Numerical Simulation of a Building Envelope with High Performance Materials

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Abstract: Simulation tools for building physics problems play an important role in design and understanding the behavior of energy efficient buildings. There are different tools available for simulation of these problems, but each simulation tool has its own advantages and limitations. In this paper, a heat transfer problem in an exterior building wall with high performance materials has been simulated in both COMSOL 4.0 and WUFI 5.0. The results show the advantage of using high performance materials in new construction systems. On the other hand, comparable results between utilized simulation tools have been found indicating that COMSOL has a high potential with special advantages for simulation of different building physics problems.

Keywords: Concrete, Aerogel, Thermal Conductivity, Phase Change, Solar Energy.

1. Introduction

Numerical modeling is indispensible in studying the efficiency of new concepts in energy design of buildings [1]. Thus having an appropriate simulation tool that will be able to consider different phenomena in real and laboratory cases is necessary for building physics engineers.

In order to achieve buildings with high energy efficiency, the construction industry needs high performance materials and new construction systems. Materials such as aerogel and PCM (Phase Change Materials) are promising materials for this purpose [2-5]. PCM absorbs heat as the temperature increases and releases heat by decrease in the temperature. mPCM (micro-encapsulated PCM) can be used inside the building materials such as concrete to save energy and increase thermal comfort [6-8]. On the other hand silica aerogel has a low thermal conductivity with high solar energy transmittance [9]. Hence, using a layer of silica aerogel in the exterior part of the façade, in a glazing system or on the external wall, can help the storage of solar energy in the building materials during the day and avoid heat loss during the night. More over, using a layer of concrete containing mPCM behind the aerogel in the exterior wall can be a good idea for saving energy in the building envelope. mPCM can absorb the passive solar energy which passes through the aerogel layer during the day time and release it at night with a low heat loss due to existence of aerogel insulation. In this paper performance of this system is studied using the programs COMSOL 4.0 and WUFI 5.0, and the results are discussed.

2. Materials and Geometry

A three layer building envelope is considered for numerical simulation. Two layers of low thermal conductive light weight concrete with and without mPCM and a thin layer of silica aerogel form the envelope. In the reference model none of the concrete layers contain mPCM but in the main model the layer in the middle is mixed with mPCM. In fact, it is possible to consider a more energy efficient envelope system by for example using electrochromic glass in the exterior part of the wall to avoid solar energy gain during the warm season, or by applying another layer of PCM at the interior part of the wall to decrease temperature fluctuation during high external heating loads and save more energy in cooling systems as well. In order to study the performance of previously described system, the envelope in Figure 1 is numerically simulated.
Average values for aerogel material properties are considered here according to the producer [10]. Concrete material properties are taken from the WUFI database. Dieckmann et al [11] have reported the graph in Figure 2 for enthalpy of a concrete containing mPCM, which has been explained in the WUFI tutorial as an example. Based on this data, two values are roughly determined for specific heat capacity of the concrete layer containing mPCM. Since the choice of PCM depends on factors such as weather, building structure, thermophysical properties and etc [1], different phase change temperatures with the same values of specific heat capacity will be considered for simulation in order to compare the effect of phase change temperature in the system. Thermophysical properties of the materials are given in Table 1.

### Table 1: Thermophysical properties of the materials.

<table>
<thead>
<tr>
<th></th>
<th>Density [Kg/m³]</th>
<th>Thermal Conductivity [W/mK]</th>
<th>Specific HeatCapacity [J/KgK]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concrete</td>
<td>400</td>
<td>0.1</td>
<td>850</td>
</tr>
<tr>
<td>mPCM Concrete</td>
<td>400</td>
<td>0.1</td>
<td>T=PCT*: 1900</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>T=PCT: 12700</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>T&gt;PCT: 1900</td>
</tr>
<tr>
<td>Aerogel</td>
<td>30</td>
<td>0.01</td>
<td>850</td>
</tr>
</tbody>
</table>

*PCT: Range of Phase Change Temperature

3. Numerical Simulation

3.1 Initial and Boundary Conditions

A heat transfer problem is solved in both COMSOL 4.0 and WUFI 5.0. The indoor temperature and initial temperature of the wall is 22 °C. The exterior boundary condition is defined as step change between a high and a low temperature (each in a period of 12 hours) to result in a sinus shape heat flux curves with less dependency on the more realistic outdoor temperature changes which usually have sinus variations as well. The high temperature is equal to indoor temperature to have an initial heat flux of zero, and the low temperature is considered as minus 10 °C to clearly see the effect of heat loss and phase changes of the PCM. Moreover, the effect of considering solar radiation is discussed in the results section. The boundary conditions are given in Table 2.

### Table 2: Boundary conditions of the heat transfer problem.

<table>
<thead>
<tr>
<th></th>
<th>Surface Heat Resistance [m²K/W]</th>
<th>Air Temperature [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indoor</td>
<td>0.125</td>
<td>22</td>
</tr>
<tr>
<td>Outdoor</td>
<td>0.0588</td>
<td>0-12 hr: -10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>12-24 hr: 22</td>
</tr>
</tbody>
</table>

3.2 Phase Change Temperature

Since the phase change temperature of the PCM affects the efficiency of the system, three different phase change temperatures of 5 °C, 15 °C and 20 °C are considered for mPCM to study this effect. The phase change range for definition of specific heat capacity was defined as 1°C higher and 1°C less than the phase change temperature.
4. Results and Discussion

Results of the numerical simulation of the reference envelope are given in Figure 3. Comparable results are obtained from COMSOL and WUFI. Considering that the outdoor temperature boundary condition is defined by the text climate file in WUFI, but an interpolation function in COMSOL, there will be some minor differences in the results. On the other hand, since COMSOL is a general multiphysics simulation tool, special care must be taken in definition of parameters such as meshing parameters. Since WUFI is a specialized building physics simulation tool (developed for studies of heat and moisture transport in building envelope systems), the WUFI results will be used for discussing the performance of the wall system. The advantages of using COMSOL for simulation of building physics problems will be discussed at the end of this part.

Figure 3. Heat flux at the interior surface of reference wall.

Figure 4 shows the differences between the heat flux at the interior surface of the reference wall and the wall containing mPCM with a phase change temperature of 5 ºC (simulated with WUFI). Although the total heat flux for both cases is similar, the difference between the maximum and minimum points of the heat fluxes is noticeable. This means that using PCM has resulted in less heat loss during cold periods and higher loss during the warm periods. Consequently, the energy consumption is shifted from the peak periods to off-peak periods by using PCM; this can result in [12]: i) Possibility of purchasing energy at lower cost in off-peak periods. ii) Reduction in cost of energy production, smaller size of equipments and more efficient operation due to time-shifting energy consumption.

Since diminution in fluctuation of the heat flux depends on interaction between phase change temperature of the PCM and changes in temperature profile of the envelope, in the next step the phase change temperature of the mPCM was considered 15ºC according to the temperature profile in the previous simulation. Figure 5 shows that this change has resulted into a more efficient system due to two phenomena: i) reduction in the peak value of heat flux that is about 30% in this case and ii) delay in the initiation of maximum heat loss that is apparent in the first 5 days and it takes time more than 10 days in this case. Therefore, using a PCM layer inside the wall can be beneficial even without considering energy gain by solar radiation.

Figure 4. Heat fluxes at the interior surfaces for the reference wall and wall containing mPCM with a phase change temperature of 5 ºC.

Figure 5. Heat fluxes at the interior surfaces for the reference wall and wall containing mPCM with a phase change temperature of 15 ºC.
regulating the heat flux fluctuation in the interior surface. This is due to the heat flux that solar energy generates from the exterior surface opposite to the heat loss direction.

Increasing the phase change temperature does not help the effectiveness of the current system, because the temperature profile in the wall will not match the phase change temperature range of the mPCM. This is shown in Figure 6. On the contrary, fluctuation in the heat flux in all the cases is less than the reference envelope and the main reason is higher specific heat capacity of the wall containing mPCM at any temperature.

Figure 6. Heat fluxes at the interior surfaces of simulated walls.

Although it is clear that this system can result in reduction in energy consumption, determination of the effectiveness of the system requires using the real climate data including the data about moisture condition, solar radiation, rain and wind data, orientation of the construction element and etc. Furthermore, by applying the real climate data, it would be possible to optimize the system by varying different parameters such as thickness or thermal conductivity of each layer, that can for instance, speed melting or slow down solidification of PCM. Therefore, a real climate database is necessary to convert COMSOL to a suitable building physics simulation tool.

On the other hand, one of the advantages of COMSOL 4.0 to WUFI 5.0 is the possibility of defining different types of functions and applying them in simulation. For example, since process of phase change in the PCM normally consists of two different heating and cooling curves for \( C_p \) of the material, it is essential to define \( C_p \) properly to get more comparable results with experimental studies [1]. On the other hand in case of having convective heat transfer in boundary conditions, for example in hot box test of a wall [13], COMSOL multiphysics can be used for simulation. And finally simulating 3D problems as well as multiphysics problems are the main advantages of using COMSOL multiphysics for building physics problems.

5. Conclusions

Applying high performance materials in new construction systems can result in: i) saving energy, ii) less waste of the materials, iii) simplicity in execution of constructions, iv) more effective space to be sold to the customers and v) even less construction costs, as a consequence of parts ii and iii.

Utilizing a PCM layer behind exterior aerogel heat insulation can be beneficial due to both gaining solar energy and increasing heat capacity of the wall. However, the effectiveness depends on the construction details and weather conditions. Thus it is necessary to do numerical simulation in order to optimize the system.

COMSOL multiphysics has a high potential with special capabilities to be used as a building physics simulation tool. However, more practical facilities such as a database for real climate data are necessary to achieve this goal.

6. References

4. K.I. Jensen et al, Development of windows based on highly insulating aerogel glazings,


