CFD vs. lumped models applied to HAM: a comparison between HAM-Tools and Comsol

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Abstract

CFD models have several advantages in comparison with zonal-models, due to the more accurate calculation of the airflow distribution within the built environment. Nevertheless, in currently available CFD software the simulation of mass transfer cannot be directly extended from the fluid region to the solid region. In the wholebuilding moisture transport studies, the mass coupling between the indoor environment and the wall system is usually achieved by third party programming. The Annex 41 research project of the International Energy Agency (IEA) was carried out to explore the complex physics governing the whole building heat, air and moisture (HAM) transfer, by developing several models to couple 3-D CFD simulations with hygrothermal models of walls.

The objective of this study is to develop a coupled CFD model able to simulate the HAM transport in a single environment (i.e. a simple test room), influenced by the room factors. A numerical method was utilized to model the indoor environment and the moisture transport process in the simple room and inside the wall system as influenced by the moisture loads and ventilation conditions.

The comparison between the CFD and a lumped model allows us to demonstrate how a simplified model can be reliable in predicting the RH variation inside a room, also taking into account the indoor material buffering effect.

1. Introduction

HAM-Tools is a building simulation software implemented on the Simulink-Matlab platform by the Chalmers University of Technology (Gotheborg, Sweden) and the Technical University of Denmark (Lygby, Denmark) within the Annex 41 project. The main objective of this tool is to run simulations of transfer processes related to building physics, i.e. heat and mass transport in buildings and building components in operating conditions. Nevertheless, results from literature demonstrate how simulations made with the HAM-Tools lumped model over-estimate about twice the moisture dampening effect than what was actually measured experimentally (Ramos et al., 2012). The authors then focused on the air-flow pattern, comparing experimental measurement results to theoretical ones. An appreciable difference between the measured hygroscopic inertia and the calculated one was found due to the air velocity field that caused the development of several dead zones inside the test chamber. This meant that the perfect mixing of the room air, a simplification commonly assumed in HAM simulations, had a clear impact on the results of this kind of problem. If perfect mixing is assumed, all the hygroscopic surfaces would be fully active; but since this is not true, the flux chamber simulations overestimated the moisture buffering effect.

The CFD model has the advantage to overcome the limitations of the zonal-model applied to HAM-Tools, but it encounters another limitation due to the calculation in different environments. The moisture flux on the wall surface calculated by CFD is used as the input for the wall model to determine the distribution of the moisture inside the wall material at each time step (i.e. using MatLab), and the mass fraction on the wall surface is calculated and sent back to the CFD model as the boundary condition for the next time step.

In the Annex 41 research project (2004-2008) of the International Energy Agency (IEA), several models were developed to couple CFD simulations with hygrothermal models of walls. For instance, Neale (2007) solved the heat and moisture transport in air and porous materials by developing a simplified hygrothermal model in MATLAB coupled to FLUENT software; Steeman et al. (2009) used the effective penetration depth (EPD) approach to couple CFD and moisture transport inside the wall which allows the simplified quantification, while it has been argued that the reliance on the moisture penetration depth concept necessitates comprehensive material properties (Janssen et al., 2007). Amissah (2005) coupled a 1D HAM model to a low-Reynolds number κ-ε turbulence model and Erriguible et al. (2006) coupled indirectly a 2-D CFD model with a 2-D hygrothermal material model. In these models, similar limitations can be found, and the main reason is that all these models are not simulated in one single simulation environment.

This paper presents the fitting between the time variation of the vapour concentration according to the CFD model and to the lumped model. The CFD output – in this case the relative humidity variation φ – is an average value over the room air volume, depending on the air velocity field.

The aim of the study is the coupling, within the COMSOL simulation environment, of the CFD and of the moisture transfer models and the comparison of the results with those obtained by the HAM-Tools lumped model.

2. Validation of the diffusion equations in COMSOL

Due to the simplified modelling of the air volume, HAM-Tools considers that each part of the wall absorbs the same amount of moisture, overestimating the material buffer. In real conditions, the influence of the ventilation system and of the air velocity pattern causes the presence of dead zones, where the moisture buffer decreased due to a higher surface vapour resistance. The calibration of the HAM-Tools simplified air ventilation lumped model will be carried out using the computational fluid dynamics from COMSOL.

This section is based on the validation, through HAM-Tools, of the equations of coupled heat and moisture transfer in building components implemented in Nusser and Teibinger (2012) using the physical approach modelled in WUFI, a wellknown and worldwide used commercial software for calculating the HAM-transfer developed at the Fraunhofer Institute for Building Physics. Regarding the transport process, the coupled heat and moisture transfer is calculated from WUFI according to the following equations:

$$\frac{dH}{dT}\frac{\partial T}{\partial t} = \nabla(\lambda\nabla T) + h_{v}\nabla[\delta_{p}\nabla(\varphi \cdot p_{v,s})] \quad (1)$$
$$\frac{dw}{d\varphi}\frac{\partial\varphi}{\partial t} = \nabla(D_{\varphi}\nabla\varphi) + \delta_{p}\nabla(\varphi \cdot p_{v,s}) \quad (2)$$

where $dw/d\varphi$, or ξ , [kg/m³] is the moisture storage capacity, D_{φ} [kg/(m s)] the liquid conduction coefficient, h_v [J/kg] the latent heat of evaporation and dH/dT [J/(m³ K)] is the volumetric heat capacity, calculated as:

$$\frac{dH}{dT} = \left(c_p + \frac{1}{\rho_0}c_{p,w} \cdot w\right)\rho_0 \tag{3}$$

where c_p and $c_{p,w}$ [J/(kg K)] are the specific heat capacities of the dry material and of water respectively. In this approach, the temperature and the relative humidity are the driving potentials. Both potentials affect both transport processes, so

they have to be deviated with respect to space in both equations.

$$\delta_{p}\nabla(\varphi \cdot p_{\nu,s}) = \delta_{p}\varphi \frac{\partial p_{\nu,s}}{\partial T}\nabla T + \delta_{p}p_{\nu,s}\nabla\varphi \quad (4)$$

With Equation (4) the heat and moisture transport equation can be described in the following way:

$$\frac{dH}{dT}\frac{\partial T}{\partial t} = \nabla \left[\left(\lambda + h_{v}\delta_{p}\varphi \cdot \frac{dp_{v,s}}{dT} \right) \nabla T + h_{v}\delta_{p}p_{v,s}\nabla\varphi \right]$$
(5)
$$\frac{dw}{d\varphi}\frac{\partial\varphi}{\partial t} = \nabla \left[\left(\delta_{p}\varphi \cdot \frac{dp_{v,s}}{dT} \right) \nabla T + \left(D_{\varphi} + \delta_{p}p_{v,s} \right) \nabla\varphi \right]$$
(6)

and can be compared to Fick's second law equation model used in HAM-Tools, here described together with the heat transfer equation in order to have a direct comparison between the two models:

$$\rho_{0}c_{p}\frac{\partial T}{\partial t} = -\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x} + \dot{g}_{a}c_{p,a}T + \dot{g}_{v}h_{v}\right) \quad (7)$$
$$\frac{\partial w}{\partial t} = -\frac{\partial}{\partial x}\left(\lambda_{l}\frac{\partial p_{c}}{\partial x} - \delta_{p}\frac{\partial p_{v}}{\partial x} + \dot{g}_{a}u\right) \quad (8)$$

Rearranging the transport equations (5) and (6) into matrix notation in order to input them in COMSOL, we finally obtain:

$$\begin{vmatrix} \lambda + h_{v}\delta_{p}\varphi \cdot \frac{dp_{v,s}}{dT} & h_{v}\delta_{p}p_{v,s} \\ \delta_{p}\varphi \cdot \frac{dp_{v,s}}{dT} & D_{\varphi} + \delta_{p}p_{v,s} \end{vmatrix} \begin{bmatrix} \nabla^{2}T \\ \nabla^{2}\varphi \end{bmatrix} = \\ = \begin{bmatrix} \left(c_{p} + \frac{1}{\rho_{0}}c_{p,w} \cdot w\right)\rho_{0} & 0 \\ 0 & \xi \end{bmatrix} \begin{bmatrix} \frac{\partial T}{\partial t} \\ \frac{\partial \varphi}{\partial t} \end{bmatrix}$$
(9)

After the implementation of the HAM transport equations in COMSOL, the validation with the HAM-Tool model was carried out. The study will match the two models by gradually increasing the level of complexity. As a first approach to the matching between the results, a simple 3-layers wall case study has been chosen: 10 cm foam insulation, 10 cm aerated concrete, 3 cm gypsum

plaster; apart from the measured plaster's properties, the other material data were taken from Annex 24 (Kumaran, 1996). Several simulations were carried out in order to evaluate the influence of the layer discretization on the hygrothermal performance results in HAM-Tools and COMSOL. As the increase of the mesh detail leads to a longer simulation time, this process aimed at defining the best detail level for an acceptable simulation time, especially with regard to COMSOL. After the detail of the wall discretization was set for the three layers at 4, 10 and 6 nodes respectively (fine mesh settings), a 1-D HAM transfer simulation was carried out focusing on the temperature and on the relative humidity trends within the wall. Both the variables were monitored at nodes no. 3, 9 and 17 (central nodes of the layers) by using the two simulation tools. In this phase, any CFD was used to solve the indoor air in COMSOL, since only the indoor boundary conditions were set because the target was the moisture diffusion process within the building component first.

The simulations were carried out using the climate data of Turin as outdoor boundary conditions, for the first two weeks of January. The indoor temperature and relative humidity were set respectively at 20 °C and 50% and maintained constant throughout the simulation period; the same values were set for the materials' starting conditions, then left floating. According to Rode et al. (2005) the moisture transfer coefficients for outdoor and indoor respectively are $\beta_{ext} = 2 \cdot 10^{-7} \text{ kg/(m^2 s Pa)}$ and $\beta_{int} = 2 \cdot 10^{-8} \text{kg/(m^2 s Pa)}$.



Figure 1 – Temperature trend for nodes n. 3-9-17 in the first 2 weeks of January (Turin weather data). The dotted and the continuous curves are related respectively to the HAM-Tools and to the COMSOL simulations.



Figure 2 – Relative humidity trend for nodes n. 3-9-17 in the first 2 weeks of January (Turin weather data). The dotted and the continuous curves are related respectively to the HAM-Tools and to the COMSOL simulations.

No solar radiation nor ventilation was taken into account for the airtight structure. The simulation results show the perfect matching between the two models both for the temperature and for the RH trends (Fig. 1 and 2), validating the implemented equations from Nusser and Teibinger (2012).

3. Influence of the ventilation configuration on the room hygroscopic performance

At the room level, the two air models were compared after ensuring that the HAM-transfer model for building components was implemented in the same way for both the simulation tools.

As the solution time for CFD calculation is still a big issue, a 2-D model was set in a specific way to solve both the air balance and the moisture transfer in porous media on the same platform. Several attempts were performed on COMSOL to test the simulation time according to the calculation regime and the meshing size. Even with high CPU capabilities, solving both the domains in a time dependent regime means a simulation time closer to real time, so it would take too long without obtaining effective advantages. Since the influence of different flow patterns and velocity fields in the air volume on the moisture buffering was investigated, transient fluctuations of the velocity field on the component response to humidity variations can be neglected in favour of a simplified model that considers local equilibrium between the fluid region turbulence and the material surface.

The air movement inside the simulated room is turbulent with mixed convection conditions. In

COMSOL, two turbulence models are available: the κ - ε model and the κ - ω model. Theoretically, the κ - ε model is based on the assumption that the Re number is moderate or high and the turbulence in boundary layers is in equilibrium. The κ - ω model provides a better prediction in the free flows close to the wall, but it is less accurate in the free-stream flow simulation. In addition, the κ - ω model is harder to reach convergence. Meanwhile, the accuracy of CFD simulation results is related not only to the turbulent model selection, but it also depends on the wall surface conditions. In this 2-D simulation of the momentum, heat and mass coupling in different regions, using κ - ε model is a fair trade-off of saved computational resources compared to the more complicated turbulence models. The balance equations for the coupled heat and moisture transfer in air and within the building components were set to be solved in sequence in the COMSOL environment according to the following order:

- Air velocity field with CFD: steady state regime. For solution time and computing memory capacity reason the use a coarse mesh (less detailed) is possible the κ-ε turbulence model has been adopted (Figure 3);
- HAM-transfer: transient regime. After the air velocity field had been calculated for each point of the considered volume, the coupled heat and moisture transfer was solved for the zone and for the building components considering the boundary conditions reported below. The moisture source was placed in the middle of the room and the average RH level over the air volume was monitored.



Figure 3 – Mesh definition for the air velocity field calculation. The inlet and outlet positions are indicated

The study has been applied to a simple room as defined by EN ISO 13791. The room volume in HAM-Tools was adapted to fit the 2-D model in COMSOL, which provides a 1 m deep third dimension for the building components for a total of 14.85 m³. For the air velocity field calculation a ventilation rate of 0.5 h^{-1} was considered. Since the inlet and outlet vents comply with the described room dimensions a 0.1×1.0 m vent area was set, considering a 1 m long development along the wall. In this way, the volumetric air flow to the zone in HAM-Tools was normalized on the vent section. Thus, the corresponding air velocity at the inlet is 0.02 m/s.

The cyclic gain in the adapted test room (200 g/h) was set considering half of the moisture load in the full-sized simple room defined by EN ISO 13791, for which an 80 g/h (medium activity in offices in accordance with UNI TS 11300-1:2014) per person was considered for a 5 people occupancy.

The room is ventilated and the outdoor air conditions (temperature and relative humidity) were set according to the weather data for Turin (EnergyPlus weather data). The start RH level in the room and within the material was set at 30% and a gypsum plaster layer was applied as interior finishing together with an aerated concrete and foam insulation envelope. The study aims at demonstrating:

- the deviation between results obtained from HAM-Tools (lumped model) and COMSOL (CFD model) with regard to the indoor relative humidity trend for both cases when the environment is subjected to a cyclic moisture gain, constant for each scenario, and when there is no moisture load. According to recent studies from literature, a higher relative humidity level is expected within the room, due to the development of "dead zones" on the finishing material surface which do not fully interact in the moisture buffer process;
- the deviation on results between simulations carried out with different inlet and outlet vent positions, in order to evaluate how the configuration can affect the RH trend and the moisture buffer.

4. Results

In Figure 4 the relative humidity trend for scenarios with and without moisture gain are shown (4 curves). The simulation is related to a 0.5 h⁻¹ ventilation rate calculated with COMSOL and HAM-Tools.



Figure 4 – Relative humidity trend for a $0.5 h^{-1}$ ventilation rate. COMSOL and HAM-Tool results for scenarios with and without moisture gain

While a good fitting is reached between the curves without any vapour generation, the moisture gains determines a deviation of the RH trend denotes between COMSOL and HAM-Tools.

The cyclic load has a lower impact on RH peaks in the COMSOL environment, as the RH curve looks flattened. This behaviour is probably due to the RH averaging above the room volume, which involves the diversification between those zones directly affected by the moisture generation and those more distant not subjected to a sudden increase in the vapour concentration. This leads to a slower rise of the RH level during the loading period (8 hours) and to a likewise unloading phase that appears more like a "stabilisation" phase, where a real discharge of the RH level due to the ventilation mechanism does not occur. The average value of relative humidity for the 4 cases is reported in Table 1. The average relative humidity μ_{φ} [-] calculated in COMSOL denotes a $\Delta RH = +7$ % for the case without moisture gain and a ΔRH = +10 % for the case with moisture gain, with respect to HAM-Tools results.

Table 1 – RH average value for the 4 simulated cases. 0,5 $h^{\mbox{-}1}$	
ventilation rate, 200 g/h moisture gain.	

Moisture load Ġ _{gen} [g/h]	μ _φ [-] (HAM-Tools)	μ _φ [-] (COMSOL)
0	0.39	0.42
200	0.57	0.63

In order to match the RH trends obtained from the two models, the following correction were applied to HAM-Tools:

- correction factor C_β = 0.4 applied to the indoor surface moisture transfer coefficient β_{int}. This aims at reducing the buffer capacity of the finishing layer by increasing its surface vapour resistance of 60 %;
- reduction of the building components area (-50%). This allows us to consider that not all the surfaces are involved in the moisture buffer.

The above correction is in accord with a recent experimental study (Ramos, 2012), which demonstrates that the final buffer effect is half of the expected one.

Figure 5 shows the two approaches. In both the cases the calibration leads to an increase of the fluctuation amplitude of relative humidity – with an average RH value μ_{φ} = 58 % in either case – and not to a trend similar to the one obtained with COMSOL.



Figure 5 - HAM-Tools calibration on the results previously obtained for the scenario with moisture gain. The graph shows both cases: 1) application of a correction factor C_{β} = 0.4 to the indoor surface moisture transfer coefficient β_{int} ; 2) and reduction of the building components area (-40 %)

The next step was the evaluation of the influence of the vents configuration on the RH trend inside the room. Five different vent positions for the inlet and outlet were considered, in order to make a sensitivity analysis. A deviation between results is expected, due to the affection of the air velocity field on the indoor surface vapour resistance of building components that leads to different amounts of buffered moisture. The scenario adopted for the sensitivity analysis is the 0.5 h⁻¹ ventilation rate, considering a 200 g/h moisture gain for the whole week (Turin weather data). In Figure 6, the air velocity field calculated in steady-state conditions and a snapshot of the respective relative humidity distribution over the air volume (transient conditions, 1-week simulation) according to vent configuration no. 1 is reported.



Figure 6 – The air velocity field calculated in steady-state conditions (above) and a snapshot of the relative humidity distribution in the air volume and within the envelope (below) for vents configuration n.1

According to the different configurations and to the resulting air flow patterns, the zones with a reduced air velocity (i.e. v < 0.02 m/s) are clearly visible and not only localized in the corners of the room, but also in the central areas of the walls. This leads to localized surface moisture transfer coefficients that are characterized by several vapour resistances; in this way the interior finishing do not interacts in the same way with the moisture flux they come in contact with, defining a more detailed response to humidity variations by the building components. The results highlight a deviation between the RH trends for the different vents configuration as expected. Figure 7 shows the humidity trend for each case, while the average value of RH is reported in Table 2. It is so possible to identify which configuration is most inconvenient for the moisture dampening inside the environment.



Figure 7 – Relative humidity trend for a 0.5 h^{-1} ventilation rate. COMSOL results for scenarios with different vents configurations

From the sensitivity analysis it is clear that configurations no. 2 and no. 3 lead to a higher RH level inside the room. This is probably due to the inlet vent position, located at the height of 2.70 m. Since the density of water vapour is lower than that of dry air, the generated moisture tends to go upwards, stratifying in the air volume in contact with the ceiling; the presence of the exhaust air vent in the upper part helps the moisture removal. A maximum Δ RH equal to 5 % is achieved between the lowest and the highest average RH value. However, configuration no. 5 does not account for any vent in the upper part of the wall but still shows an average RH level close to the first solutions.

Table 2 – RH average value for the 5 simulated vent configurations cases. 0,5 $h^{\text{-1}}\,$ ventilation rate, 200 g/h moisture gain.

μ _{φ,1} [-]	μφ,2 [-]	μφ,3 [-]	μφ,4 [-]	μφ,5 [-]
0,63	0,68	0,67	0,63	0,64

The air velocity field is also responsible for the removed amount of moist air through the mechanical ventilation system, but how much this depends on one variable or another is still to be investigated.

5. Conclusion

COMSOL Multi-physics provides a simulation environment by coupling HAM equations and heat and moisture transfer between indoor air and enclosure without a third party programming. In the present work, the fully coupled model was established in this single simulation environment. This model has several advantages: 1) it overcomes the main limitations of the currently available CFD coupling models in simulating the whole building HAM transport, and 2) it has great application potential for the aspects related to ventilation design, HAM-transport through wall system and prediction of the room hygric inertia. The influence of the position of ventilation vents on the indoor RH trend, especially under low ventilation rates has been evaluated. The comparison between the lumped model (HAM-Tools) and the CFD model (COMSOL), when the HAM-transfer is applied, generated uncertainties. The first part of the investigation resulted in a good matching with regard to the diffusion equation implementation in COMSOL, validated by means of numerical simulation with HAM-Tools. The component behaviour with regard to the moisture transfer has been evaluated and both the simulation tools produce the same results.

The second phase, where the air zone has been solved with the CFD in COMSOL instead of using lumped conditions, was found critical with respect to the matching between the two software. The original intention to "rectify" the lumped model with another closer to reality generated difficulties to find a correction coefficient able to match the results. The CFD-HAM model on COMSOL should be validated by experimental data and needs to be improved and implemented. For this reason, we cannot assume it as the reference model and calibrate the lumped model with non-validated results.

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7. Nomenclature

Symbols

D_{ϕ}	liquid conduction coefficient (kg/ms)
c _p	specific heat capacity (J/kgK)
\dot{g}_{a}	density of air flux (kg/m ² s)
ġ _v	density of moisture flux (kg/m ² s)
Н	volumetric heat capacity (J/m ³ K)
h _v	evaporation enthalpy of water (J/kg)
Т	absolute temperature (K)
t	time (s)
p _c	suction pressure (Pa)
$p_{\rm v}$	vapour pressure (Pa)
$p_{v,s}$	vapour pressure at saturation (Pa)
u	moisture content by mass (kg/kg)
W	moisture content by volume (kg/m ³)
Х	thickness (m)
δ_p	vapour permeability (kg/m s Pa)
λ	thermal conductivity (W/m K)
λ_1	liquid conductivity (s)
Q0	density of dry material (kg/m3)
φ	relative humidity (-)
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ξ moisture storage capacity (kg/m³)

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