Full scale validation and sensitivity analysis of a CFD-HAM model

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SUMMARY

CFD (Computational Fluid Dynamics) is a useful tool to study air flow patterns in a room. Current CFD models are able to simulate air flow combined with temperature distributions and species distributions. In this paper a coupled CFD-HAM model is shortly discussed. This model combines CFD with a HAM model (Heat, Air and Moisture) for hygroscopic materials. This coupled model is able to simulate air flow around a porous material and combines this with heat and moisture transport in the porous material. Validation with a small scale experiment showed good results. In this paper a further validation of the model is discussed based on a sensitivity analysis of some model parameters.

INTRODUCTION

Temperature and relative humidity are two important parameters for damage risk assessment of buildings. E.g. too high levels of indoor relative humidity can cause mould growth on the surfaces of the building envelope. When moisture migrates through the building envelope, interstitial condensation can occur which can lead to rot, deterioration of surface finishing materials or other damage phenomena. Even if humidity levels are kept low enough, damage can still occur due to too strong variations. E.g. paintings and artefacts can show cracks when exposed to fluctuating temperatures and humidity levels [1]. Having a good knowledge of the heat, air and moisture transport in a building is also of great importance for many other applications. Moisture buffering by hygroscopic materials levels out indoor relative humidity fluctuations. This can reduce the energy use of HVAC systems [2] and improve the indoor air quality at the same time [3]. In literature some examples are found where the importance of knowing the relative humidity in the design stage of a HVAC system is highlighted [4,5].
A new trend in Heat, Air and Moisture modelling (HAM) is the coupling of these models to CFD (Computational Fluid Dynamics). However, these models still need proper input data like boundary conditions, initial conditions and material property data. Extensive databases for these material properties can be found in literature [6,7,8], but recent studies revealed a large spread of some of these material properties when the same material was measured by different laboratories [8,9]. It is often not clear how this will affect the model outcome. This paper highlights the importance of a sensitivity analysis for newly developed coupled HAM models.

COUPLED CFD-HAM MODEL

Standard CFD packages do not include a HAM model to simulate the interaction with porous materials. Therefore a new model was added to an existing CFD package (Fluent®). This model is discussed more detailed in Steeman et al. [10]. In this paper only a short overview of the modelling approach is given.

A direct coupling approach is used. This implies that the computational domain encloses the air region as well as the porous material and only one solver is used. Nevertheless, for each region (porous material or air) a different set of equations has to be solved.

Heat and moisture transfer in the air

The air is modelled as an incompressible fluid. In this case the energy and moisture transport equations reduce to equations (1) and (2). Note that for the transported variables, temperature, T, is chosen for the energy equation and the mass fraction of water vapour, Y, for the moisture transport equation. The same transport variables are used in the transport equations for the porous material.

$$\frac{\partial}{\partial t}(\rho_{air} CT) + \nabla.(\vec{v}\rho_{air} CT) = \nabla.\left(\lambda_{air}\nabla(T) - (C_{vap} - C_{air})\vec{g}T\right) \quad (1)$$

$$\frac{\partial}{\partial t}(\rho_{air} Y) + \nabla.(\rho_{air}\vec{v}Y) = \nabla.(\rho_{air} D\nabla(Y)) = -\nabla.\vec{g} \quad (2)$$

with

$$C = YC_{vap} + (1 - Y)C_{air} \quad (3)$$

In these equations ρ_{air} [kg/m³] is the density of the humid air, C_{vap} [J/kgK] is the specific heat capacity of water vapour, C_{air} [J/kgK] the specific heat capacity of air and C [J/kgK] the weighed average specific heat capacity according to equation (3), λ_{air} [W/mK] is the thermal conductivity of air and g [kg/m²s] the water vapour diffusion flux. D [m²/s] is the diffusion coefficient of water vapour in air. The first term on the left hand side of each transport equation is the storage term, the second term represents the convective term; the right hand side represents the transport by diffusion.

Heat and moisture transfer in porous materials

For the porous material zone the following assumptions are made in the model:

-No air transfer occurs
-Liquid transfer is not dominant
-Moisture storage only depends on relative humidity
-The temperature remains below the boiling point
-There is no radiative transfer inside the porous material

The model is only valid in the hygroscopic range (RH <98%). Here moisture transfer by vapour transfer is dominant. This implies that the moisture transfer can be modelled by a single water vapour diffusion coefficient. Equations (4) and (5) describe the moisture transfer and the heat transfer in the porous material. Again temperature T and vapour mass fraction Y are used as the transported variables. Note how latent heat of vaporization L_{vap} appears in equation (5). Due to the capillary action of the porous material, part of the water vapour entering the porous material condenses (or when the porous material dries out, liquid water evaporates from the pores). This phase change is accompanied by a latent heat effect.

$$\frac{dw}{dt} = -\nabla.\vec{g} \Leftrightarrow \frac{\partial w}{\partial RH}\frac{\partial RH}{\partial Y}\frac{\partial Y}{\partial t} + \frac{\partial w}{\partial RH}\frac{\partial RH}{\partial T}\frac{\partial T}{\partial t} = \nabla\left(\rho\frac{D}{\mu}\nabla(Y)\right) \quad (4)$$

$$\frac{dE}{dt} = \nabla.\left(\lambda_{mat}\nabla(T) - \left(\left(C_{vap} - C_{air}\right)T + L_{vap}\right)\vec{g}\right) \Leftrightarrow$$

$$\rho_{mat} C \frac{\partial T}{\partial t} + C_{liq} T \frac{\partial w_{liq}}{\partial t} + \left(C_{vap} T + L_{vap}\right)\frac{\partial w_{vap}}{\partial t} = \nabla.\left(\lambda_{mat}\nabla(T) - \left(\left(C_{vap} - C_{air}\right)T + L_{vap}\right)\vec{g}\right) \quad (5)$$

with

$$E = \rho_{mat} C_{mat} T + C_{liq} w_{liq} T + \left(C_{vap} T + L_{vap}\right) w_{vap} \quad (6)$$

$$C = C_{mat} + \frac{C_{liq} w_{liq}}{\rho_{mat}} + \frac{C_{vap} w_{vap}}{\rho_{mat}} \quad (7)$$

$$w_{liq} = \frac{\phi - \dfrac{w}{\rho_{vap}}}{\dfrac{1}{\rho_{liq}} - \dfrac{1}{\rho_{vap}}} \quad (8)$$

$$w_{liq} = \frac{\dfrac{w}{\rho_{liq}} - \phi}{\dfrac{1}{\rho_{liq}} - \dfrac{1}{\rho_{vap}}} \quad (9)$$

In equations (4) to (9) *mat* refers to material properties, *liq* stands for liquid water and *vap* for water vapour. In the material model described by equations (4) to (9) the following material properties have to be known: the sorption isotherm which states the relation between the equilibrium moisture content w [kg/m³] and the relative humidity RH [%], the vapour resistance factor μ [-] as function of the relative humidity, the thermal conductivity λ_{mat} [W/mK] of the porous material as function of the relative humidity, the dry density ρ_{mat} [kg/m³], the heat capacity C_{mat} [J/kgK] and the open porosity Φ [-].

REFERENCE CASE

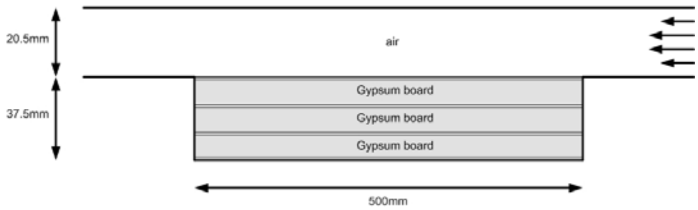

Figure 1. Reference case setup

In order to perform a sensitivity analysis on the coupled CFD-HAM model, a reference case was chosen first. The same case was used by Steeman et al. [10] to validate the coupled model. The case is based on an experimental setup discussed in detail by Talukdar et al. [11]. Figure 1 shows a schematic representation of the test setup. Preconditioned air enters on the right and flow over a pile of gypsum boards (three gypsum boards with a thickness of 12.5mm were stacked on top of each other). The gypsum board was preconditioned at 30%RH and 23.3°C. During the first 24 hours the air had an average relative humidity of 71.9% and an average temperature of 23.8°C. After these 24 hours a step change was applied to the air conditions. The temperature changed to 22.5°C and the relative humidity to 29.6%. During this test the temperature and relative humidity between the gypsum boards were monitored.

MATERIAL PROPERTIES

The material properties used for the reference case were taken from IEA Annex 41 [8]. These properties are needed to solve equations (4) to (9). Report 2 of Annex 41 comprises an elaborate round robin test for some of these porous material properties. Samples of the same gypsum board were sent to different laboratories where the material properties were determined. Figure 2 and 3 show the average sorption isotherm and vapour resistance factor calculated from the data of Annex 41 [8] together with the upper (+) and lower (-) measured values. Differences up to 20% are found.

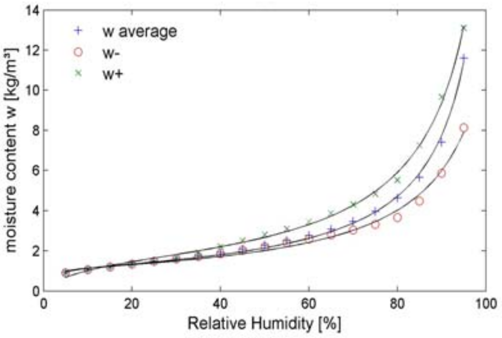

Figure 2. Sorption isotherm for gypsum board (data from [8])

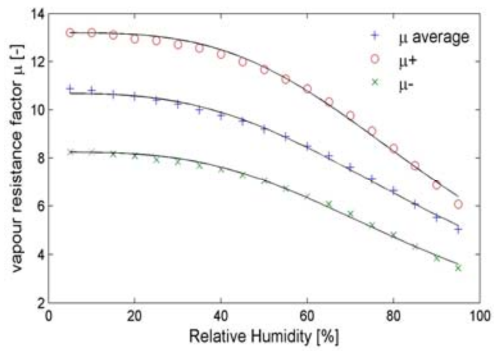

Figure 3. Vapour resistance factors for gypsum board (data from [8])

The following analytical functions (10) and (11) are used for sorption isotherm and vapour resistance factor of gypsum board. The coefficients are determined by fitting the functions to experimental data.

$$w_a = \frac{RH}{aRH^2 + bRH + c} \qquad (10)$$

$$\mu = \frac{\mu_0}{1 + aRH^n} \qquad (11)$$

SENSITIVITY ANALYSIS

Studies of [8] and [9] showed a large variability of measured material properties, which stresses the importance of a sensitivity analysis. For this sensitivity analysis different cases ware simulated. In each case only one parameter was altered. Temperature and relative humidity at a depth of 12.5mm and 25mm in the bed of gypsum board are simulated and a comparison between the different cases is made. In order to compare the results of the different simulations, figure 4 proposes five parameters derived from a typical response of temperature and relative humidity inside gypsum board (ΔRHa, ΔRHd, RHmax, Tmax and Tmin).

Tables 1 and 2 show the simulation results for the different cases. A change of 5% (decrease as well as increase) in density, thermal conductivity and heat capacity has almost no effect on the model outcome.

Changes in sorption isotherm and vapour resistance factor on the other hand have a more severe impact. Table 4 shows that an increase in sorption isotherm (w+) results in a decrease of the maximum relative humidity by 1.72% points and a decrease of the sorption isotherm (w-) results in an increase of the relative humidity by 0.94% points. These values are relatively low compared to the differences between the sorption isotherms. Changes in sorption isotherm also affect the simulated temperature. The temperature change due to latent

heat effects is slightly smaller for a lower sorption isotherm and slightly larger for a higher sorption isotherm. These results correspond with what can be physically expected. An increased sorption isotherm will result in a higher moisture content and a higher specific moisture content ($\partial w / \partial RH$). This reduces the water vapour diffusion within the vapour phase and thus the relative humidity. Temperature change due to phase change increases because more vapour condenses during absorption and evaporates during desorption.
Changing the vapour resistance factor by a higher or lower curve again changes the model outcome. Similar to the higher sorption isotherm, a higher vapour resistance factor results in a lower relative humidity during the absorption phase and a higher relative humidity during the desorption phase. The opposite counts for a lower vapour resistance factor. The effect is again more pronounced deeper in the material.
A higher vapour resistance factor corresponds with a lower vapour permeability. Thus it is more difficult for the water vapour to penetrate the porous material. This explains why a lower relative humidity is found during absorption and a higher relative humidity is found during desorption. Simultaneously the temperature change due to the latent heat effect is less pronounced for a higher vapour resistance factor and the other way around for a lower vapour resistance factor.
Finally the effect of modelling gypsum board as layered or as uniform was investigated. Gypsum board is normally built up out of three layers: a layer of paper on each outside surface and a layer of gypsum in between. In the ‘uniform’ case the gypsum board was modelled as a uniform material and a weighed average isotherm and vapour resistance was used. The ‘layered’ case models each layer of material separately. However, the two modelling approaches show almost no difference. The material properties of the layered gypsum board are taken from [12] and are slightly different from the material properties used in the previous test cases. Therefore the results can differ.

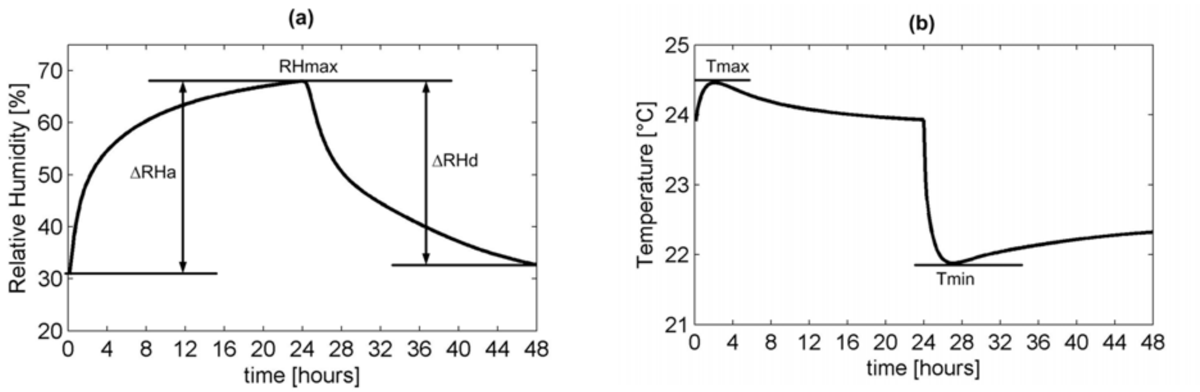

Figure 4. Typical response of the temperature (a) and relative humidity (b) in gypsum board at a depth of 12.5mm for a step change induced in the relative humidity of the surrounding air (29.6%RH-71.9%RH).

Table 1. Simulation results for temperature and relative humidity at 12.5mm in the gypsum board

	@12.5mm				
	ΔRHa[%]	ΔRHd[%]	RHmax[%]	Tmax [°C]	Tmin [°C]
Reference case	38.02	35.31	68.02	24.46	21.88
ρ+5%	38.02	35.32	68.02	24.44	21.89
ρ-5%	38.02	35.31	68.02	24.47	21.86
λ+5%	38.02	35.32	68.02	24.46	21.88
λ-5%	38.01	35.30	68.01	24.46	21.88
C_{mat}+5%	38.02	35.32	68.02	24.44	21.89

C_{mat}-5%	38.02	35.31	68.02	24.48	21.86
Sorption isotherm +	36.30	31.27	66.30	24.57	21.83
Sorption isotherm -	38.96	37.26	68.96	24.41	21.91
μ+	36.84	32.58	66.84	24.37	21.97
μ-	39.18	37.97	69.18	24.57	21.75
Layered	40.18	39.11	70.18	24.51	21.83
Uniform	40.15	39.07	70.15	24.52	21.81

Table 2. Simulation results for temperature and relative humidity at 25mm in the gypsum board

	@25mm				
	ΔRHa[%]	ΔRHd[%]	RHmax[%]	Tmax [°C]	Tmin [°C]
Reference case	35.64	30.83	65.64	24.54	21.81
ρ+5%	35.64	30.84	65.64	24.53	21.82
ρ-5%	35.64	30.83	65.64	24.56	21.79
λ+5%	35.66	30.86	65.66	24.54	21.81
λ-5%	35.62	30.80	65.62	24.55	21.80
C_{mat}+5%	35.64	30.84	65.64	24.53	21.82
C_{mat}-5%	35.64	30.83	65.64	24.56	21.79
Sorption isotherm +	33.03	24.32	63.03	24.66	21.78
Sorption isotherm -	37.07	33.96	67.07	24.50	21.83
μ+	33.77	26.27	63.77	24.44	21.92
μ-	37.51	35.45	67.51	24.68	21.65
Layered	39.12	37.08	69.12	24.62	21.72
Uniform	39.08	37.01	69.08	24.63	21.71

PRELIMINARY FULL SCALE VALIDATION

The previous paragraphs showed simulation and validation results for a small scale benchmark experiment. However, the question still remains how well the model will perform in a more realistic situation. Therefore a second test setup was developed witch represents a small room. A schematic representation of the room is shown in figure 5. The room measures 1.8m wide by 1.8m high by 1.89m long. Conditioned air is supplied at the top of the room and extracted at the bottom. Figure 6 shows a detail of the test sample in the room. Here a sample of calcium silicate is placed in an isolated and impermeable wall. The sample measured 20cm by 20cm and has a thickness of 10cm. The surfaces on the side and back of the sample are covered with wax to prevent moisture transfer through these faces and thus ensure a 1D moisture transfer. Insulation around the sample does the same for heat transfer.

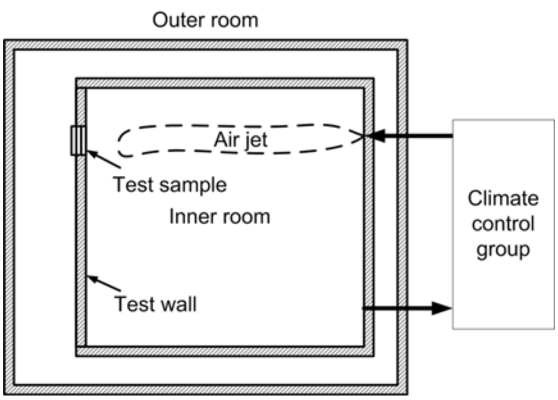

Figure 5. Schematic representation of the test facility

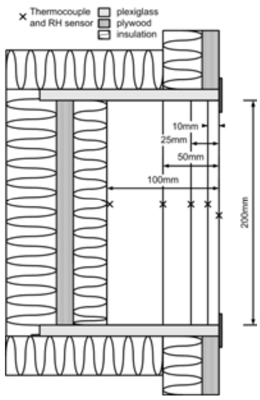

Figure 6. Detail of the test sample

Relative humidity sensors and thermocouples are located at a depth of 10mm, 25mm and 50mm of the sample. An outer chamber shields the test room and test sample from outdoor influences.
Figure 7 and 8 show some preliminary results of simulations and measurements in the test room. The sample was preconditioned at 25.4°C and 47%RH. It was then exposed to a supply air of 25°C and 70%RH during 8 hours. Afterward the relative humidity was lowered to 50% during 16 hours. Measurement and simulations show relative good agreement. However no perfect match was found. Previous paragraphs already showed the importance of the material properties, especially sorption isotherm and moisture permeability. This would explain the deviations found here. However, boundary conditions are more complex in this case as well as the modelling of these conditions. This could also explain some of the discrepancies.

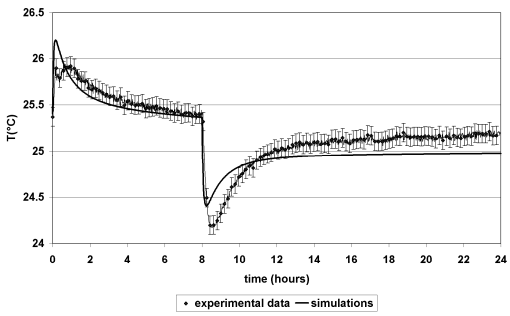

Figure 7. Temperature at a depth of 10mm in calcium silicate. Error bars are included for the measurements.

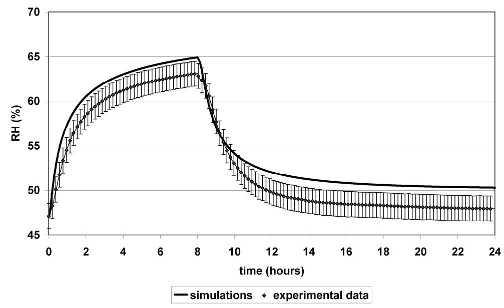

Figure 8. Relative Humidity at a depth of 10mm in calcium silicate. Error bars are included for the measurement.

CONCLUSIONS

An extensive sensitivity analysis was performed on a recently developed coupled CFD-HAM model. This model uses CFD to calculate the indoor air distributions around a porous material and combines this with a HAM model to incorporate the heat and mass transfer between air and the porous material. By using a direct coupling method, no external data exchange between the two models is needed which increases the calculation speed of the model.
Data from a benchmark transient heat and mass transfer experiment performed during IEA Annex 41 were used as a reference case for the sensitivity analysis. The material data used for this case were the averaged values found in a round robin test also performed during IEA Annex 41. This test showed that large discrepancies could occur between material properties measured at different laboratories.
In this paper it is shown that the coupled CFD-HAM model is rather insensitive to deviations in most of the material properties. For density, heat capacity and thermal conductivity of the porous material no significant effect on simulated temperature and relative humidity was found when these properties were changed by 5%. The impact of sorption isotherm and vapour resistance factor was more severe. These properties are often harder to measure, resulting in large uncertainties. Deviations up to 2%RH were found for the different isotherms and resistance factors. Changing both at the same time would lead to even larger deviations. These hygroscopic properties also have their impact on the calculated temperature although this is limited. Finally, modelling gypsum board as layered had no impact on the results.

Some preliminary results of a full scale validation experiment were shown in the last paragraph. These results again stress the importance of a sensitivity analysis before final conclusion on the modelling accuracy can be drawn.

ACKNOWLEDGEMENT

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