Multi-Scale Modeling of Thermophysical Properties of Phase-Change Nanocomposites for Energy Applications

Alessandro Ribezzo [S], Luca Bergamasco, Matteo Fasano and Eliodoro Chiavazzo [C]
Department of Energy "Galileo Ferraris", Politecnico of Turin, Turin, Piedmont, Italy
eliodoro.chiavazzo@polito.it

With the increasing exploitation of intermittent renewable sources of energy, the energy storage sector has become progressively more important: thermal energy storage is currently the largest single energy storage application field in Europe [1]. An efficient way to store thermal energy is based on the use of phase-change materials (PCM), which – due to phase transition – can assure a sufficiently higher energy density as compared to traditional sensible heat storage. However, overall performance of PCM-based storage systems are limited by poor thermal conductivity, which hinders heat transfer process and lowers key figures of merit such as power density and effective energy capacity [2-3]. A possible way to alleviate that issue is offered by modern nanocomposites, where highly conductive nanofillers (e.g. graphite flakes, carbon nanotubes) are dispersed into PCM matrices [4-5]. A comprehensive multi-scale approach to predict thermophysical properties of PCM-based nanocomposites is the main focus of this work. In particular, molecular dynamics simulations are performed to study nanoscale interactions at the filler-matrix interface [5]. Afterwards, relevant quantities at the atomistic scales are used as key inputs for mesoscopic and continuum simulations. The aim is to construct a consistent model that, spanning from nano- to meso-scale, can accurately predict heat transfer phenomena in nanocomposites. The phase change of such nanocomposites will be investigated as well by analysing the impact of the presence of nanofillers on latent heat and supercooling behaviour of the PCM.

References:

[1] European Association for Storage of Energy, Thermal Storage Position Paper, Brussels, July 2017 (https://easestorage.eu/thermal-storage-position-paper/)

[2] Neri *et al*, Journal of Energy Storage, vol. 32 (2020)

[3] Li *et al*, Renewable Energy, Vol. 147 (2020)

[4] Fasano *et al*, Renewable and Sustainable Energy Reviews, vol. 41 (2015)

[5] Nejad *et al*, , International Journal of Thermal Sciences, vol. 159 (2021)