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Published in:
Journal of Physics: Conference Series (Online)

DOI:
10.1088/1742-6596/2116/1/012023

Publication date:
2021

Document version:
Final published version

Journal of Physics: Conference Series

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Abstract. Optimal selection of domain discretization for numerical Phase Change Material (PCM) models is useful to establish confidence in model predictions and minimize the time consumption for conducting design analysis. Very detailed and geometrically complex models are usually applied utilizing several million cells. A 2D numerical PCM model of a climate module for thermal comfort ventilation is investigated. The mesh independence was conducted on 22 different mesh sizes ranging from 70 to 10.870 nodes. Convergence criteria was evaluated based on average air supply temperature and total heat transfer between the PCM and the air within the simulation time interval. Less than 0.1 % change in the air supply temperature and the heat transfer between the PCM and the air was achieved with 5250 and 9870 nodes, respectively. Thereby highlighting that a relatively small amount of nodes can be considered to achieve sufficient accuracy to conduct analysis of PCM applications.

1. Introduction

Investigating the impact of domain discretization for numerical models is needed in order to identify the least detailed mesh that can be used by the numerical model while being able to accurately predict the behavior of the considered dynamics to the required precision. The use of mesh independence studies are especially applied within the field of Computational Fluid Dynamics (CFD) and other numerical models. Numerical modeling has become an increasingly standard approach used in product development in engineering fields, allowing testing of various design scenarios without the need for multiple prototypes produced [1]. CFD models are frequently applied within the field of Phase Change Material (PCM) analysis. Detailed models are needed to predict the behavior of the PCM in the phase transistion [2, 3]. Bejan et al. (2019) [4] found that a mesh of 5.3 million cells was needed to eliminate visual variations between the velocity profiles for a CFD model of an air-solar collector with PCM. Melting heat transfer was analysed by Sheikholeslami et al. (2017) [5], where a CFD model of the dynamic melting of CuO-water nanofluid was utilized. Mesh independence was found by evaluating the average Nusselt number for different mesh sizes resulting in a mesh of 14.981 nodes. Five different grid sizes were investigated in the range of 15.000 to 120.000 elements for an inclined PV/PCM system by Yildiz et al. (2020) [6]. Reporting that the grid of 88.500 elements has achieved grid independent solutions of the mean Nusselt number with reasonable computational time. Giovannelli et al. (2017) [7] studied a PCM based short term thermal storage for a solar dish micro gas turbine to handle large temperature variations in the working fluid. For the developed CFD model four different meshes of between 445.065 - 4.037.561 cells were investigated and the independence was evaluated using the average hot wall temperature, the outlet working fluid temperature and the PCM liquid fraction. However, no mesh was chosen as optimal

Journal of Physics: Conference Series **2116** (2021) 012023 doi:10.1088/1742-6596/2116/1/012023

and both increasing and decreasing tendencies were observed for the output parameters with increasing mesh resolution. Mesh independence studies are often conducted within this modeling field utilizing few meshes, and relying on changing or unspecified criteria for convergence of the solution. This contribution will conduct a detailed domain discretization study using suggested parameters of a 2D numerical model, of a climate module with PCM for Heating, Ventilation and Air Conditioning (HVAC) purposes. The analysis is based on accumulated heat transfer, supply air temperatures from the ventilation system and average temperature of the PCM.

2. The Model

A validated 1D finite difference model of a PCM based climate module developed earlier by the authors was upgraded and expanded to a 2D model by including air dynamics [8]. The developed climate module model is intended to be used for design purposes, optimization and control strategy investigations. For this objective, the modeling has to consider time periods of up to one year with changing data inputs, hysteresis and partial melting. The mesh independence study is performed on a data set that includes sharp temperature gradients and discontinuities that have to be modeled accurately. A 3D drawing of the climate module that the model is applied to is presented to the left of Figure 1. The climate module functions as an add-on to a ventilation system that will supply cooling or heating to a climate zone, as a replacement to conventional compressor based technologies [9]. Ambient air is drawn in through the ventilation system and runs in small channels between the PCM plates in order to either charge or discharge the PCM. A number of simplifications are made in order to simplify the model while maintaining representation of the PCM and air in the climate module. These simplifications can be seen in Figure 1. Here it is assumed that there is uniform air distribution between the PCM, meaning that all

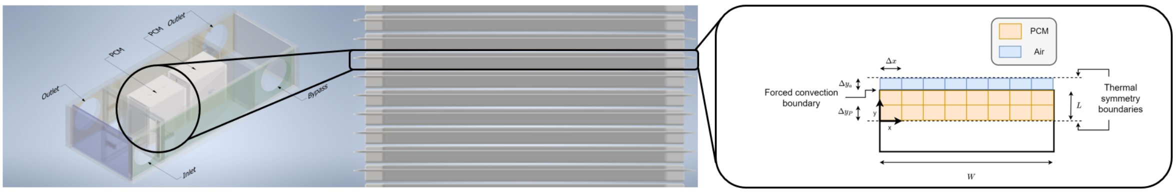


Figure 1: Left: 3D drawing of climate module with PCM. Middle: 2D view of the PCM plates with PCM inside them. Right: Discretization of the PCM and air into nodes.

the plates will behave in the same way and only one of the plates needs to be modeled. The buoyancy forces that arise as a result of density changes with variations in temperature and phase are not considered and therefore a symmetry boundary through the middle of the PCM plate can be assumed. Likewise, only half of the air channel needs to be considered. Thus, the discretization domain is made up of half the PCM plate thickness and half of the air channel height. The heat transfer at the air and PCM interface is modeled using a convective heat transfer coefficient estimated from the Nusselt number and the air velocity in the channel [10] and the end points of the PCM panels orthogonal to the air flow direction are assumed adiabatic,

$$-k_P \frac{\partial T}{\partial y}\bigg|_{y=0} = 0 \quad , \quad -k_P \frac{\partial T}{\partial y}\bigg|_{y=L} = h\left(T_a - T_P(y=L)\right) \quad , \quad -k_P \frac{\partial T}{\partial x}\bigg|_{x=0,W} = 0 \quad (1)$$

Where $-k_P$ is the thermal conductivity of the PCM, L is half of the thickness of the PCM plate, h is the convective heat transfer coefficient, T_a is the air temperature, T_P is the PCM temperature and W is the length of the air channel. A 2D finite difference scheme is used for the modeling of the heat equation of the PCM and the backward-difference representation is used for the air [11],

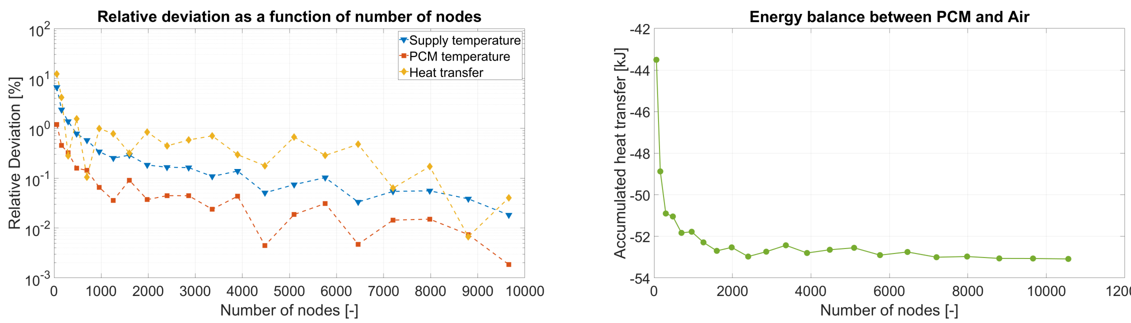
$$PCM : \frac{dT_{i,j}^{t+1}}{dt} = \alpha_P \left(\frac{T_{i-1,j}^t + T_{i+1,j}^t - 2T_{i,j}^t}{\Delta x^2} + \frac{T_{i,j-1}^t + T_{i,j+1}^t - 2T_{i,j}^t}{\Delta y_P^2} \right) \tag{2}$$

$$Air : \frac{dT_{i,j}^{t+1}}{dt} = \frac{2h}{\rho_a c_{p,a}} \frac{T_{i,j-1}^t - T_{i,j}^t}{\Delta y_a} + \alpha_a \frac{T_{i-1,j}^t + T_{i+1,j}^t - 2T_{i,j}^t}{\Delta x^2} - u_x \frac{T_{i,j}^t - T_{i-1,j}^t}{\Delta x} \tag{3}$$

Where t is the time step, i is the number of the node in the x direction, j is the number of the node in the y direction, T is the temperature of the node, u_x is the velocity of the air in the x direction, ρ_a is the density of the air, $c_{p,a}$ is the isobaric specific heat capacity of the air, α_P is the thermal diffusivity of the PCM, α_a is the thermal diffusivity of the air, Δx is the node length in the x direction, Δy_P is the PCM node length in the y direction and Δy_a is the air node length in the y direction. The equations are solved using the Ordinary Differential Equation (ODE) solver: ODE15s in MATLAB.

3. Methodology and Findings

The domain discretization analysis purpose is two-fold, both to investigate the meshing level of detail needed to accurately depict the behavior of interest but also determining the point at which model results are independent of further mesh resolution increase. In this analysis 22 different mesh resolutions were investigated. Fixed increases in the number of nodes in the x and y direction where employed investigating number of nodes between 70 and 10.870. Air inlet temperature changing between 35°C and 10 °C every 15 mins, is considered for an hour simulation. Uniform initial conditions at 15°C are assumed for the PCM. The initial condition for the air temperature is assumed to have a linear gradient starting at the inlet temperature to 1°C above or below the PCM temperature at the outlet. The meshes are compared through the heat transfered from the air to the PCM, calculated by integrating the energy change of the air ($\dot{m}_a c_{p,a} dT dt$), the average PCM temperature and the average difference in air supply temperature. Mesh independence will be assumed to have been achieved when the difference between the present solution and the previous solution is less than 0.1 % for two consecutive meshes. Evaluating the average PCM temperature and the supply temperature for the meshes, less than 0.1 % difference is obtained with 1330 and 5250 nodes, respectively, see Figure 2a. The heat transfer between the PCM and the air over the entire time period can be seen as a function of the number of nodes on Figure 2b. Clear



(a) Percentage deviation between concequtive meshes as a function of number of nodes.

(b) Heat transfered from the air to the PCM in the entire time interval with mesh sizes.

Figure 2: Left: Percentage deviation for heat transfer and supply temperature. Right: Total heat transfer as a function of number of nodes.

convergence tendency is observed. However, the heat transfer is more mesh sensitive than the supply temperature not showing less than 0.1 % change with 5250 nodes. For this parameter 9870 nodes are needed to meet the established accuracy requirement for the total heat transfer between the PCM and the air.

4. Discussion and Conclusion

The mesh independence analysis conducted analyzed meshes between 70 and 10.870 nodes and found that a meshing detail of 9870 nodes was needed in order to achieve the required accuracy. Compared to the literature this number of nodes is less than what is typically observed for PCM modeling [4, 7]. The main reason is that many of these models are of larger systems or are 3D meaning that fewer symmetry considerations can be included in the model or the increased level of meshing needed to capture fluid motion in the PCM. The numerical geometry analyzed here is relatively simple due to the purpose of the model being to evaluate large time series data and control of the module, which limits the complexity that can be applied while maintaining reasonable overhead time consumption.

Acknowledgments

This work was financed by the NeGeV project [9] which is funded by the Danish Energy Agency under the Energy Technology Development and Demonstration Program (EUDP Project no 64017-05117). The authors would like to acknowledge the contribution from lector Martin Winther-Gaasvig and engineering student Anders Dyreborg Schmidt who provided the 3D drawing of the climate module.

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