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Quality criteria for phase change materials selection

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ABSTRACT

Selection guidelines are primary criterion for optimization of materials for specific applications in order to meet simultaneous and often conflicting requirements. This is mostly true for technologies and products required to meet the main societal needs, such as energy. In this case, gaps between supply and demand require strategies for energy conversion and storage, including thermal storage mostly based on phase change materials. Latent heat storage is also very versatile for thermal management and thermal control by allowing high storage density within narrow temperature ranges without strict dependence between stored thermal energy and temperature. Thus, this work addressed the main issues of latent heat storage from a materials selection perspective, based on expected requirements of applications in thermal energy storage or thermal regulation. Representative solutions for the kinetics of latent heat charge/discharge were used to derive optimization guidelines for high energy density, high power, response time (from fast response to thermal inertia), etc. The corresponding property relations were presented in graphical forms for a wide variety of prospective phase change materials, and for wide ranges of operating conditions, and accounting for changes in geometry and mechanisms.

1. Introduction

Limitations of fossil fuels and other primary energy sources combined with their environmental impact have stimulated increasing emphasis on renewable energies in order to sustain the development and quality of life in modern societies, without excessive environmental impact. Emphasis on renewable energies also imply ability to develop strategies of conversion and storage to bridge gaps between energy harvesting and consumption. This is the case of solar heat stored as latent heat in phase change materials for heating or cold storage for air conditioning, which represent important fractions of total energy needs for domestic, office and industrial levels, often relying on combustion of fossil fuels or valuable electricity, due to its widespread distribution. Consumption of these energies may be minimized by alternative concepts of storage, regulation and management.

Though solar heat represents about 50% of the solar spectrum, its effective use is limited by gaps between daytime and night, often varying from heat excess in daytime hours to cold nights. Classical concepts to overcome these deviations from the comfort range have relied on thermal isolation with highly porous materials, double or multiple windows, or thermal inertia, with transient loading and unloading of sensible heat in heavy structures (e.g. thick stone walls). Still, these strategies have limited heat storage flexibility if one seeks minimum temperature fluctuations for precise thermal regulation and management. Thus, representative applications of phase change materials include thermal management in buildings, by incorporation of phase change materials in bricks [1] or as a component of composites [2]. Other identified applications can be found in relevant reviews [3] and are summarized in Table 1, often based on encapsulated phase change materials [4] to minimize undue interaction with the surrounding media. In this case, the dynamics of heat transfer may include limitations imposed by low thermal conductivity of paraffins [5] and most organic phase change materials, in series with additional limitations imposed by encapsulating materials and/or heat transfer to a cooling fluid or surrounding medium, as discussed below. Attempts to enhance performance also comprise a variety of experimental developments combined with modelling [6], as often used for applications of PCM materials in cold storage [7]. Prospective application of latent heat storage materials has also been proposed for cooking in developing countries with hot climate, to extend the versatility of solar kilns [8].

Phase change materials also find applicability in thermal management, as required for pharmaceutical products [9] or heat sensitive electronics [10], and to sustain other exothermic processes. In these cases, requirements of fast heat dissipation lead

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Table 1
Summary of main requirements for different PCM applications.

Application	Requirements		
	Amount of stored energy/thermal inertia	Discharge power	Discharge time
Climatization/thermal comfort in:	✓		
(i) Buildings [1,2];			
(ii) Vehicles [3,4];			
(iii) Greenhouse [5,6];			
(iv) Air conditioning [7]			
Solar kiln [8,9]	✓		
Thermal protection of:	✓		
(i) Food [4,10];			
(ii) Medical products/equipment [9,10];			
(iii) Electronic devices [9,10].			
Energy storage for:	✓	✓	
(i) Solar systems [11,12];			
(ii) Sanitary hot water [11–13];			
(iii) Ice banks [4,14];			
(iv) Central solar for energy production [4,10].			
Power dissipation in:			✓
(i) Electronic systems [15,16];			
(ii) Exothermic chemical reactions [9,10].			

to different strategies to enhance thermal conductivity, based on incorporation of conducting phases with different geometries [11]. Other applications depend mainly on high storage ability, as required to support hot water systems [12], and to minimize temperature decrease at night [13]. In fact, latent heat storage in phase change materials offers advantages in terms of power density and prospects for heat discharge under nearly isothermal conditions.

Applicability in sub-zero or even cryogenic conditions [14] includes prospects to sustain power failures or intermittent renewable electricity in refrigeration. These applications also require high storage ability and differ from the requirement of fast dissipation of short heat peaks in electronics, which may rely on additions of lightweight conducting phases such as carbon foams [15] and/or carbon nanotubes [16] to enhance thermal conductivity of phase change materials.

The representative applications listed in Table 1 are classified for their main requirements of (i) stored energy or thermal inertia, (ii) discharge power and (iii) discharge time. This must be taken into account for the purpose of materials selection in the development of engineering concepts and commercial products, to seek high efficiency, robustness and viability of the products. Selection is based on previous identification of relevant thermophysical properties, such as latent heat, thermal conductivity and melting temperature, and their interactions in representative quality criteria. Thermophysical properties may also be optimized in order to minimize size or weight of storage systems, and to lower charge/discharge times in high power appliances. Other applications require thermal inertia (e.g. transportation of temperature sensitive products such as food and blood), or PCM materials for temperature regulation upon temporary failure of the normal supporting equipment (e.g. refrigerators with frequent power cuts). Selection of PCM materials may also be extended to account for differences in unit cost, encapsulation and other processing costs, as well as other relevant issues of durability, safety, corrosion, environmental impact, etc.

Quality criteria of phase change materials for specific requirements should also be as simple as possible to ensure facile implementation. Still, these criteria must be based on sound descriptions of the dynamics of solidification and melting, as known for the classical heat conduction solution for planar geometry [17]. This model behavior does not account for slow nucleation of the transformed phase causing undercooling on freezing or overheating on melting, and also fails to describe the impact of encapsulation with poorly conducting materials, or limited heat transfer coefficients to heat transfer fluids. These conditions of mixed control require alternative numerical methods [14].

Reliable numerical methods are needed for other representative geometries, as shown by the schematic representations in Fig. 1, with emphasis on spherical symmetry, as commonly utilized for encapsulated PCM materials [15], or cylindrical symmetry. Still, these numerical solutions are ill-suited for ready applicability in selection procedures, thus requiring simpler approximate solutions for charge/discharge rate, such as quasi-steady-state solutions for discharge time, as summarized in Table 2. These are expressed as a function of relevant physical properties (density, latent heat and thermal conductivity), combined with a representative encapsulation size, the temperature difference acting as the driving-force. A scaling factor is also introduced for differences in geometry of encapsulation which depends on dimensionality, and also to account for mixed control, as shown below.

The kinetics of charge/discharge of latent heat is the basis for materials selection based on suitable combinations of thermophysical properties of PCM materials, as proposed by Ashby [18] and guided by sound kinetic models of latent heat charge/discharge for different geometries, such as flat slab geometry [19] or spherical encapsulation [19,20]. Information on relevant physical properties for a wide variety of PCM materials is available online [21], and may be used to generate the required quality maps for PCM selection intended for applications with specific requirements of high energy density, high power or response time.

The main objective of this work is, thus, focused on guidelines for selection of PCM materials. Selection criteria are based on sound solutions for the dynamics of latent heat charge or discharge, under conditions imposed by representative types of applications. These criteria are the basis to compile performance maps containing a wide variety of PCM materials; this is quite diverse from recent reviews, which were focused on general decision making in energy conversion and managements, without corresponding selection maps [22].

Performance maps may be designed to assist selection of PCM materials for established applications requiring high energy density, such as residential thermal management, as well proposals to enhance the efficiency of other solar energy-based processes such as desalination in dry hot climates [23].

Similarly, performance maps for fast discharge time or high power provide selection guidelines to extend the applicability of phase change materials to novel energy conversion systems [24]. These maps were designed to be user friendly, accounting for