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New database to select phase change materials: Chemical nature, properties, and applications

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ABSTRACT

Today, thermal energy storage materials are proposed as a promising solution to increase the energy efficiency in building sector and to reduce the total energy demand because building sector accounts up to 34% of total energy consumption. Under this situation, phase change materials (PCM) are well-considered as materials to store energy allowing high energy densities (between 50 and 600 MJ/cm^3). Available materials to be used as PCM for building application in literature were added to a database for to be used with CES Selector software. More than three hundred PCM whit phase change temperatures between −50 °C and 150 °C and considering commercial and non-commercial PCM were listed and classified by their properties and the values available of the materials have been introduced in this database. The main objective of this study is to generate a PCM database and draw on it in order to facilitate the selection of the most suitable PCM depending on the building application.

1. Introduction

Today, thermal energy storage materials are proposed as a promising solution to increase the energy efficiency in building sector and to reduce the total energy demand because building sector accounts up to 34% of total energy consumption in developed countries as state International Energy Agency [1,2]. In Fig. 1 the energy consumption in building sector divided by world areas and differentiating between residential and commercial buildings is shown. Notice that developed countries account more energy consumption in commercial buildings than in residential ones.

Materials used to store thermal energy are divided in three types concerning the method used to store the energy. The first one consists on the heat stored produced when a temperature gradient is applied to a media (solid, liquid or gas) which is known as sensible heat (SHTES) [3]. The second is the one concerning the latent heat stored or released during a phase change state (LHTES) [3]. This method used phase change material (PCM) to store thermal energy. The last one consists on store the thermal energy produced when a reaction takes place. This method is known as thermochemical storage (TCS) and thermochemical materials (TCM) are used for storage [4]. Thermal energy storage (TES) is proposed as one way to improve the gap between energy consumption and energy supply [5]. Actually, there are different compilations to collect all the reported information about PCM properties, not only the thermophysical ones but also other relevant properties [6,7].

In addition, phase change materials (PCM) are well-considered as materials to store energy allowing high energy densities (between 50 and 600 MJ/cm^3). The phase change temperature range will define the final application where this material/substance can be implemented: heating, cooling, domestic hot water, cold storage, etc. Therefore, it is a material selection parameter. Moreover, PCM are divided in several groups of PCM depending on their chemical nature: paraffin, fatty acids, salt hydrates, sugar polyol, etc. [8].

CES Selector is a software database developed by Granta Design [9]. This software is a very intuitive tool to help researchers and designers to select the most appropriate material for a determined application taking into account the constrains. CES Selector was used by Navarro et al. in order to define the best material candidate to store thermal energy as sensible heat [10], as well as Khare et al. [11]. This software has been used as a tool being the aim of this paper to build a new database and to use this tool for the first time in order to obtain proper graphs that will help PCM selection.

Therefore, this paper aims to show the scope of creating a PCM database for CES Selector. The main source of data of PCM

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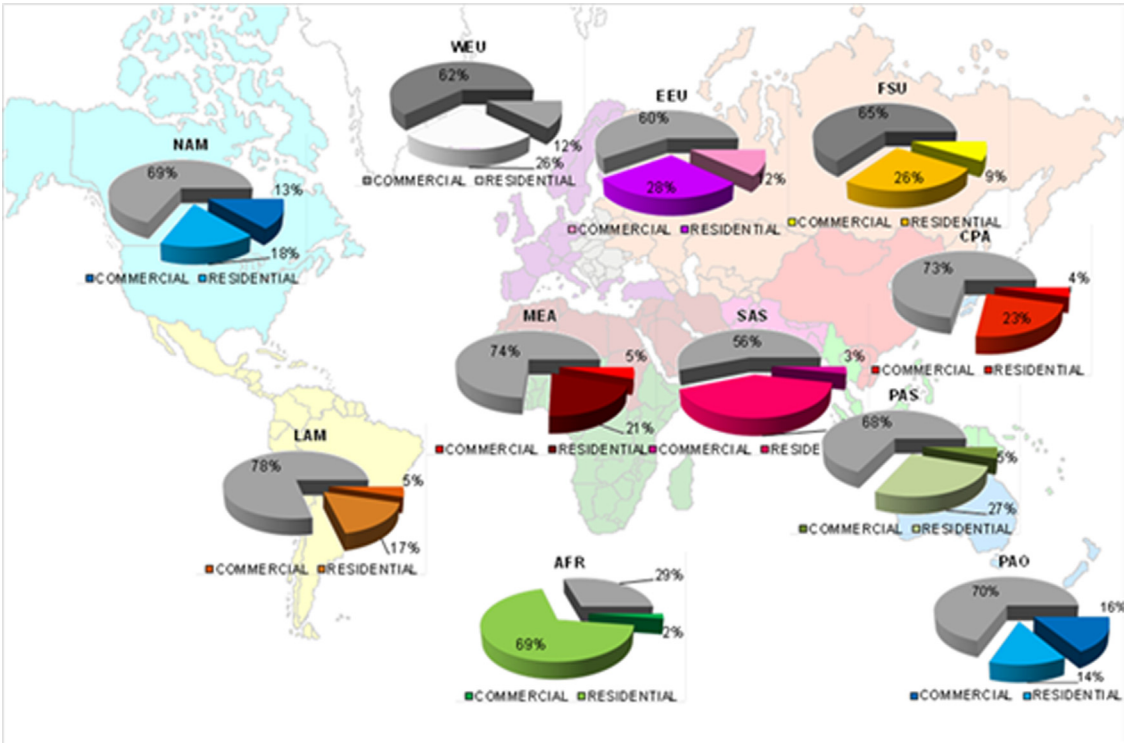

Fig. 1. World zones energy consumption distribution divided by commercial and residential subsectors and others for 2010 [2].

for building applications is the one considered in the review that Cabeza et al. published in 2011 [12]. Available materials to be used as PCM (commercialized and standard substances) for building applications in literature were listed in this review [12] as well as materials commercialized as PCM. More than three hundred PCM were listed and classified by their properties and introduced in this database. This database is a simple and intuitive method to obtain a general PCM list for certain application depending on the thermophysical properties required.This tool is very used in material science field but it is non-existent in the PCM field.

The main objective is to create a database that facilitates the selection of the most suitable PCM depending on the application. Moreover, the information that can be extracted from the data presented in this paper will be discerned by presenting a case study for domestic hot water application in buildings.

2. Selection materials methodology

Following a materials selection strategy the main goal is to obtain a small number of materials candidates among a given database taking into account a specific application. The systematic selection of the best materials for a given application begins by knowing the most relevant properties that has to be considered. CES Selector is software from GRANTA Design at the University of Cambridge that allows combining the information on materials from its specific database and presenting the results in friendly material charts. Moreover, it has a tool, the CES constructor, that allows creating your own data base to apply the materials selection methodology comparing different materials from your database, the CES Selector database and also those found in the literature that are used in the desired application.

One of the main purposes of this work is to create a new database of PCM to select them depending on their properties and their application. Therefore, a new database was created using the CES Constructor software to introduce the main properties such as melting point and latent heat of fusion from the PCM found in the literature and also from commercial PCM.

More than 300 PCM references were introduced in this software to be used to select material candidates for TES in several applications for building sector. The data introduced is based on the review published in 2011 by Cabeza et al. [12]. Moreover, the main cited classification of PCM by groups is used in this database which considered the chemical nature of the substances used to store energy by their latent heat of phase change and the main properties that will characterize the thermal behaviour of a PCM are the working temperature range (based on the peak temperature of the phase change) and the heat of fusion (energy that one substance is able to store as latent heat). These two properties are considered for all the PCM available in the new database. It is also important to remark that there are several properties that are very relevant as density, thermal conductivity, specific heat, etc. which were also introduced in the new database even though there is not data available for all References

3. Results and case study for domestic hot water

There are 6 main groups or families that PCM are divided depending on their chemical nature which are represented in Fig. 2. Each PCM family has its own characteristics:

- Organic/Eutectic Organic/Paraffin/Fatty acids: these substances almost do not present corrosion problems. However, it is difficult to ensure the thermal stability of cycling stability after many thermal cycles.
- Inorganic/Eutectic Inorganic/Salt hydrate/water solution: are the PCM with the highest capacity to store energy but they present corrosion problems that must be taken into account from the beginning of the system design.

However, one of the most important parameter to take into account during the PCM selection step is the energy density which