RESEARCH ARTICLE OPEN ACCESS

Energy Storage: CFD Modeling of Phase Change Materials For Thermal Energy Storage

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ABSTRACT
To optimize the utilization of thermal conversion systems it is needed to integrate them with thermal energy storage. Between many types of base materials, the phase change materials (PCMs) are the most adequate mediums to store and release the thermal energy. PCMs have high latent heat of fusion and, in general, low thermal conductivity, therefore, nanomaterials are used as additives to enhance the properties of base materials as PCMs.

Paper presents an exhaustive classification of PCMs and nanomaterials used in thermal energy storage technologies in addition an assessment about their modeling through computational fluid dynamics (CFD).

Goal was to emphasize CFD use as an effective tool to increase engineering development of thermal energy storage technologies.

Keywords-CFD, Nanofluids, Nanomaterials, Nanoparticles, PCM,TES.

I. INTRODUCTION

In nature, many types of energy sources are intermittent as solar energy; accordingly, thermal energy storages (TES) are primary in heat recovery and in improving the performance of the thermal systems.

TES are able to store the thermal energy and release the stored thermal energy to recompense for the shortage in the main thermal source. Commonly, the storing medium is a fluid or phase change material (PCM). In general, the thermal conductivity of these TES is poor leading to a slow charging and discharging rate. The charging and discharging rate can be enhanced by applying the heat transfer enhancement methods.To enhance the thermal conductivity of the TES materials there are numerous methods varying from extended surfaces and fins, bubble agitation, metal ring and metal matrix insertion, encapsulation, and many others; among them are the nanoadditives [1, 2, 3].

Many researchers published studies on the thermophysical properties of different PCM and/or nanomaterials for different applications. Investigations on the characteristic mechanism enhancement (conductive and convective heat transfer) by these advanced materials have been carried out experimentally, numerically and theoretically [4,5,6,7].

CFD utilization is expected to be an effective way to save money and time and to deliver optimization tools for maximum efficiency of these systems.

Article focuses on the enhancement of TES by using nanomaterials as additives to the base storage materials. It critically reviews the existing studies dealing with the use of nanocomposites in TES applications. First, classifications of PCMs and of the nanomaterials were presented and discussed and then CFD utilization to study nanocomposites are analyzed.

Goal was to emphasize CFD application as an effective tool to increase engineering development of thermal energy storage technologies.

This study involved the author in the task FP7: "Feasibility study for the synthesis of Nano PCM with attractive properties for using in TES" of STAGE_STE, an Integrated Research Program (IRP) on the topics Concentrating Solar Thermal Energy that engages all major European research institutes. [8].

II. PCMsANDNANOPARTICLES: CLASSIFICATIONS

Phase change materials are the most satisfactory mediums to store and release the thermal energy due to their high latent heat of fusion. Because, in general, it have low thermal conductivity, use of

nanoparticles dispersed enhances the thermal properties of the phase change materials.

For the reasons mentioned above, first the classification of PCM and then classification of dispersed nanoparticles were carried out.

Solid-liquid PCMs are classified into three categories named Organic Compounds, Inorganic Compounds and Eutectics Compounds. Detail

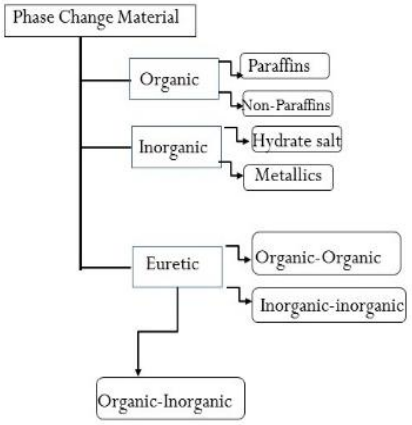

Figure 1. Basic categories of phase change materials

classification is givenin Figure 1. [9,10,11]

Paraffins are mostly hydrocarbons. Non-paraffins are fatty acids and form the largest group in the phase change materials. Inorganic PCMs are separated into salt hydrate and metallic. Hydrate salt undergoes hydration and dehydration of the salt during the phase change but not all of the hydrate salts melt congruently. Metallics are low melting metals and eutectics. These metallics are very light and have a high thermal conductivity like metal but are low in terms of the latent heat of fusion. Another alternative in PCMs is eutectics. Eutectics are compositions of two or more components such as a combination of organic and organic, inorganic and inorganic, and inorganic and organic. Eutectics have shown a positive sign to solve the incongruent melting of hydrate salts. Mixing two types of hydrate salts, (inorganic and inorganic) as an example, to form a eutectic, helps to prevent incongruent melting and atthe same time reduces the melting point and improves the thermal conductivity.

Although organic PCMs possess lower latent heat compared to inorganic PCMs, the thermal cycles are stable and have a low super cooling effect. It is important to have stable thermal cycles. In such, the storage and release of the latent heat will be stable with no weight loss happening [12]. However, the thermal conductivity of PCMs is low. The introduction of nanomaterials mixed with PCMs will enhance the thermal conductivity.

Nanomaterials are classified into organics and inorganics

Organic nanomaterials:

- ✓ fullerenes,
- ✓ carbon nanotubes (CNT),
- ✓ single-walled carbon nanotubes (SWCNT),
- ✓ multi-walled carbon nanotubes (MWCNT), graphite and nanofibers.

Inorganic nanomaterials:

- ✓ aluminium,
- ✓ zinc,
- ✓ copper,
- ✓ iron,
- ✓ aluminium oxide,
- ✓ iron oxide,
- ✓ titanium oxide

Quantum dots, such as CdSe, ZnS, and ZnOetc are metalloid nanomaterials and are categorized as inorganic nanomaterials.
Finally, hybrid nanomaterials are the combination of organic and inorganic nanomaterials.

III. NUMERICALSOLUTIONOF PCM AND NANO_PCM

Many studies on conductive and convective heat transfer in the PCMs with and without dispersed nanoparticleshave been carried out. In this section, numerical and analytical solutions and CFD use for these problems were explored.

CFD can be in fact an effective tool to increase engineering development of thermal energy storage technologies. Furthermore, CFD utilization is expected to be an effective way to save money andtime and to deliver optimization tools for maximum efficiency of these systems.

The mathematical formulation of a phase transient noted as a phase change is governed by a partial deferential equation that can be solved either analytically or numerically. The analytical solution of PCMs is difficult because of the nonlinear phase front interfaces, complex geometries, and nonstandard boundary condition; the few analytical

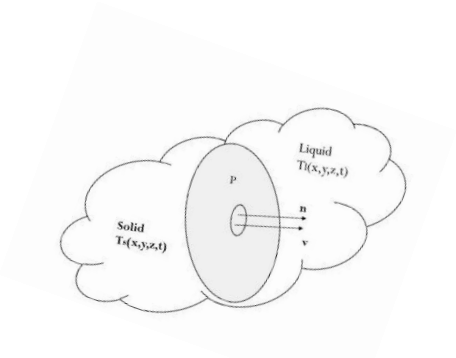

Figure 2. Solid–liquid interface for a multidimensional situation

studies available are on 1D cases with regular geometries and a standard boundary condition.

In addition, numerical solution is difficult because of its inherent nonlinear nature at moving interfaces, for which the displacement rate is controlled by latent heat lost or absorbed at the boundary.

Nevertheless, the heat transfer phenomena in solid–liquid PCMs can be analyzed using two main methods:

temperature-based
enthalpy-based

In the first method, temperature is considered a sole dependent variable. The energy conservation equations for the solid and liquid are written separately; thus, the solid–liquid interface position can be tracked explicitly to achieve an accurate solution for the problems.

$$\frac{\partial T_s}{\partial n} k_s = \frac{\partial T_l}{\partial n} k_l + \rho L K v_n \quad (1)$$

Where T_s temperature of solid is phase, T_l is temperature of liquid phase$k_s$is thermal conductivity of solid phase, k_l is thermal conductivity of liquid phase, n is the unit normal vector to the interface, and v_n is the normal component of the velocity of the interface. L is the latent heat of freezing. As shown in Figure 2

In the second method, the solid–liquid interface position need not be tracked. We often use the enthalpy formulation because of the following advantages:

the governing equation are similar to single phase equation;

no explicit conditions need to be satisfied at the solid–liquid interface;

the enthalpy formulation involves the solution within a mushy zone, involving both solid and liquid materials, between the two standard phases;

The phase change problem can be solved more easily

$$\frac{\partial \rho H}{\partial t} + \nabla \cdot (\rho \bar{v} \mathrm{H}) = \nabla \cdot (k \nabla T) + S \quad (2)$$

Where T is the temperature, k is the thermal conductivity, $\rho$is the density of the PCM, $\bar{v}$is the fluid velocity, His the enthalpy, S is the source term.

IV. CFD ANALYSIS

Researchers simulating melting and solidification processes in engineering problems and the heat transfer phenomena in PCMs, use self-developed programs with language(C++, Fortran, Matlab and also numerous commercial software as COMSOL Multiphysics , Star-CMM and Fluent by ANSYS [13,14,15].

In this paper, we focused use of Fluent software by ANSYS to simulate melting and solidification processes in engineering problems and the heat transfer phenomena in PCMs.

The Fluent processor,tool of workbench ANSYS 15.0is used [16,17] successfully to simulate different engineering problems;it has a specific model that can simulate a range of different melting and solidification problems. The program can be used to solve the phase change that occurs at a single temperature or over a range of temperatures.The applications and limitations of Fluent can be found in Ref. [16,17]. First, physical engineering problem is meshed in a specific geometric modeling using mesh generation tools that include the workbench ANSYS 15.0. After the physical configuration is drawn and meshed, the boundary layers and zone types are defined, and the mesh is exported to the Fluent software.

Different grid sizes and time steps should be applied to the numerical model to ensure that the numerical results are independent of the parameters. Small grid sizes and time steps are preferred for a short simulation time in the computer.

The mathematical equations used to solve the solidification and melting models in Fluent depend on the enthalpy porosity technique [18,19,20] and on the finite volume methods. In the former, the melt interface is not tracked explicitly. A quantity called liquid fraction, which indicates the fraction of the cell volume in liquid form, is associated with each cell in the domain. The liquid fraction is computed at each iteration based on enthalpy balance. The mushy zone is a region wherein the liquid fraction lies between 0 and 1. The mushy zone is modeled as a ‘‘pseudo’’ porous medium in which the porosity decreases from 1 to 0 as the material solidifies. When the material has fully solidified in a cell, the porosity becomes zero, resulting in the drop of velocities to zero. In this

section, an overview of the solidification/melting theory is given [18].

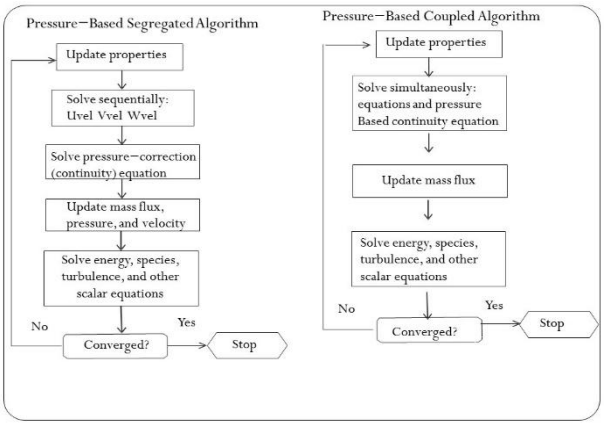

Figura 3. Overview of thepressure-based solution methods

The energy equation is:

$$\partial_t(\rho H) + \nabla(\rho \bar{v}\, \mathrm{H}) = \nabla(k\nabla T) + S \qquad (3)$$

Whereρ is the density of the PCM, $\bar{v}$ is the fluid velocity, K is the thermal conductivity, H is the enthalpy, and S is the source term.

The sensible enthalpy can be expressed as:

$$h = h_{ref} + \int_{T_{ref}}^{T} c_p\, \Delta T \qquad (4)$$

In addition, H can be defined as:

$$\mathrm{H} = h + \Delta H \qquad (5)$$

Where h_{ref} is the reference enthalpy at the reference temperature T_{ref} , c_p is the specific heat, Δ H is the latent heat content that may change between zero (solid) and 1 (liquid), L is the latent heat of the PCM, and γ is the liquid fraction that occurs duringthe phase change between the solid and liquid state when the temperature is$T_l > T < T_s$.

Thus, γmay be written as:

$$\gamma = {}^{\Delta H}/_{L} \qquad (6)$$

$$\gamma = 0 \quad \text{if} \quad \mathrm{T} < T_s \qquad (7)$$

$$\gamma = 1 \quad \text{if} \quad \mathrm{T} > T_l \qquad (8)$$

$$\gamma = \frac{(T - T_s)}{(T_l - T_s)} \text{if} T_l > T_s \qquad (9)$$

The Fluent software has two main solvers: the pressure-based solver and the density-based coupled solver. Only the first method can be used to simulate the melting and solidification problems.

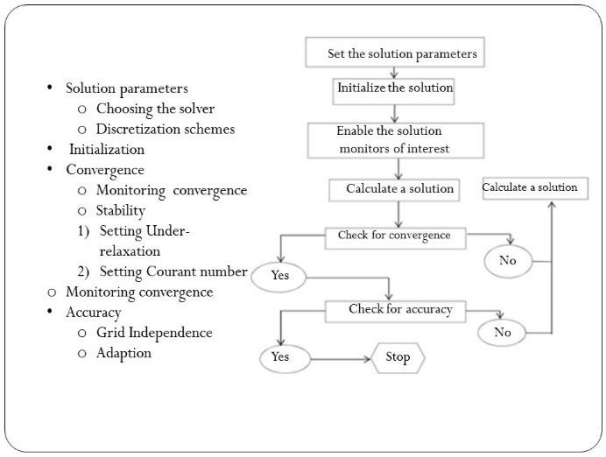

Figure 4.Solution Procedure for Fluent

Figure3 shows two pressure-based solver algorithms, namely, a segregated algorithm and a coupled algorithm, these are available in Fluent. Different discretization schemes are available for the convection terms in Fluent.The first-order upwind, power law, and second-order upwind schemes are mostly used with solidification and melting problems.

Figure4 shows, instead, the solution procedure overview. More details about the solution, initialization, and discretization methods can be found in Ref. [16,17].

The physical properties of materials, such as density, thermal conductivity, heat capacity, and

viscosity, may be temperature dependent and/or composition-dependent. The temperature dependence is based on a polynomial, piecewise-linear, or piecewise-polynomial function. Individual component properties are either defined by the user or computed via kinetic theory. Nevertheless, these physical properties can be defined as a constant value, a temperature-dependent function, or a user-defined function (UDF) that can be written in a specific programming language to define the temperature-dependence of the thermophysical properties.

Sometimes the thermophysical properties of PCMs, as density and viscosity,can be considered as dependent on temperature changes and are determined by specific correlations.

$$\rho = \rho_1/(\beta(T - T_1) + 1)(10)$$

$$\mu = \exp(A+B/T)(11)$$

Whereρ_1 is the density of PCM at the melting temperature T_1 , β is the thermal expansion coefficient, and A, B are constant coefficients.PCM Storage System composed by the relationship between PCM and nanoparticles is described by aspecific model called the volume of fluid (VOF). This model defines the PCM–Nanoparticles system with a moving internal interface, but without inter-penetration of the two-phase fluid.

V. NUMERICAL RESULTS

Goal of this paragraph is summary of main numeric studies of nanostructured materials suitable to implement the efficient thermal storage systems in Concentrated Solar Power.

This study involved the author in the task FP7: "Feasibility study for the synthesis of Nano PCM with attractive properties for using in TES" of STAGE_STE, an Integrated Research Program (IRP) on the topics Concentrating Solar Thermal Energy that engages all major European research institutes.

Author et al [13] numerically investigated on variations on variations of thermos-physical properties of phase change material (PCM) due to dispersion of nanoparticles presented. We focused on investigation of the melting of paraffin wax dispersed with three different metal oxide that is heated from one side of rectangular enclosure of dimensions of 25 mm×75 mm. The integrated simulation system ANSYS Workbench 15.0 for the numerical study was used including mesh generation tool ICEM and FLUENT software.

Aim was examining effects of nanoparticles suspended

Inparaffin wax respect to thermos-physical properties and to heat transfer rate. For all nano-PCM and for all volumetric concentration considered [13], results showed that:

- Thermal conductivity of nano-PCM is greater than the simple PCM.
- Dynamic viscosity of nano-PCM increases with the increase in the volumetric concentration of nanoparticles.

The variation in thermal conductivity and dynamic viscosity

ofnano PCM with temperature and volume fraction agreed well with the experimental reported in literature. Examining effect of volumetric concentration of the nanoparticles on the melting performance, we showed that melting rate decreases with the increase in thevolumetric composition of adding nanoparticles.

In summary, although phase change material due to dispersion of nanoparticles have great potential for demanding thermal energy storage applications, the selection of proper nanoparticlesand its concentration is essential to improve theheat transfer performance of PCM.

Next numerical investigations will concern inorganic materials used such as PCMs. Coming soon, a transient numerical investigation of the melting and solidification process of sodium nitrate (NaNO3), which is used as phase change material, also will be presented.

VI. CONCLUSION

Paper shows exhaustive classification of PCMs and nanomaterials used in thermal energy storage technologies and an assessment about their modeling through computational fluid dynamics (CFD).

Goal was to emphasize CFD use as an effective tool to increase engineering development of thermal energy storage technologies.

The application of CFD in designing PCM thermal storages is a feasible method because of the highly accurate results. CFD also delivers optimization tools to help users achieve maximum efficiency while saving time and money.

Author shows effects of nanoparticles suspended in paraffin wax respect to thermos-physical properties and to heat transfer rate. Results showed that although phase change material due to dispersion of nanoparticles have great potential for

demanding thermal energy storage applications, the selection of proper PCM , nanoparticles and its concentration is essential to improve the heat transfer performance.

Acknowledgements
Author would like to acknowledge IFN (TRENTO) of CNR for collaboration under scientific agreement cooperation signed (2016) with IM of CNR

REFERENCES

Journal Papers:

[1] W.Yu; H.Xie; A review on nanofluids: preparation, stability mechanisms, and applications. *J. Nanomater., 2012, 43, 187-193.*

[2] S.K. Das; S.U.S.Choi; H.E. Patel:Heat transfer in nanofluids - a review. *Heat Transfer Eng., 2006, 27, 3-19.*

[3] X.Wang; A.S.Mujumdar; Heat transfer characteristics of nanofluids: a review. *Int. J. Therm. Sci., 2007, 46, 1-19.*

[4] X. Wang; A.S. Mujumdar;A review on nanofluids - part II: experiments and applications. *Braz. J. Chem. Eng., 2008, 25, 631648.*

[5] X. Wang; A.S. Mujumdar; A review on nanofluids - part I: theoretical and Numerical Investigations. *Braz. J. Chem. Eng., 2008, 25, 613-630.*

[6] M.U.Niemann; S.S.Srinivasan; A.R. Phani;Nanomaterials for hydrogen storage applications: a review. *J. Nanomater., 2008, 23, 1-7.*

[7] S.Kakaç; A. Pramuanjaroenkij; Review of convective heat transfer enhancement with nanofluids. *Int. J. Heat Mass Tran., 2009, 52, 13-14.*

[9] Z.Haddad; H.F.Oztop; E. Abu-Nada; A review on natural convective heat transfer of nanofluids. Renew. *Sust. Energ. Rev., 2012, 16, 5363-5378.*

[10] J.Fan; L.Wang, Review of heat conduction in nanofluids. *J. Heat Transf., 2011, 133(4), 133-138.*

[11] A.Joulin; Z.Younsi; L.Zalewski; S.Lassue; D.R.Rousse; J.P.Cavrout, Experimental and numerical investigation of a phase change material: thermal energy storage release. *Appl. Energ., 2011, 88, 2454-2462.*

[12] B.Zalba; J.Marin; L.F.Cabeza; H.Mehling, Review on thermal energy storage with phase change materials: heat transfer analysis and applications. *Appl. Therm. Eng., 2003, 23, 251-283.*

[13] M.Auriemma;A.Iazzetta; Numerical Analysis of Melting of Paraffin Wax with Al2O3, ZnO and CuO Nanoparticles in Rectangular Enclosure, *Indian Journal of Science and Technology, 2016, 9(3), pp. 1-8.*

[14] A.Joulin;Z.Younsi; L.Zalewski; DR.Rousse;S.Lassue; A numerical study of the melting of phase change material heated from a vertical wall of a rectangular enclosure. *International Journal of Computational Fluid Dynamics 2009;23:553–66.*

[15] N.Mostafavinia; S.Eghvay;A.Hassanzadeh; Numerical Analysis of Melting of Nano-Enhanced Phase Change Material (NePCM) in a Cavity with Different Positions of Two Heat Source-Sink Pairs, *Indian Journal of Science and Technology, 2015, 8(S9), pp. 49–61* .

[18] V.R.Voller; C.Prakash; A fixed grid numerical modelling methodology for convection-diffusion mushy region phase-change problems. *International Journal of Heat and Mass Transfer 1987;30:1709–19.*

Chapters in Books:

[8] STAGE-STE www.stage-ste.eu

[16] http://www.fluent.com/

Proceedings Papers:

[19] V.R.Voller; A.D.Brent;KJ.Reid; A computational modeling framework for the analysis of metallurgical solidication process and phenomena. Technical report. *Conference for Solidication Processing. Ranmoor House, Sheffield; 1987.*

[20] VR. Voller Modeling solidification processes. *Technical report. Mathematical modeling of metals processing operations conference. Palm Desert (CA): American Metallurgical Society; 1987.*