the phenomenon, the Stephan problem. Then, it provides basic mathematical descriptions used as basis for numerical modeling using either first or second law approaches and fixed or adaptative meshes. The next section, considered by the authors as the major contribution, is a model collection of most recent works published on the subject. This survey is organized according to the problem geometry (Cartesian, spherical, and cylindrical) and specific configurations or applications (packed beds, finned surfaces, porous and fibrous materials, slurries). A synthesis is provided at the end and several recommendations are formulated.

2. The Stephan problem

Phase transition of a material is described by a particular kind of boundary value problems for partial differential equations, where phase boundary can move with time. This question has been first studied by Clapeyron and Lamé in 1831 when analyzing the formation of the Earth's crust when it cooled. In that case, the problem was simplified from a spherical geometry to a one-dimensional semi-infinite slab [9]. This solution was found independently by Franz Neumann, who introduced it in his lectures notes of 1835–1840 [10]. Nevertheless, this type of problems is named after Jožef Stefan, the Slovene physicist who introduced the general class of such problems in 1889 [11] in relation to problems of ice formation. Existence of a solution was proved by Evans in 1951 [12], while the uniqueness was proved by Douglas in 1957 [13].

Very few analytical solutions are available in closed form. They are mainly for the one-dimensional cases of an infinite or semi-infinite region with simple initial and boundary conditions and constant thermal properties. Under these conditions, these exact solutions usually take the form of functions of the single variable $x/t^{1/2}$ and are known as similarity solutions [14,15]. A collection of similarity solutions and references is to be found in [16,17].

3. Numerical solution

The problem of predicting the behavior of phase-change systems is difficult due to its inherent non-linear nature at moving interfaces, for which displacement rate is controlled by the latent

Table 1
Common heat storage materials.

Property	Materials			
	Rock	Water	Organic PCM	Inorganic PCM
Density [kg/m^3]	2240	1000	800	1600
Specific heat [kJ/kg K]	1.0	4.2	2.0	2.0
Latent heat [kJ/kg]	–		190	230
Latent heat [MJ/m^3]	–	–	152	368
Storage mass for 10^9 J, avg [kg]	67,000 (Δt = 15 K)	16,000 (Δt = 15 K)	5300	4350
Storage volume for 10^9 J, avg [m^3]	30 (Δt = 15 K)	16 (Δt = 15 K)	6.6	2.7
Relative storage mass	15 (Δt = 15 K)	4 (Δt = 15 K)	1.25	1.0
Relative storage volume	11 (Δt = 15 K)	6 (Δt = 15 K)	2.5	1.0