Study of thermal protection devices using molecular alloys as phase change materials (MAPCM) by heat transfer simulation methods

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ABSTRACT: Molecular alloys as phase change materials are used for thermal protection and energy storage in many industrial sectors. A simple and easy-to-build, thermal protection device using molecular alloys is presented. This enables us to obtain excellent results for thermal protection of macromolecule monocrystals at a controlled temperature (more than two days at 20±2ºC). We show how fundamental studies are helpful to choose the right composition that is able to work at the temperature required for the application in question, and the design, development and test of thermal protection devices used during transport. All the results have been tested using heat transfer simulation methods with the TDYN software (2 dimensions case), and experimentally.

KEY-WORDS: Molecular Alloys Phase Change Materials (MAPCM), thermal protection, n-alkane and macromolecule monocrystals.

INTRODUCTION

The MAPCMs offer opportunities in the fields of energy storage and thermal protection, where the classics Phase Change Materials (PCM) don't exist or they are difficult to find. Their originality relies on the idea of alloy, they are thermo-adjustable materials by means of their composition. It means that it is possible to talk about the selection of the proper composition to allow the best scenario of energy storage and/or usage temperature (application temperature = phase transition temperature).

Our group works on the development of a wide range of molecular alloys which may be used in any application that requires the application temperatures that correspond to the phase transition of these materials. Our objective is to offer a "material menu" for any economic sector that requires the usage of a controlled temperature. Basic research is needed to understand the stability, the structural and energetic behaviour of molecular alloys. To that end and rather than studying isolated systems, our research is invariably focused on families of systems whose components are members of a chemically coherent group of substances (more than 100 binary and ternary systems have been studied)[1-2]. Some of these families studied by us are: n-alkanes, n-alkanols, fatty acids etc that allow us to offer MAPCMs for application temperatures from –30ºC to 120ºC. The authors of this paper are members of the REALM group (*Réseau Européen sur les Alliages Moléculaires*). The REALM group works on mixed molecular crystalline materials pursuing fundamental scientific knowledge and the application of molecular alloys. This European network is member of the "*Xarxa Temàtica dels Alliatges Moleculars*" as well as other European groups and industries. The REALM group has studied and developed different kinds of applications using MAPCMs:

- an isothermal bag for blood transport (application temperature of +6ºC)[3]
- an "active" packaging for fresh drink protection (application temperature of +10ºC)[4]
- a device for the dissipation of heat produced by electronic components (application temperature of +70ºC).

- a packaging for thermal protection of ice-cream during transport[5].
- a thermal protection device for telecommunication components (application temperature of +35ºC).
- and at the present, we are elaborating a thermal protection system for the catering sector (application temperature of +90ºC).

In this communication we present a simple and easy-to-build, thermal protection device using molecular alloys. This enables us to obtain excellent results for thermal protection of macromolecule monocrystals at a controlled temperature. We show how fundamental studies are helpful to choose the right composition that is able to work at the temperature required for the application, and the design, development and test of thermal protection device used during transport. In order to design and test the different prototypes used during the transport process, heat transfer simulation methods, in this case using the TDYN software (2 dimensions case), take an important role. They permit us to test the effect of different parameters as: the different properties of the materials used to build the prototype, the usage of different geometries, the boundary conditions etc. This supposes a considerable economisation of time and expenses, as we are allowed not to do an experimental test for all the considered prototypes.

SEARCH OF THE MAPCM

To formulate, elaborate and characterize Molecular Alloys as Phase Change Materials to be used for this application, we have choose the n-alkanes family to provide especially interesting MAPCMs. Within this family, it is possible to elaborate MAPCMs for a large domain of applications covering temperatures from -30ºC to 120ºC. In a first stadium we have choose pure compounds with a melting temperature close to the application temperature (20ºC), and with a high latent melting heat. The objective was use, these compounds as components of the binary, ternary or multicomponent systems. The phase diagrams determined with these compounds allowed us to select, among several compositions, different candidates to be used as MAPCMs for the required application (Figure 1).

The material selected for this application has a liquidus temperature (temperature where disappeared the last solid particle) around 21ºC, its melting enthalpy (ΔH) is around 155J/g and the difference between the solidus (temperature where appeared the first liquid particle) and liquidus temperatures (δ) is around 3.5°C. The thermal behaviour of this MAPCM tested by DSC over cycles of heating and cooling at a milligram scale showed no differences after cycling.

THE PROTOTYPE

The device tested (Figure 2) consist of a cardboard box (2mm thickness) covered by a layer of expanded polystyrene whose thickness is 50mm at the top and bottom, and 22mm at the sides. This device contain four plastic containers (used normally in portable ice chests) inside, with a total quantity 2.8 liters of MAPCM. Two of them are placed at the bottom of the box, and the other two at the top, leaving the monocrystal box in the middle.

To design and test the prototype, heat transfer simulation methods were used. The software used to model the heat transfer inside the prototype was TDYN 4.4b[6]. TDYN is a fluid dynamic (CFD) simulation environment based on the stabilized finite element method which permits the simulation of heat transfer problems in fluids and solids. This software includes fully integrated pre/post-processing modules GID7.3b[7]. The materials properties and the conditions used during the calculation are summarized in the Table I.

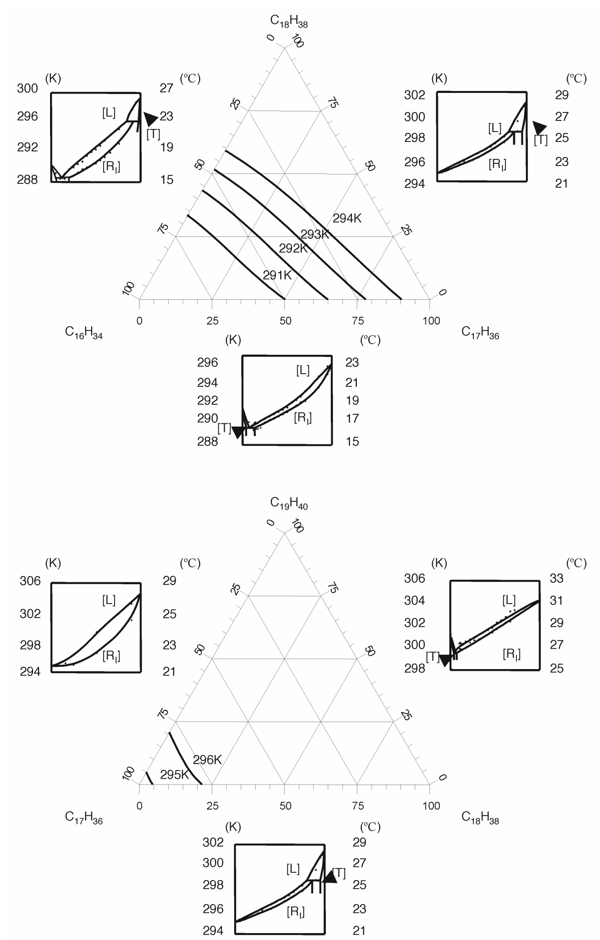


Fig 1: Phase diagrams used to select several compositions, to be used as MAPCMs for the required application.

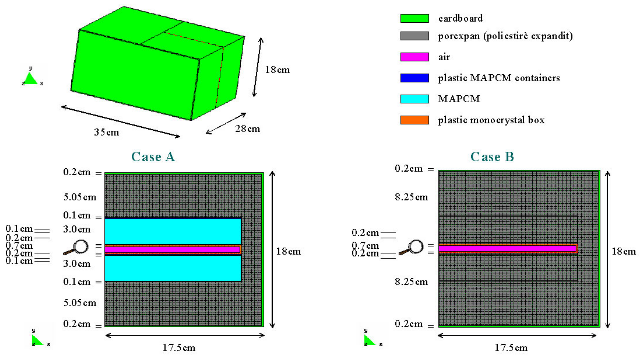
The results obtained with the simulation program are agree with those obtained experimentally (Figure 3) using a thermal device to control the ambient temperature during transport, and several Pt probes placed in the different parts of the prototype.

Materials proprieties	d(kg/m^3)	λ(W/mK)	Cp(J/kgK)
Cardboard	930	0.18	1340
Expanded polystyrene (EPS)	25	0.033	1210
Air	1.22	0.02	1006
Plastic MAPCM containers	900	0.2	1800
Plastic monocrystal box	900	0.2	1800
MAPCM	870	0.2	(255K) 1800, (275K) 1800 (278.23K) 2170 (280.03K) 2380 (282.03K) 2860 (284.03K) 3430 (285.33K) 3990 (286.43K) 4770 (287.53K) 5610 (288.63K) 7310 (290.23K) 10490 (291.63K) 14240 (292.83K) 19190 (294.33K) 26960 (295.13K) 37160 (297K) 2400 (298K) 2400

Boundary conditions:
External temperature (transport temperature) 298K
Heat flux of the air 20*298 W/m^2
Reactive heat flux 20 W/m^{2}K
Internal conditions:
Initial temperature of the cardboard, Expanded polystyrene (EPS), air inside de prototype and Plastic monocrystal box 293K
Initial temperature of the MAPCM and Plastic MAPCM containers 255K

Table I. Material properties and conditions used during the simulation process using the TDYN 4.4b software. d: density, λ: thermal conductivity and Cp: specific heat.

Fig 2: Prototype used.



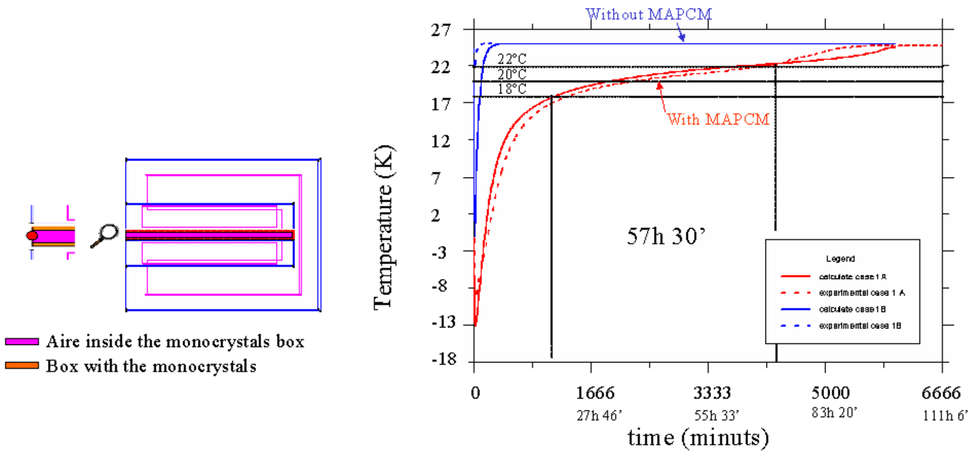


Fig. 3: Experimental and calculated temperature versus time evolution using MAPCM and without MAPCM.

CONCLUSION

The basic knowledge of the properties of a family of substances (in this case n-alkanes), particularly their capacity to form stable molecular alloys, permits us to conduct the search for suitable molecular alloys as phase change materials for a particular application.

The results obtained with the prototype proposed show that the effect of the MAPCM is important (57h 30' at 20±2ºC). This thermal device can be also used to protect any kind of food product or biomedical supplies which needs to be distributed at this controlled temperature.

REFERENCES

[1] D. Mondieig, A. Marbeuf, L. Robles, P. Espeau, B. Poirier, Y. Haget, T. Calvet, M.A. Cuevas-Diarte, *High Temperatures-High Pressures,* **1997**, *29*, 385-388.

[2] H.A.J. Oonk, D. Mondieig, Y. Haget, M.A. Cuevas-Diarte, *J Chem Phys*. **1998**, *108*, 715-722.

[3] D. Mondieig, F. Rajabalee, A. Laprie, H.A.J. Oonk, T. Calvet, M.A. Cuevas-Diarte, *Transfusion and apheresis science,* **2003**, *28*, 143-148.

[4] P. Espeau, D. Mondieig, Y. Haget, M.A. Cuevas-Diarte, *Package technol sci*. **1997**, *10*, 253-260.

[5] L. Ventolà, T. Calvet, M.A. Cuevas-Diarte, D. Mondieig, H.A.J. Oonk, *Mat Res Innovat.* **2002**, *6,* 284-290.

[6] TDYN 4.4b developed by COMPASS enginieria y sistemas **2002**.

[7] GID 7.3b developed by CIMNE (International Center for Numerical Methods in Engineering **2002**.