Thermal Modeling in a Historical Building – Improving Thermal Comfort through the Siting of a Passive Mass of Phase Change Material

F. Herbinger, L. Desgrosseilliers, D. Groulx*
Mechanical Engineering Department, Dalhousie University, Halifax, NS, Canada
*Corresponding author: P.O. Box 15 000, Halifax, Nova Scotia, Canada, B3H 4R2, dominic.groulx@dal.ca

Abstract: A model of an office room was created in COMSOL Multiphysics 4.4 to simulate heat transfer and study the impact of siting a mass of phase change material (PCM) in a room to increase thermal comfort. This study determined that incorporating the selected PCM, butyl stearate, in the ceiling and in the floor did not alter the temperature of the room significantly after one hour. Incorporating the PCM in the floor near the windows proved to even slightly increase the temperature in the room. This was due to the high absorptivity of the PCM enclosure. With the PCM in the ceiling, the temperature decreased marginally: 0.1 °C in comparison to the room with no PCM. However, the room temperature started to decrease near the end of the simulation for both PCM configurations. Longer simulation times are needed to see if this trend continues. Additionally, further study is required to determine optimal PCM enclosure surface properties and a mass of butyl stearate that will achieve complete melting over a period of a day.

Keywords: Heat Transfer, Phase Change Materials, Radiation, Building, Thermal Comfort

1. Introduction

Thermal discomfort of occupants in building is an issue that arises when the thermal load received by and removed from the building are in such misbalance that indoor room temperature and/or humidity fall well outside acceptable ASHRAE guidelines. Thermal discomfort occurs in historical buildings due to the occupation incompatibility with the building's original intent as well as poor building envelope performance. A building's heritage status makes modifying the building envelope more difficult or even impossible. The Toronto Carpet Factory located in downtown Toronto, Ontario, Canada is a heritage building which was retrofitted into office spaces. Some of these offices are subject to space temperature fluctuations outside of the ASHRAE comfort level guidelines (*i.e.*, 23°C < T < 26°C during the cooling season, with no more than 1.7°C of temperature fluctuation [1]).

One way of passively controlling and reducing those temperature fluctuations is with the use of a passive mass of phase change material (PCM) inserted in the space. To that regard, a research collaboration is underway with Internat Energy Solution, a Toronto based company, to investigate the anticipated performance of such a heat storage strategy in improving the thermal comfort of occupants in select rooms. Ongoing COMSOL Multiphysics 4.4 simulations performed in Dalhousie University's Lab of Applied Multiphase Thermal Engineering have the goal of simulating the heat transfer in the room and study the impact of siting a PCM on the temperature history of the room.

Phase change materials have been under study for several decades and extensive research has been carried out on their applications in buildings. PCMs can be incorporated passively in several different parts of the building, including the wallboards, concrete, insulation, and ventilation system [2]. One of the possible objectives of passively integrating PCMs into a building is to reduce the internal space temperature span to a more desirable range (*e.g.* reducing a measure temperature range from 20 °C – 27 °C to 22 °C – 25 °C). The addition of a PCM mass achieves this through the storing of thermal energy when it melts once its melting point is reached and the release of the stored energy during solidification when the freezing point of the PCM is reached.

In this research project, heat transfer was simulated in a small, west-facing office room with three windows, accounting for solar radiation, natural convection in the space and phase change heat transfer in the PCM. Studying the impact of siting a PCM on the temperature recorded in the room was the primary goal of the simulations. A mass of PCM was added as a 1 cm layer near the windows on the floor and on the ceiling.

2. Geometry and Materials

Figure 1 shows the geometry of the room used in the simulations. The room is 9.9 m wide, 8.1 m deep and 4.21 m high. The three shaded rectangular prisms represent the window sills where the sun rays enter the room. The wall with contact to the outside air is a four layer brick wall which is 0.46 m thick, and the interior walls measuring 0.2 m in thickness are gypsum wallboard with white paint. Wood oak flooring makes up the ceiling (0.5 m in height) and floor (0.13 m in height), and the interior domains in the room and window sills are composed of air. The domain of air delimited by the first 2 m of the room from the window as seen in Fig. 1 is referred later in this paper as the "close to the wall" volume while the remaining domain of air is referred as "away from the wall". Table 1 outlines the thermophysical properties of the above materials and Table 2 gives the solar radiative properties.

Table 1: Thermophysical properties of room materials used in the simulation

Material	***ρ*** **(kg/m^3)**	***k*** **(W/mK)**	***C_p*** **(J/kgK)**
Brick	1670	0.66	838
Wood (Oak)	820	0.3	2390
Gypsum Wallboard	800	0.17	1000
Air	COMSOL Materials Database		

Table 2: Solar radiative properties of room materials used in the simulation

Material	**Solar Absorptivity**	**Surface emissivity**
Brick	0.63	0.93
Wood (Oak)	0.35	0.89
White Paint	0.25	0.89
PCM Enclosure	0.99	0.99

Table 3: Butyl Stearate properties

Melting Temperature (°C)	26.3
Latent Heat of Fusion (kJ/kg)	167
Solid Thermal Conductivity (W/mK)	0.16
Liquid Thermal Conductivity (W/mK)	0.16
Solid Heat Capacity (kJ/kgK)	1.6
Liquid Heat Capacity (kJ/kgK)	1.9
Density (Solid/Liquid) (kg/m^3)	850

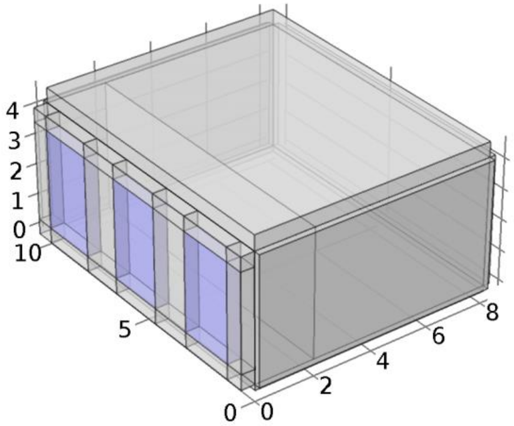


Figure 1: COMSOL geometry of the office room.

The PCM chosen for the particular room conditions was butyl stearate ($C_{22}H_{44}O_2$) having a melting temperature of 26.3 ºC. The PCM thermophysical properties are summarized in
.

The PCM was implemented as a 1 cm layer extending 2 m from the brick wall either in the floor or in the ceiling. The PCM ran the full 9.9 m length of the wall.

3. Mesh

It was determined that the most appropriate mesh for this model was a swept quadrilateral one (see Fig. 2). The general mesh size was set to normal; however, distribution nodes were used for the PCM domain to split it more finely as can be seen in Fig. 3. There were 2064 elements used which still resulted in simulations taking in excess of 2 days to simulate one hour of solar radiation, heat transfer and thermal storage in the room.

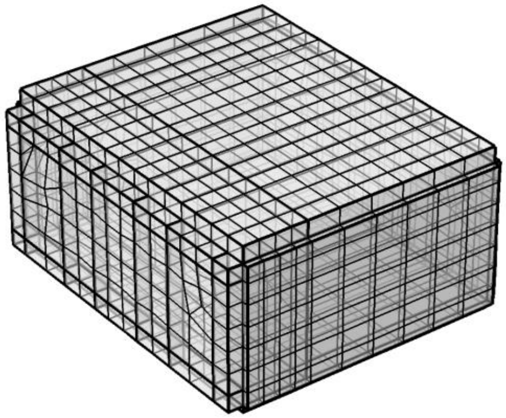


Figure 2: General mesh used in model.

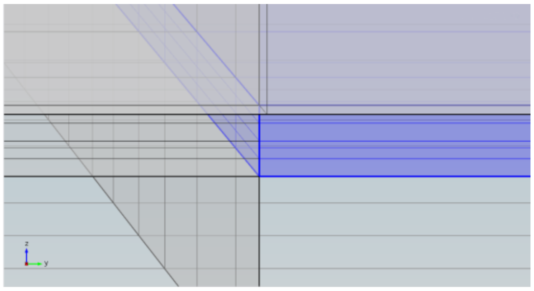


Figure 3: Mesh distribution in the PCM.

Table 4: Values used in the built-in solar model

Latitude (+ to N)	Longitude (+ to E)	Time zone (+ UTC)
43.639	-79.425	-4
Day	**Month**	**Year**
15	08	2013
Hour	**Minute**	**Second**
0	0	*t*

4. Use of COMSOL Multiphysics

The two parent physics nodes used in this work were heat transfer with radiation in participating media, including heat transfer from surface-to-surface radiation, and laminar flow. A coupling was created between the fluid velocity calculated in the laminar flow node and the temperature calculated in the heat transfer with radiation in participating media. Equation (1) was introduced as the volume buoyancy force acting in the *z* direction in the laminar flow physics:

$$F_{\hat{z}} = g_{const} \cdot \rho_0 \cdot \beta \cdot (T - T_0) \qquad (1)$$

where g_{const} is the gravitational constant, ρ_0 is the reference density, which is approximately equal to 1.18 kg/m^3 at 298.15 K and 1 atm, and β is the thermal expansion coefficient which is the reciprocal of the reference temperature T_0.

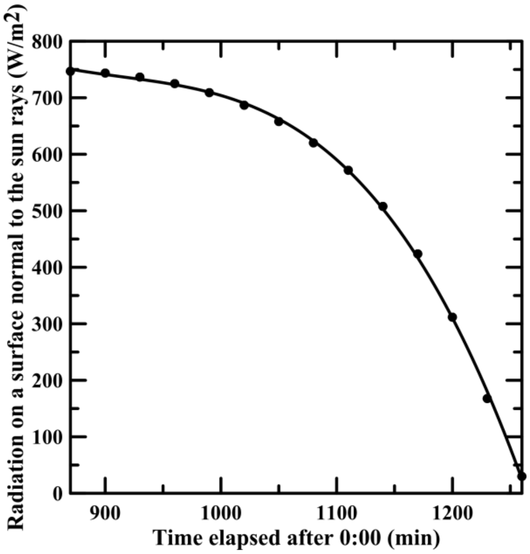


Figure 4: Normal radiation from 14:30 to 21:00 on August 15, 2013. 0:00 indicates midnight.

The important sub-nodes included an external radiation source to model the path of the sun in the Toronto sky and determine incoming radiation, and heat transfer with phase change to model the PCM. Table 4 shows the parameters used in the built-in solar model.

The solar intensity, which is defined as the radiation on a surface normal to the sun rays, was not kept at the default 1000 W/m^2. A time dependent analytical function was used. The function was based on the excel *SolRad_v1.2* model from the department of ecology from the State of Washington [3], which has values for the solar azimuth, elevation, and radiation for any position on the earth and on any given day. Equation (2) was determined by fitting a trendline to the relevant data outputted by this excel model (see Fig. 4). Only the second half of August 15, 2013 was simulated since the sun does not shine in the west facing room until approximately 14:30.

$$R_N = 12381 - 37.658t + 0.040892t^2 - 1.4911 \cdot 10^{-5}\, t^3 \qquad (2)$$

The exterior of the floor, ceiling, and gypsum walls were thermally insulated and the interior boundaries of the room experienced natural convection and surface-to-surface radiation. The exterior of the brick wall underwent external natural convection based on a vertical wall height of 4.21 m and an ambient temperature based on Eq. (3). This analytical function was determined by the ambient temperatures recorded on August 10, 2013 (an average day in terms of temperature near August 15th) at the Toronto City weather station (latitude: 43°40' N; longitude: 79°24' W). Figure 5 shows the trend line fitted to the data, which was retrieved from Environment Canada.

$$T = -0.76766 + 0.051603t - 2.8293 \cdot 10^{-5} t^2 \qquad (3)$$

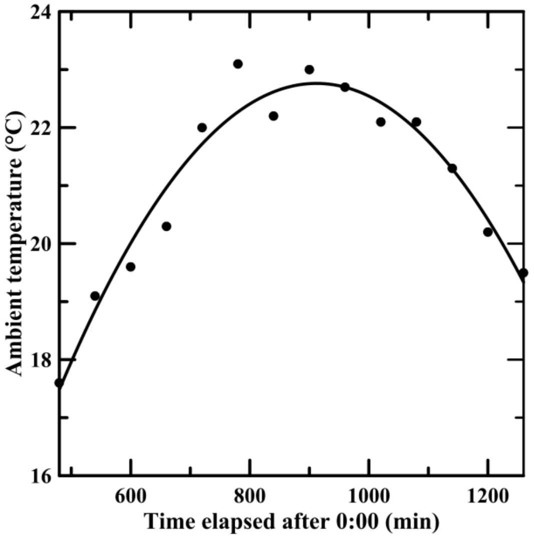


Figure 5: Ambient temperature from sunrise to sunset on August 10, 2013.

The built-in heat transfer with phase change node in COMSOL was used to simulate the PCM melting and solidifying. Thermophysical properties were inputted into the interface as necessary. It is important to note that the simulations assume constant density, as the model does not deal with fudged values to ensure mass conservation. The transition interval between the solid and liquid phase was set to 2 °C.

4. Results

4.1 Without PCM

The first time-dependent simulations that were completed had the goal to successfully modeling the heat transfer in the room through accounting for conduction, convection, and radiation. Figure 6 shows the temperature distribution and resulting fluid motion from natural convection in the room after a simulated hour at 15:30, when an initial uniform temperature of 25 °C was set for 14:30. Based on real-time data collected by Internat, 25 °C is the approximate temperature at this time of day in the room in mid-August. The surface temperature color range is limited to 25 - 29 °C in order to highlight the hot spots created on the floor and the left wall from solar radiation entering through the windows.

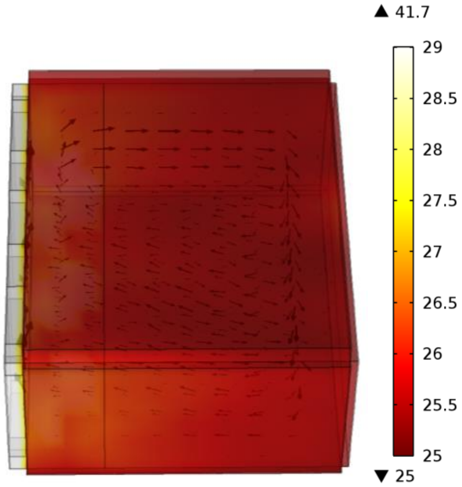


Figure 6: Surface temperature distribution and fluid motion in the room at 15:30.

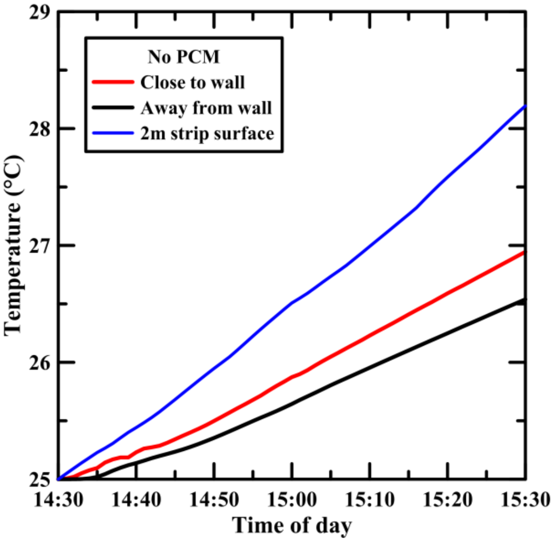


Figure 7: Average temperature in the first 2 m of the room (close to the wall) and in the rest of the room (away from the wall) as well as the average temperature on the surface of the 2 m strip on the floor.

Figure 7 shows the development of the temperature in the two volumes of air defined in the geometry section. Also detailed is the temperature averaged over the surface of the 2 m strip on the floor near the brick wall. It can be observed that without any thermal storage of energy from PCM, the room temperature increases by 1.5 to 2 °C on average. As expected, the strip of floor closer to the windows, which receives direct solar radiation sees its temperature increase more than 3 °C.

4.2 PCM in the floor

The second simulation included PCM in the floor. The comparison between the temperature history of the room without the PCM and with the PCM in the floor is shown in Fig. 8. Due to the high absorptivity of the PCM enclosure (99%) versus the regular flooring use in the previous simulation (35%), a large amount of radiation was absorbed by that surface. Consequently, the air temperature in the room was marginally higher with the PCM in the floor than without PCM, despite the fact that 25% of the PCM did melt, storing thermal energy through this process, as seen in Figure 9.

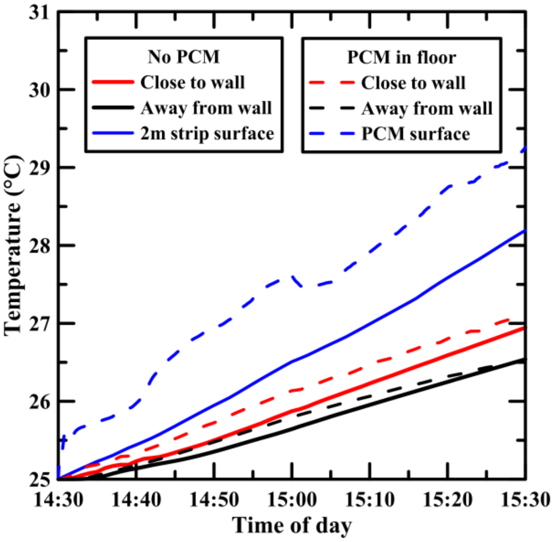


Figure 8: Comparison between the temperature history in the room without the PCM and with the PCM in the floor.

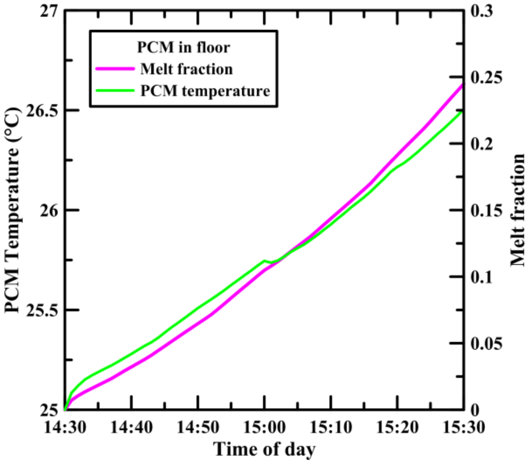


Figure 9: The melt fraction and temperature of the PCM in the floor.

However, careful examination of Fig. 8 reveals that the temperatures in the two air domains with PCM in the floor appear to be increasing at a smaller rate then the temperature in the no PCM case. This suggest, through extrapolation, that with longer simulated times, it is probable that the PCM will in fact reduce the temperature in the room through latent heat storage.

4.3 PCM in the ceiling

The final simulation evaluated the effectiveness of incorporating PCM in the ceiling at reducing the temperature in the room. Figure compares the temperature history in the room without the PCM and with the PCM in the ceiling.

The PCM in the ceiling did not modify the temperature in the room significantly. However, similar to the PCM in the floor configuration, the temperature starts to decrease near the end of the simulation. At 15:30, the temperature in both domains had dropped by about 0.1 °C compared to the no PCM case. Even though the PCM did not melt as significantly (see Figure 10), the room temperature decreased because the PCM absorbed heat from the room, both from radiation reflected from the floor and walls in which case the high-absorptivity of the PCM enclosure played an important role and from high temperature air flow carrying heat to the ceiling by natural convection.

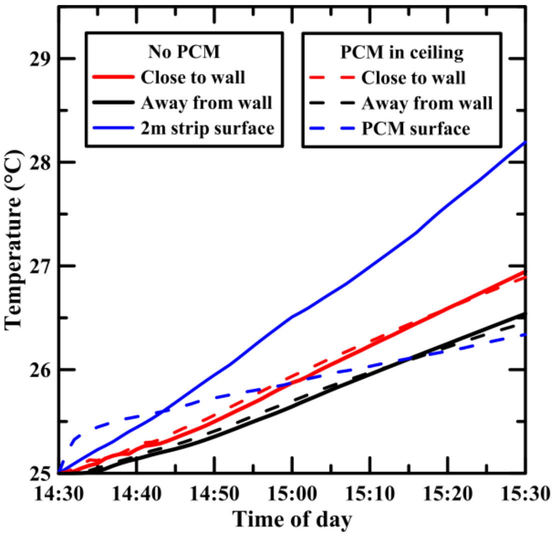


Figure 10: Comparison between the temperature history in the room without the PCM and with the PCM in the ceiling.

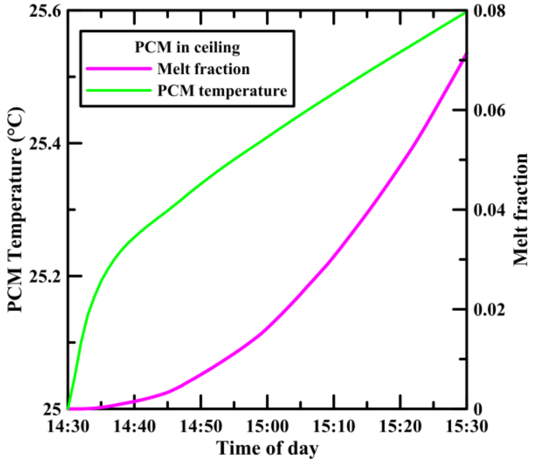


Figure 10: The melt fraction and temperature of the PCM in the ceiling.

Judging by what is shown in Figure 12 and Figure 12, for both PCM configurations, the PCM melts almost entirely at the surface exposed to the room (the top image) and very little on the opposite surface (bottom image). A PCM with a higher thermal conductivity than Butyl Stearate would be beneficial to achieve more complete melting; however, it is important to remember that only one hour is simulated. Longer simulation times are needed to determine the overall melting behavior of the PCM.

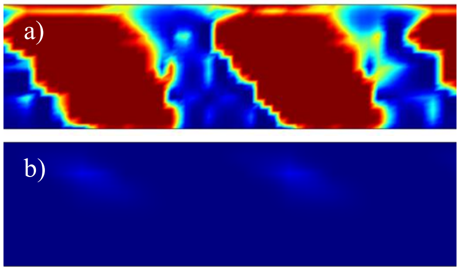
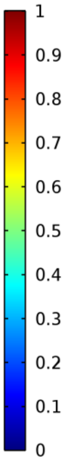


Figure 11: Surface melt fractions for the PCM in the floor: a) exposed surface, b) opposite surface.



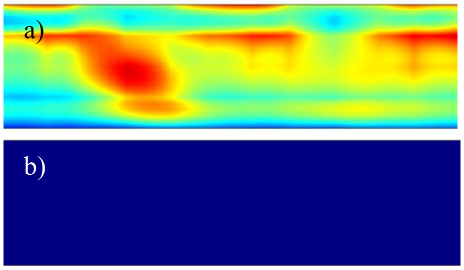


Figure 12: Surface melt fractions for the PCM in the ceiling a) exposed surface, b) opposite surface.

5. Conclusions

From these preliminary studies it was determined that there is promise for reducing the temperature in the office room through the use of a mass of butyl stearate and improving the thermal comfort for occupants. Near the end of the simulations, the temperature in the room with both PCM cases begins to reduce its rate of increase compare to the no PCM case. However, a more careful selection of PCM enclosure surface properties is required.

For the PCM incorporated in the floor, approximately 25% of the PCM had melted after one hour of simulation. Nonetheless, the temperature in the room increased slightly compared to the room without the PCM due to the high absorptivity surface of the PCM enclosure. For the PCM incorporated in the ceiling, the temperature after an hour was approximately 0.1 °C lower than the temperature for the same air volume in the no PCM case; approximately 7% of the PCM had melted.

Further study is required to find optimal PCM enclosure surface properties and a mass of butyl stearate that will achieve complete melting over a period of a day. This will involve more simulations with different surface property and, more importantly, longer simulation time that model the PCM melting behavior throughout the rest of the day. Additionally, a mesh convergence study should be carried out to determine if a finer mesh density will significantly alter the results.

6. References

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