Heat and Moisture Modeling Benchmarks using COMSOL

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Abstract: Benchmarks are important tools to verify computational models. In the research area of building physics, the so-called HAMSTAD (Heat, Air and Moisture STAnDardization) project is a very well known benchmark for the testing of simulation tools. In this paper we evaluate the use of COMSOL regarding this benchmark.

Keywords: Heat, air, moisture, benchmark construction

1. Introduction

Multiphysics tools for modeling heat and moisture transport in constructions, might encounter numerical problems. Especially the multi-layered mixed moisture transport (i.e. vapour and water) part can be tricky to solve. A guideline on how to implement up to 3D heat air and moisture (HAM) transport models using COMSOL (2008) is already provided (van Schijndel 2006). Another recent development concerning COMSOL is presented in Tariku et al. (2008). This work shows a successful implementation of 1D HAM transport using relative humidity as moisture potential. This paper presents two major extensions to work of van Schijndel (2006) and Tariku et al. (2008), described in the following sections: First, the implementation of LPc as moisture potential for including both vapour and liquid transport and second, the implementation of material and boundary functions for calculating the PDE coefficients from the material properties. The implementation of the two new extensions is verified using the HAMStad benchmark 1 (Hagentoft et al 2002).

2. Model

The heat and moisture transport can be described by the following PDEs using LPc as potential for moisture transfer.

\[
C_T \frac{\partial T}{\partial t} = \nabla \cdot (K_{11} \nabla T + K_{12} \nabla \text{LPc})
\]

\[
C_{\text{LPc}} \frac{\partial \text{LPc}}{\partial t} = \nabla \cdot (K_{21} \nabla T + K_{22} \nabla \text{LPc})
\]

With:

\[
\text{LPc} = 10 \log(P_c)
\]

\[
C_T = p \cdot c
\]

\[
K_{11} = \lambda
\]

\[
K_{12} = -l_v \cdot \delta_p \cdot \phi \cdot \frac{\partial \text{LPc}}{\partial \text{LPc}} \cdot P_{\text{sat}} \cdot \frac{M_w}{\rho_a RT}
\]

\[
C_{\text{LPc}} = \frac{\partial w}{\partial \text{LPc}} \cdot \frac{\partial \text{LPc}}{\partial \text{LPc}}
\]

\[
K_{22} = -K \cdot \frac{\partial \text{LPc}}{\partial \text{LPc}} - \delta_p \cdot \phi \cdot \frac{\partial \text{LPc}}{\partial \text{LPc}} \cdot P_{\text{sat}} \cdot \frac{M_w}{\rho_a RT}
\]

\[
K_{21} = \delta_p \cdot \phi \cdot \frac{\partial P_{\text{sat}}}{\partial T}
\]

Where \( t \) is time [s]; \( T \) is temperature [°C]; \( P_c \) is capillary pressure [Pa]; \( p \) is material density [kg/m³]; \( c \) is specific heat capacity [J/kgK]; \( \lambda \) is thermal conductivity [W/mK]; \( l_v \) is specific latent heat of evaporation [J/kg]; \( \delta_p \) vapour permeability [s]; \( \phi \) is relative humidity [-]; \( P_{\text{sat}} \) is saturation pressure [Pa]; \( M_w = 0.018 \) [kg/mol]; \( R = 8.314 \) [J/molK]; \( \rho_a \) is air density [kg/m³]; \( w \) is moisture content [kg/m³]; \( K \) is liquid water permeability [s].

3. Implementation of advanced material and boundary functions.

The second extension is the implementation of advanced material and boundary functions using MatLab. These functions are used to convert measurable material properties such as \( K \), \( \phi \), \( \delta_p \) and \( \lambda \) which are dependent on the moisture content into PDE coefficients which are dependent on the LPc and \( T \). This is schematically shown in figure 1.
Figure 1. The conversion from measurable material properties into PDE coefficients.

The results for two materials (based on HAMstad benchmark 1) are presented in figure 2.

Figure 2 PDE coefficients $C_{ij}$ as functions of $LPC$ and $T$ calculated from the provided HAMSTAD benchmark no.1 material properties for the load bearing (a) and insulation (b) material.

For each material and at each point the vapour pressure can be calculated using similar corresponding functions.

4. HAMSTad benchmark 1

This Section summarizes the HAMSTAD benchmark no.1: ‘Insulated roof’. The roof structure is analyzed in 1D regarding dynamic heat and moisture transport. The thermal insulation is facing the interior and there is a moisture barrier facing the exterior. The structure is perfectly airtight. Figure 3 shows the structure:

Figure 3 A schematic of the structure of the benchmark

The properties of the layers are provided in the benchmark including initial conditions.

The boundary conditions are at the (i)nternal (connected with material A):

$$q = h_i \cdot (T_i - T) + l_i \cdot \beta \cdot (p_i - p)$$

$$g = \beta \cdot (p_i - p)$$ (3)

And at the (e)xternal (connected with material B)

$$q = h_e \cdot (T_e - T)$$

$$g = 0$$ (4)

Where $q$ is heat flux [W/m$^2$]; $h$ is convective heat transfer coefficient [W/m$^2$K]; $\beta$ is vapour transfer coefficient [kg/Pam’s]; $p$ is vapour pressure [Pa]; $g$ is moisture flux [kg/m$^2$s]. The boundary conditions $T_e$, $T_i$, $p_i$ and $p_e$ are hourly based values provided by benchmark.
5. The COMSOL model

The COMSOL model presented in this paper is public domain and is downloadable from the HAMLab (2008) website. A short summary is presented below. The sub domains are shown in figure 4.

The governing PDE equations (1) are implemented using the coefficient form. Table 1 shows PDE coefficients for both domains.

Table 1. PDE coefficients

<table>
<thead>
<tr>
<th>Sub domain 1</th>
<th>Sub domain 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>{K_{11\text{afun}(LPC,T)},K_{12\text{afun}(LPC,T)}; K_{21\text{afun}(LPC,T)},K_{22\text{afun}(LPC,T)}}</td>
<td>{K_{11\text{bfun}(LPC,T)},K_{12\text{bfun}(LPC,T)}; K_{21\text{bfun}(LPC,T)},K_{22\text{bfun}(LPC,T)}}</td>
</tr>
<tr>
<td>{C_{T\text{afun}(LPC,T)},0;0,C_{L\text{afun}(LPC,T)}}</td>
<td>{C_{T\text{bfun}(LPC,T)},0;0,C_{L\text{bfun}(LPC,T)}}</td>
</tr>
</tbody>
</table>

As explained before the functions of table 1 are already presented in figure 2. The boundary numbers are:

- Boundary 2-3, 5-6: \{0;0\}
- Boundary 1: \{25*(tetfun(t)-T);0\}
- Boundary 7: \{7*(titfun(t)-T);2e-8*(pvitfun(t)-Pvbfun(LPC,T))\}

As explained before, the boundary conditions \(T_e\), \(T_i\), \(p_i\) are hourly based values provided by benchmark. The vapour pressure \(p_v\) at the inside surface can be expressed as a function of \(LPC\) and \(T\) similar to the coefficients of figure 2.

In this case, a coarse grid (presented in figure 6) seems to be quite sufficient.
The model simulates over a period of time (1 year) the LPc and temperature (T) distributions. An exemplary result of the temperature distribution is shown in figure 7 (LPc distributions are similar).

**Figure 7.** A typical temperature distribution.

### 6. Comparing the results with the benchmark

**Heat**

We start with comparing the heat flow from the interior to the wall, during the first 500 hours. The results are shown in figure 8.

**Figure 8.** The heat flow from the interior to the wall of the benchmark (top) and the COMSOL model (bottom)

Figure 8 (top) shows the bandwidth of the benchmark result. The result of the COMSOL simulation (bottom) is quite satisfactory.

**Moisture**

The moisture content distributions can be calculated from the simulated LPc distributions using the material properties. We proceed with comparing the average moisture content in the insulation during the first year. The results are presented in figure 9.

**Figure 9.** The average moisture content in the insulation of the benchmark (top) and the COMSOL model (bottom)

Again, figure 9 (top) shows the bandwidth of the benchmark result. The result of the COMSOL simulation (bottom) is quite satisfactory beside some spikes related with numerical instability. At this point it is emphasized that all results are obtained using default settings of the grid and solvers. We expect even better results if more attention is paid to these settings. This is left over for future research.

Confronting the results with the benchmark, it is overall concluded that the results are within the provided bandwidths. Other benchmarks will be evaluated in near future. Moreover, the ‘benchmark 1 model using COMSOL (2008) and companying report are published at the HAMLab (2008) research and education website.
Conclusions

It is concluded that the following two main guidelines provide a stable numerical solutions for several benchmarks on heat and moisture transfer and for Multiphysics FEM packages COMSOL:

(1) Use the LPc (the natural logarithmic of the suction pressure Pc) as moisture potential.

(2) Use 2-D interpolation (table lookup) based on LPc and temperature for all PDE coefficients.

The COMSOL model presented in this paper is public domain and is downloadable from the HAMLab (2008) website.

References

HAMLab (2008), http://sts.bwk.tue.nl/hamlab/