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Computational Modeling in studying phase change materials

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Abstract

Phase-change materials (PCMs) are a well-known class of materials with a wide range of uses, from temperature stability to heat or cold storage. The primary premise of PCMs is to store energy by using the latent heat of a phase change. The major rationale for combining several chemicals to make a PCM is to attain a certain melting temperature for a specific application. However, these mixed PCMs necessitate precise and reliable techniques for estimating their physical characteristics, as the thermal properties of materials and their right determination are a significant challenge for numerical modeling that has a substantial impact on accuracy and credibility.

Keywords: energy saving; energy; insulation; building; sustainability; renewable energy; nature

Public Interest Statement

While many of the advances in materials science have been driven by breakthroughs in material design and fabrication, understanding the changes that occur in a material during its utilization or operation in devices is of immense importance for its successful integration. Considering these aspects and the continued growth in materials research, there is a clear need for new topical journals which can serve researchers to understand the phase transitions and exploit the phenomena to current, state-of-the-art research in the field of materials science, moreover with full accessibility.

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Introduction to modeling PCM

Each of the components of energy storage devices play important roles to improve their energy efficiency by reducing the mismatch between supply and demand. For this purpose, phase-change materials are particularly attractive since they provide a high-energy storage density at a constant temperature, which corresponds to the phase transition temperature of the material. Nevertheless, the incorporation of phase-change materials (PCMs) in a particular application calls for an analysis that will enable the researcher to optimize the performance of systems using different techniques such as modeling and simulation (Dutil et al., 2011).

Modeling techniques are receiving ever increasing interest in different scientific and technological areas. There are several modeling techniques that are being utilized by the researchers from different application perspectives. Here we propose a new and fast one-dimensional analytical model for simulating the long-term behavior of low energy efficient materials, especially for the design and optimization of Thermal Energy Storage (TES). It has been concluded that advanced instrumentation strategies and technical advancements are necessary in TES technology and systems. Higher computation time and anomalous behaviors of applied phase change materials (PCM) are the major drawbacks we face for modeling a PCM system.

Computational Fluid Dynamics (CFD) codes are commonly used in PCM simulation. Experimental data have been used for qualitative and/or quantitative validation of the CFD simulations in many cases. Several researchers tried to model PCM behavior using a RC-circuit concept. In order to evaluate the performance of the RC model, a computational fluid dynamics (CFD) model is developed.

"Modeling and simulation" are considered as efficient tools in science and engineering that link physical/chemical phenomena and characteristics of complex systems. In this regard, multiscale modeling is becoming of fundamental importance for the study of phase change material, especially for their energy optimization. A new material, for instance, has a well-defined molecular structure, but, obviously, its thermal performance is observed at macroscopic scale. So, its thermal properties have to be analyzed considering the impact they may have at different time- and space- scales. Nowadays, one of the major challenges in chemical engineering resides in the description of complex phenomena, which are essentially multiscale in nature. Chemical engineers are trying to describe these complex phenomena by formulating (and solving) multiscale models (Fermeglia & Pricl, 2007).

A multiscale approach, therefore, requires a detailed study both at microscopic and macroscopic scales, which characterize the system behavior, and the identification of some linking parameters allowing a proper transition (coarse-graining) between different scales. No single simulation method can provide the detailed insights of real processes considering their multiscale natures. In addition, there exist no general and comprehensive methodology, which can suggest how to link and couple the phenomena occurring at different scales. Multiscale simulations, instead, allow properly modeling and analyzing the connections between the different scales, and hence to determine how a change or even a perturbation at one scale may influence the results of the other scale.

However, there remained a challenge for the proper integration of data and simulations across different space scales and timescales (Amaro & Mulholland, 2018).

Stefan problem is attributed to the type of problems associated with changing phase boundary with respect to time. Corresponding solutions are mostly one-dimensional and defined in semi-infinite or infinite regions. On the other hand, numerical techniques are used to model boundary of phases as well as to calculate the velocity of mushy region. In the case of latent heat, when it is absorbed or desorbed at the boundaries, can be expressed by Stefan condition:

$$\rho\lambda\frac{ds(t)}{dt} = Ks\frac{\partial Ts}{\partial t} - K_f\frac{\partial T_f}{\partial t} \tag{1}$$

where ρ density (kgm-3), λ *is* latent heat ((kJ/kg), K is thermal conductivity (W/mK), s is surface position (m), *t is* time (s) and T = temperature (K)

The conservation of energy can be expressed in terms of total volumetric enthalpy (H) and the temperature (T) as:

$$H = \int_{T_{ref}}^{T} c_p dT + \beta\rho\lambda \tag{2}$$

Where Cp is specific heat (J/kg K) , β is liquid fraction.

Here, the first and second terms represent the sensible enthalpy and the latent heat, respectively. Therefore, the energy equation in the PCM can be written as:

$$\frac{\partial}{\partial t}(\rho H) + \nabla.\left(\rho \underset{u}{\rightarrow} H\right) = \nabla.(K\nabla T) + S \tag{3}$$

where S is the source term.

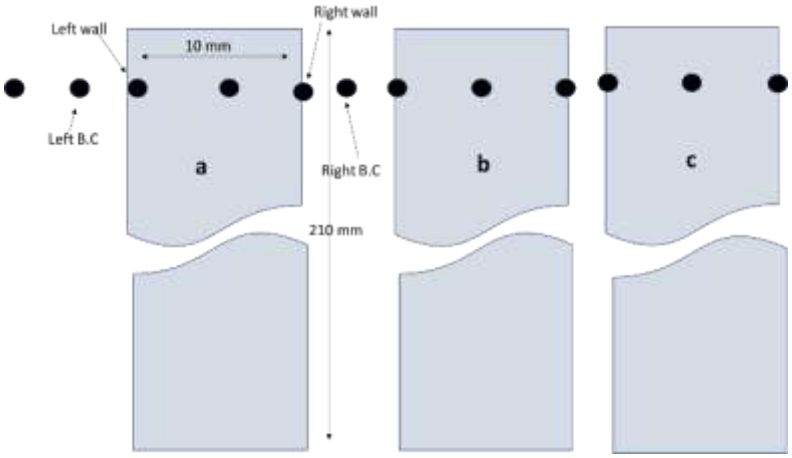

Figure 1. One dimensional modeling of the PCM sheet (a) only one phase, (b) two-phases and (c) three-phases. Here the number of nodes represents the coexistence of phases

The proposed Stefan model is indirectly validated as shown in Figure 1. A MATLAB code is developed to evaluate the performance of the proposed model. As discussed earlier, the number of nodes represents the coexistence of phases. The distance between nodes is also calculated based on equation given in the previous section. The proposed model automatically switches between one, two, and three nodes depending on the temperature imposed by left and right boundaries. It means that a two-dimensional computational fluid dynamics (CFD) model based on enthalpy equations can be utilized effectively for phase transitions.

Conclusion

The application of phase change materials (PCMs) in green buildings has been increasing rapidly. However, for that we need efficient models to design optimum materials. Computational models, especially advanced multiscale modeling techniques are of fundamental importance for developing a high-performance material in the shortest possible time. To design a TES material that could meet the necessities of green buildings, multiscale modeling techniques must be the integral part of building design. A reliable and fast simulation-based tool such as MATLAB can be employed for the design and optimization of PCMs for their TES applications such as in green buildings.

References

Amaro, R. E., & Mulholland, A. J. (2018). Multiscale methods in drug design bridge chemical and biological complexity in the search for cures. *Nature Reviews Chemistry 2018 2:4*, *2*(4), 1–12. https://doi.org/10.1038/s41570-018-0148

Dutil, Y., Rousse, D. R., Salah, N. Ben, Lassue, S., & Zalewski, L. (2011). A review on phase-change materials: Mathematical modeling and simulations. *Renewable and Sustainable Energy Reviews*, *15*(1), 112–130. https://doi.org/10.1016/J.RSER.2010.06.011

Fermeglia, M., & Pricl, S. (2007). Multiscale modeling for polymer systems of industrial interest. *Progress in Organic Coatings*, *58*(2–3), 187–199. https://doi.org/10.1016/j.porgcoat.2006.08.028