Guidelines for heat and moisture modelling in constructions using multiphysics FEM software

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1. Introduction

Multiphysics treats simulations that involve multiple physical models or multiple simultaneous physical phenomena mostly using the Finite Element Method (FEM). The commercially available software packages like ANSYS Multiphysics, LS-DYNA, COMSOL Multiphysics, and FlexPDE are very promising for application in the area of building physics. However, using these Multiphysics tools for modeling heat and moisture transport in constructions, one might encounter numerical problems. Especially the multi-layered mixed moisture transport (i.e. vapour and water) part can be tricky to solve. Amongst other possibilities, the multiphysics modeling approach of van Schijndel (2007) is selected. 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. Extension 1: Implementation of LPc potential

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

\[
\begin{align*}
C_T \frac{dT}{dt} &= \nabla \cdot (K_{11} \nabla T + K_{12} \nabla \text{LPc}) \\
C_{\text{LPc}} \frac{d\text{LPc}}{dt} &= \nabla \cdot (K_{21} \nabla T + K_{22} \nabla \text{LPc})
\end{align*}
\]

With:

\[
\text{LPc} = \log(Pc)
\]
\[
C_T = \rho \cdot c
\]
\[
K_{11} = \lambda
\]
\[
K_{12} = -I_{12} \cdot \delta_p \cdot \phi \cdot \frac{d\text{PC}}{d\text{LPc}} \cdot Psat \cdot \frac{M_w}{\rho_p RT},
\]
\[
K_{21} = \delta_p \cdot \phi \cdot \frac{dPsat}{dT},
\]

\[
K_{22} = -K \cdot \frac{dPC}{d\text{LPc}} - \delta_p \cdot \phi \cdot \frac{dPC}{d\text{LPc}} \cdot Psat \cdot \frac{M_w}{\rho_p RT},
\]

\[
C_{\text{LPc}} = \frac{\partial \omega}{\partial \text{LPc}} \cdot \frac{d\text{PC}}{d\text{LPc}}
\]
Where \( t \) is time [s]; \( T \) is temperature [°C]; \( P_c \) is capillary pressure [Pa]; \( \rho \) is material density [kg/m\(^3\)]; \( c \) is specific heat capacity [J/kgK]; \( \lambda \) is thermal conductivity [W/mK]; \( \delta_v \) is specific latent heat of evaporation [J/kg]; \( \delta_p \) vapour permeability [s]; \( \varphi \) is relative humidity [\( - \)]; \( P_{sat} \) is saturation pressure [Pa]; \( M_w = 0.018 \) [kg/mol]; \( R = 8.314 \) [J/molK]; \( \rho_a \) is air density [kg/m\(^3\)]; \( w \) is moisture content [kg/m\(^3\)]; \( K \) is liquid water permeability [s].

3. Extension 2: 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 \( K \), \( \varphi \), \( \delta_p \) 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.

![Fig 1. The conversion from measurable material properties into PDE coefficients](image)

The results for material B (based on HAMstad benchmark 1) is presented in figure 2.

![Fig. 2. PDE coefficients \( C_T, C_{LPc}, K_{ij} \) as functions of LPc and \( T \) calculated from the provided HAMSTAD benchmark no.1 material properties for the insulation b material (please note that this figure relies on colour, see digital version)](image)
For each material and at each point the vapour pressure can be calculated using similar corresponding functions.

4. Verification using HAMSTad benchmark 1

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 reference for the testing of simulation tools. This Section summarizes the results for 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 a there is moisture barrier facing the exterior. The structure is perfectly airtight. Figure 3 shows the structure:

\[ q = h_i \cdot (T_i - T) + l_{i0} \cdot \beta \cdot (p_i - p) \]
\[ g = \beta \cdot (p_i - p) \]
\[ q = h_e \cdot (T_e - T) \]
\[ g = 0 \]  

Where \( q \) is heat flux \([\text{W/m}^2]\); \( h \) is convective heat transfer coefficient \([\text{W/m}^2\text{K}]\); \( \beta \) is vapour transfer coefficient \([\text{kg/Pam}^2\text{s}]\); \( p \) is vapour pressure \([\text{Pa}]\); \( g \) is moisture flux \([\text{kg/m}^2\text{s}]\); The boundary conditions are hourly based values provided by benchmark. The results are shown in figure 4.

**Fig. 3. A schematic of the structure of the benchmark**

**Fig. 4. Left. The simulated total mass in the load bearing material (top) and insulation material (bottom) during the first year. Right. The simulated heat flows interior (bottom) and exterior (top) to the wall during the first year**
Confronting these results with the benchmark, it is 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.

5. 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 and (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.

6. Ongoing research

Application of system identification. This technique seems promising in reducing the large simulation times of (linear approximated) models with large degrees of freedom (DOF) such as 3D HAM models of constructions.

Evaluation of full 3D indoor climate and constructions HAM models. Preliminary results show that it is possible and relatively easy to model the interaction between constructions and air in Comsol. Furthermore, it seems possible to get reliable simulation results in cases for convective airflow and forced airflow. However, due to the limited computer resources used in this research, the simulated volumes were small: less than 0.1 m3 and 2 m3 for respectively the convective and forced airflow case.

Inverse modeling. An inverse problem is the task that often occurs in many branches of science and mathematics where the values of some model parameter(s) must be obtained from the observed data (Wikipedia 2008). The main goal of this work is to investigate whether material properties can be obtained using an inverse problem technique. A second goal is to evaluate this technique for heat and moisture engineering.

Application scale of DNS techniques. For full size buildings, turbulence models are necessary to solve CFD equations. One of the problems is that there are a lot of different turbulence models and they all give more or less different results. Without turbulence modeling (i.e. Direct Numerical Solving (DNS) techniques), accurate results on turbulent flow can only be obtained using very small domains compared to buildings. For DNS the following statement seems to be valid: The smaller the turbulence the bigger the domain that can be handled. Another problem is the grid dependency of the solution. This gives rise to the following main research question: “At what scale is the DNS technique still usable in relation with indoor airflow and HAM Constructions?”

REFERENCES

[3] Gothenburg, Department of Building Physics, Chalmers University of Technology.