Finite element simulations of encapsulated phase change Materials with density change upon melting: Thermal energy storage technologies

Antonio M. Puertas, Sabina Rosiek, Manuel S. Romero-Cano, F.Javier de las Nieves, F.Javier Batlles

Section of Physics, Department of Chemistry and Physics, University of Almería, 04120 Almería, Spain and
CIESOL, Joint Centre University of Almería-CIEMAT, 04120 Almería, Spain

Introduction

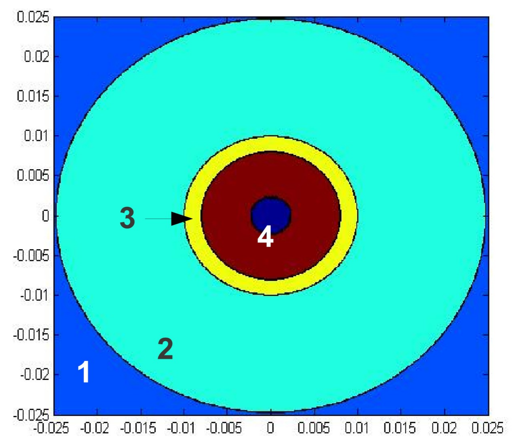
The solar-assisted cooling/heating systems are usually designed to handle the maximum expected load, requiring efficient storage systems to bridge the mismatch between energy production and demand. Thermal energy storage techniques have developed rapidly in recent years, especially latent heat storage systems, that takes advantage of the solid/liquid phase change using so-called phase change materials (PCM). Although nodules of different PCM are already commercialized, there are only a few studies of theoretical models that describe quantitatively the melting of the PCM, and thus can be used to predict the optimal characteristics of the PCM-nodule for a particular application.

In this work, simulations of the melting of encapsulated PCM are presented. The heat equation is solved by the finite differences method, in a two dimensional system. In the model, the capsule is rigid but the PCM decreases its density discontinuously upon melting. We follow the kinetics of melting due to an external heat source by monitoring the temperature profile and solid fraction. A simple theoretical model is also proposed to compare our simulation results. Simulation and theory are in very good agreement.

Numerical method

Model

1. Thermostat ($T_H > T_m$)
2. Bath (Water)
3. Capsule (PVC)
4. PCM ($CaCl_2$)



Initially, the PCM is frozen, with a void due to the different densities of liquid and solid phases

The solid PCM melts only in the vicinity of a fluid phase or the void.

MATERIAL PROPERTIES OF PCM ($CaCl_2 \cdot 6H_2O$), WATER AND PVC: CONDUCTIVITY σ, SPECIFIC HEAT c, AND DENSITY ρ. [23]

	$\sigma\,(W/m\cdot K)$	$c\,(J/(kgK))$	$\rho\,(kg/m^3)$
Solid PCM	1.088	1500	1710
Liquid PCM	0.54	2220	1562
Water	0.58	4180	1000
PVC	0.19	1000	1300

Equations for heat conduction:

$$T_{ij}(t+\delta t) = T_{ij}(t) + \frac{\dot{q}_{ij}\delta t}{\Delta^3\, \rho_{ij}\, c_{ij}} \qquad x_{ij}(t+\delta t) = x_{ij}(t) - \frac{\dot{q}_{ij}\delta t}{\Delta^3\, \rho_{ij}\, L}$$

Details:

Grid: 500x500 (5cm x 5cm). Δ=0.1mm. $\delta t = 5\cdot 10^{-3}$s.
R_{ext} =10 mm, R_{int}=8 mm, R_{thermo}=25 mm, R_{void}=2.4 mm

Theory:

Heat conduction

$$\nabla(\sigma\nabla T) = \rho c \frac{\partial T}{\partial t}$$

Heat equation in the steady state (2D):

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) = 0 \quad \Rightarrow \quad T = A\ln r + B$$

Constant flux and continuity of temperature at the interfaces:

$A_2 \ln R_H + B_2 = T_H$	Thermostat
$A_2 \ln R_{ext} + B_2 = A_3 \ln R_{ext} + B_3$	Bath-capsule
$\sigma_2 A_2 = \sigma_3 A_3$	
$A_3 \ln R_{int} + B_3 = A_4 \ln R_{int} + B_4$	Capsule - PCM
$\sigma_3 A_3 = \sigma_4 A_4$	
$A_4 \ln R_0 + B_4 = T_m$	Melting front

R_0: R_{int} (Initial stage); R_{void} (Final stage)

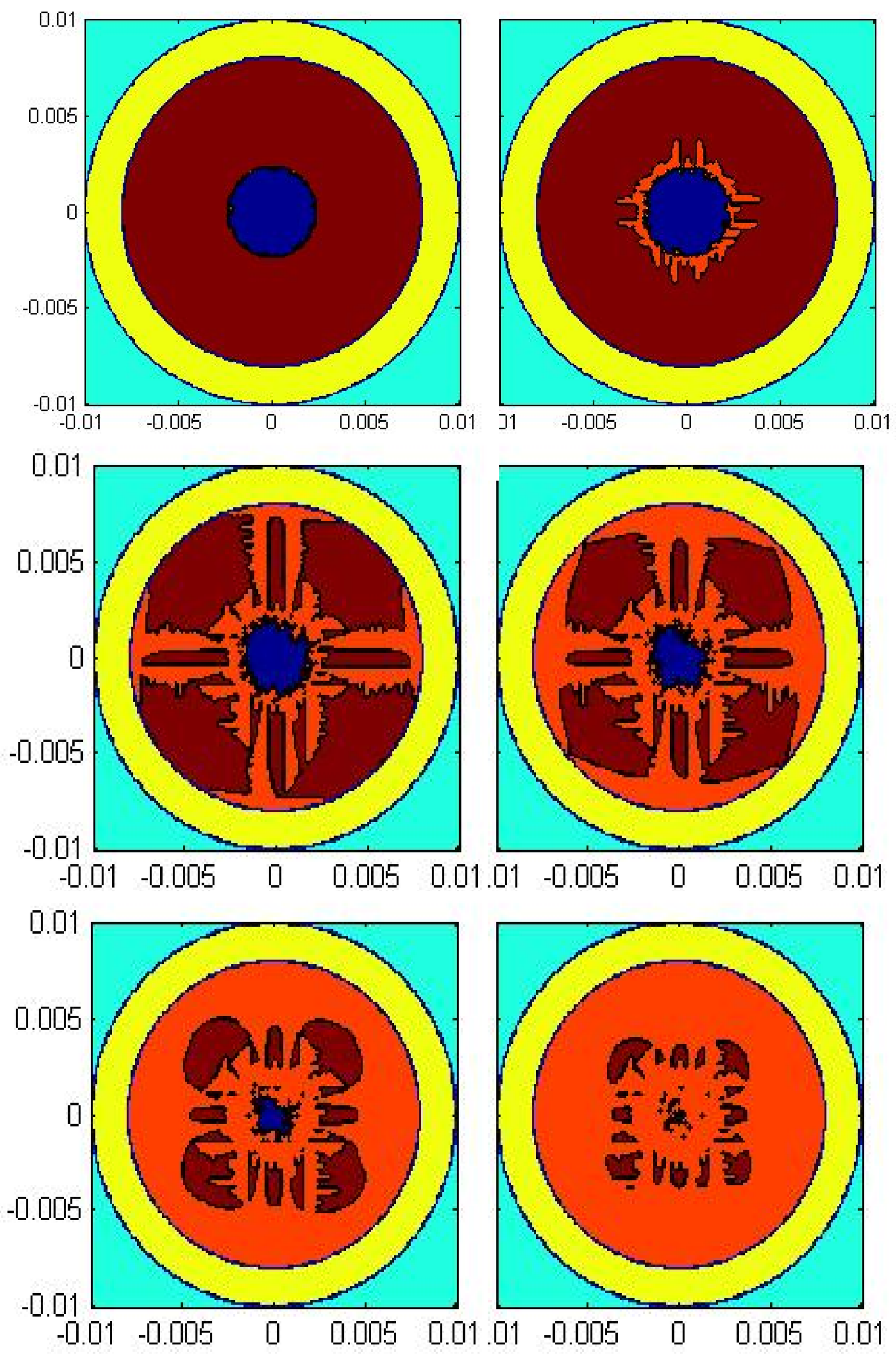
With the solution of the constants, the total flux is:

$$\dot{q} = \sigma \left.\frac{\partial T}{\partial r}\right|_{r=\rho} S = \sigma\frac{A}{\rho}2\pi\rho\Delta$$

Results

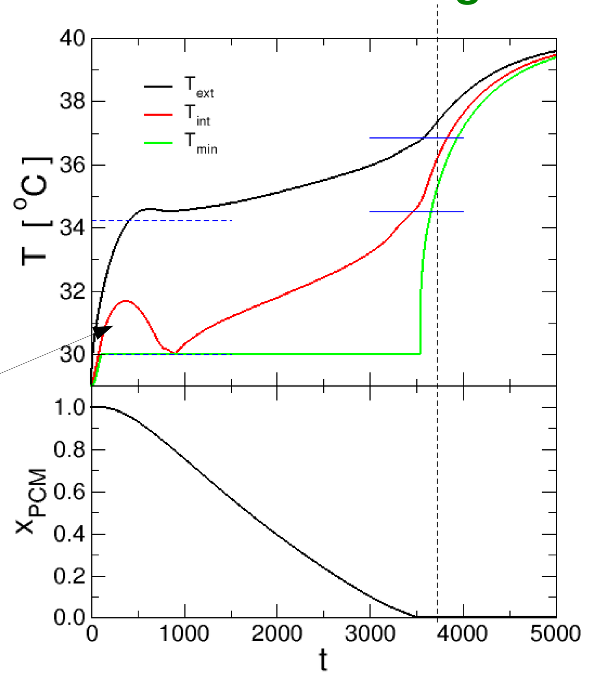
General behaviour

Snapshots

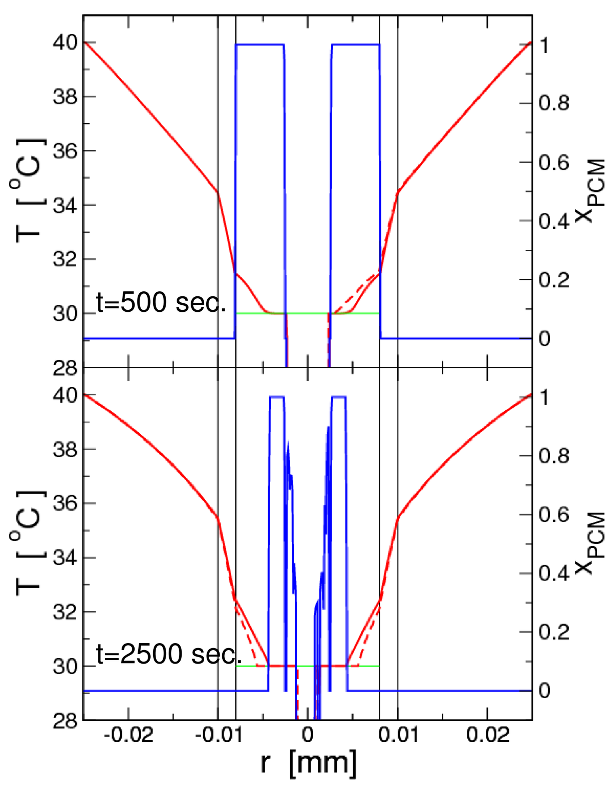


t=0, 750, 1500, 2000,2750, 3500 seconds

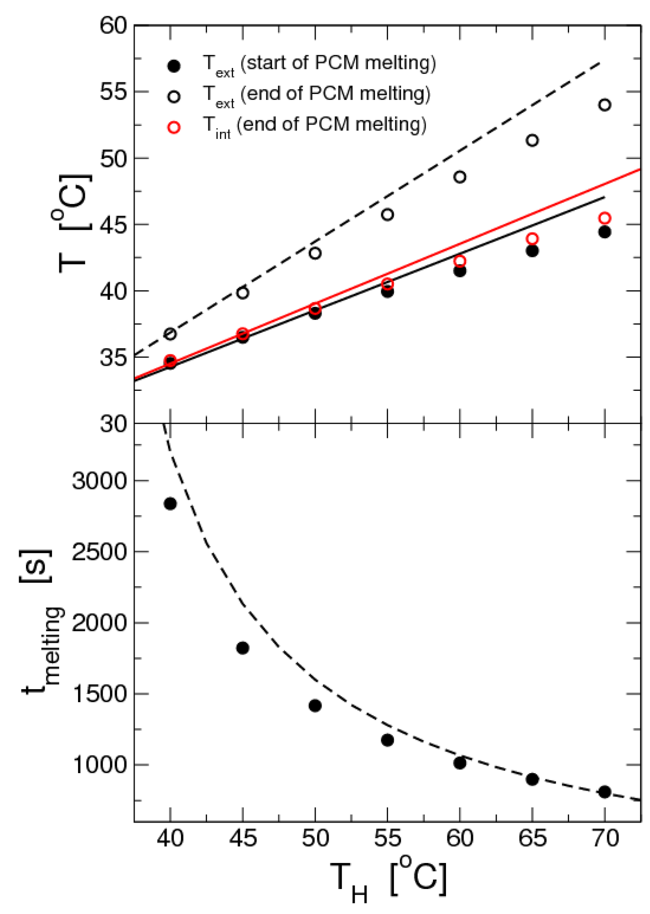
Kinetics of melting



Temperature profile

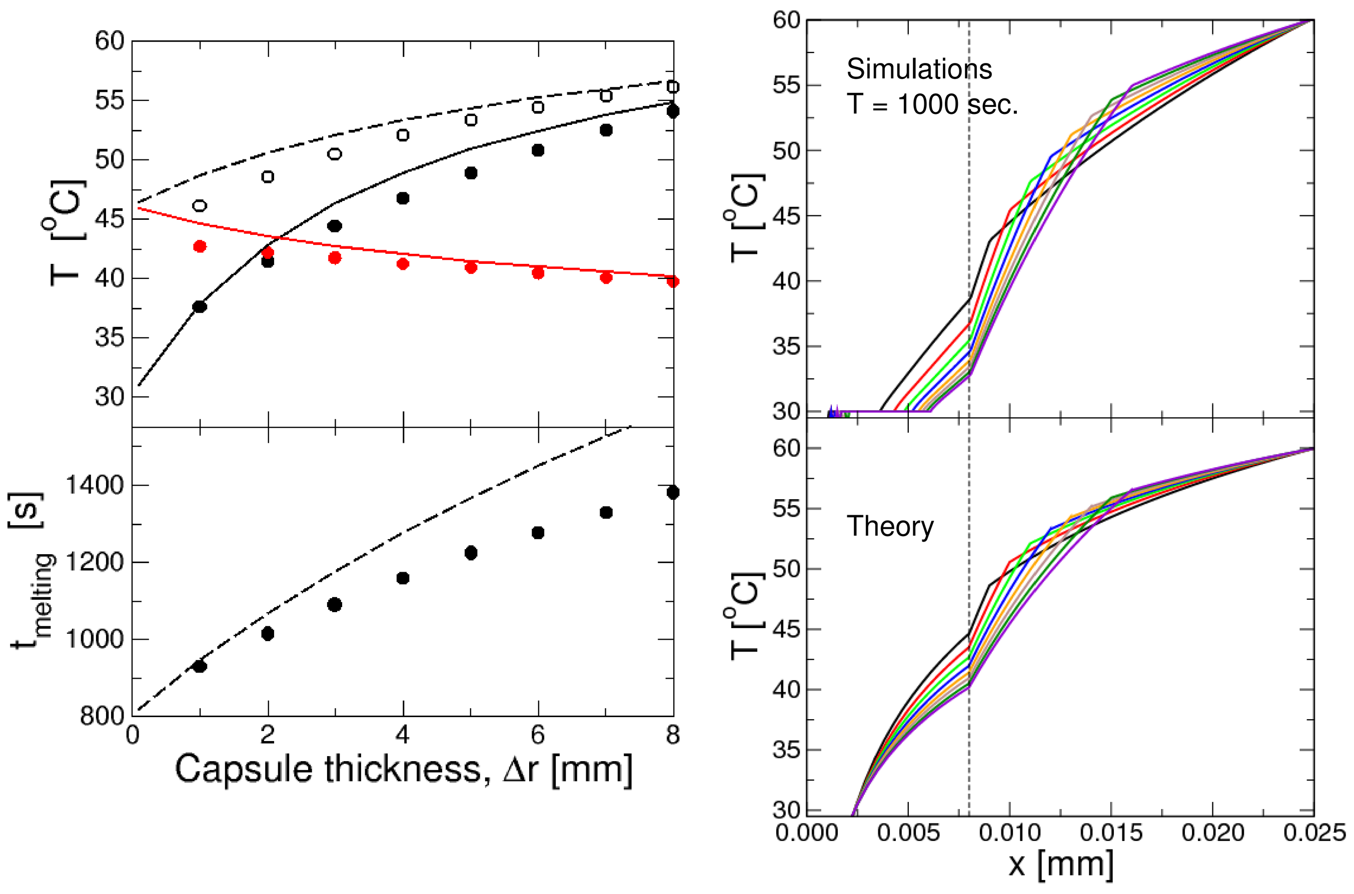


Effect of thermostat temperature



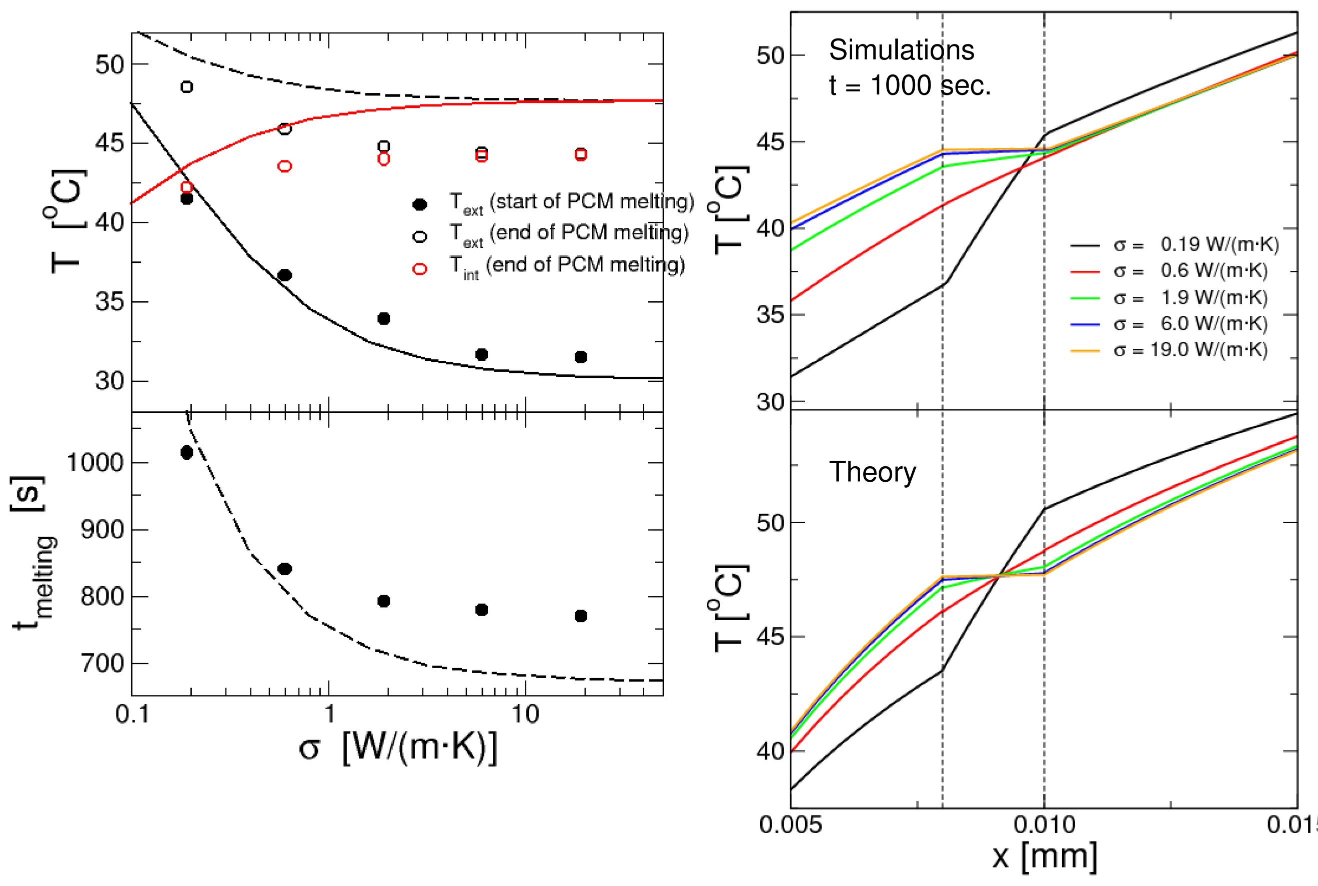
In a hotter environment the PCM melts faster and the surface temperature is higher

Effect of capsule thickness



A thicker capsule isolates the PCM more efficiently; thus it melts more slowly and the surface temperature is higher

Effect of capsule material



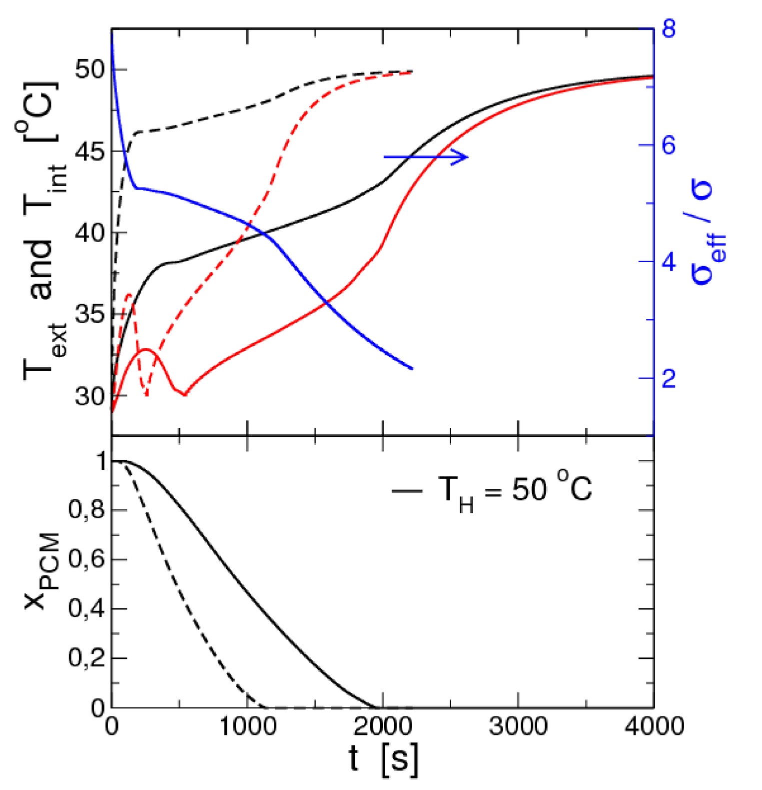
If the capsule is more conductive, the PCM melts faster and surface temperature is lower

Effect of convection in the bath

Effective thermal conductivity

$$\frac{\sigma_{eff}}{\sigma} = 0.386\left(\frac{Pr}{0.861+Pr}\right)^{1/4}(F_{cyl}Ra_D)^{1/4}$$

[Raithby and Hollands, 1975]



With convection in the bath, the PCM melts faster and the temperature is higher

Conclusions

We have developed a simulation and theory models to study the melting kinetics of an encapsulated PCM

In our model, the PCM can melt only in the vicinity of fluid PCM or the void

The model have been used to study the effects of different geometric and physical properties, including the relevance of convection

Acknowledgements

This work has been financially supported by the TERBIOR project, WaterWorks2014 ERANET COFUNDED CALL under the H2020 ERANET scheme, supported by the Spanish Ministry of Economy and Competitiveness, Ref. PCIN-2015-258.