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Implementation and benchmarking of a 3D hygrothermal model in the COMSOL Multiphysics software

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Abstract

Many buildings physics problems are difficult to evaluate properly without looking at the problem in three dimensions. For instance, it can be difficult to assess moisture transport in a brick masonry wall segment as it consists of a relatively complex system of brick and mortar. Still, most hygrothermal simulations are likely done in 1D or 2D, but development in computer hardware and software makes 3D simulations easier accessible. This paper looks into benchmarking of a hygrothermal simulation model created in the COMSOL Multiphysics software. The results show COMSOL to have promising applicability for 3D hygrothermal simulations.

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1. Introduction

In building physics, hygrothermal simulations are required in a number of different evaluative tasks, such as when evaluating structural performance with regard to transfer, absorption and release of heat and moisture, often with a final aim of looking for unwanted condensation and moisture damage. Hygrothermal simulations have mainly in the past been limited to 1D or 2D application, often with the use of dedicated software with limited or no user access to the mathematical equations describing the physics involved. However, a combination of development in computer processing capacity and the developing of so called multiphysics software have in the recent years made it

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Nomenclature

$c_{p,v}$	specific heat capacity of vapour [J/(kg K)]	R_w	specific gas constant H_2O [J/(kg K)]
$c_{p,w}$	specific heat capacity of water [J/(kg K)]	T	Temperature [K]
D_ϕ	capillary transport coefficient [kg/(m s)]	w_w	water moisture content [kg/m^3]
g	gravity constant [m/s^2]		
$g_{v,j}$	water vapour mass flux vector [kg/(m^{2}s)]	Greek letters	
$g_{w,j}$	liquid water mass flux vector [kg/(m^{2}s)]	δ_v	vapour diffusion coefficient [kg/(m s Pa)]
h_w	enthalpy of evaporation [J/kg]	ρ_s	dry density of solid material [kg/m^3]
K_l	liquid permeability coef. [kg/(m s Pa)]	ρ_w	water density [kg/m^3]
P_{sat}	vapour saturation pressure [Pa]	ϕ	relative humidity [-]

possible to conduct even 3D hygrothermal simulations with a complete user access to the mathematical equations describing the physics. The COMSOL Multiphysics software [1] have shown great promise in this regard, already having been applied by several researchers [2-9] in solving hygrothermal simulations. Except for [2, 7], this has been limited to 1D and 2D. Tariku [5] applied COMSOL, as part of his own created HAMfit model, existing in both a 1D and 2D version, on all the Hamstad Benchmarks [10] with good results. Hygrothermal 3D models in COMSOL has not been found, however, to previously been benchmarked.

In this paper implementation for COMSOL 3D modeling of heat and moisture transport is described. The heat and moisture transport mechanisms of the COMSOL model has been verified by applying the mathematical model on two benchmarks, namely Hamstad benchmark #1 and #2 [10]. The Hamstad benchmarks are all 1D benchmarks, meaning the heat, air and moisture transport is one-directional. However, the benchmarks are still valid in a 3D model given that the boundary conditions allow no heat and mass exchange over the boundaries normal to the two other directions. Further work will however be necessary to stress test the full 3D-functionality of the model on problems with results known to be correct, either in the form of benchmarks or results from laboratory tests.

2. Mathematical description of modeled physics

2.1. Moisture transport

Transport of moisture in porous materials is usually divided into three mechanisms; vapour diffusion due to gradients in vapour pressure, capillary suction due to gradients in suction pressure and vapour transfer by air transport due to gradients in air pressure. In order to implement the three mechanisms into a single partial differential equation (PDE) the mechanisms needs to become a part of a transient moisture balance having a common dependent variable. Traditionally this dependent variable has been either moisture content or relative humidity, where the latter is used here due to its benefit of being continuous over interfaces between materials having different moisture sorption capabilities. The following describe the mathematical expression for vapour diffusion and capillary suction.

Vapour diffusion can be expressed by Fick's law, i.e the negative product of a diffusivity constant δ and the gradient of vapour pressure, which with the vapour pressure expanded for, and having relative humidity (RH) as dependent variable, gives the following flux in direction j=1,2,3 [11]

$$g_{v,j} = -\left(\delta \cdot P_{sat} \frac{d\phi}{dx_j} + \delta \cdot \phi \frac{dP_{sat}}{dT} \frac{dT}{dx_j} \right) \tag{1}$$

Capillary suction is commonly based on Darcy's law, which with the use of a liquid permeability coefficient K_l becomes [6]

$$g_{w,j} = -K_l \left[\rho_w R_w \left(\frac{T}{\phi} \frac{d\phi}{dx_j} + \ln(\phi) \frac{dT}{dx_j} \right) + \rho_w g \cdot \vec{e_z} \right] \quad (2)$$

Inserting expressions (1) and (2) in the continuity equation for moisture content, expanding the transient term as well as writing the terms in (2) with a capillary transport coefficient D_ϕ [kg/(m^2 s)] instead of K_l [kg/(m s Pa)], and finally rearranging the terms according to occurrence of ϕ gives the following PDE for moisture transport.

$$\frac{dw_w}{d\phi}\frac{d\phi}{dt} = \frac{d}{dx_j}\left(\left[\delta_v P_{sat} + D_\phi \right] \cdot \frac{d\phi}{dx_j} + \left[\left(\delta_v \frac{dP_{sat}}{dT} + D_\phi \frac{1}{T} \ln(\phi) \right) \frac{dT}{dx_j} + \frac{D_\phi}{R_w} \frac{1}{T} g \cdot \vec{e_z} \right] \cdot \phi \right) \quad (3)$$

2.2. Heat transport

The PDE for heat transport is based on the enthalpy equation on conservative form. The heat storage term is modified for a porous material, taking into account both the porous solid and the water content at any given time, while neglecting the contribution of any vapour located inside the pores.

$$\rho_s c_{p,eff} \frac{d(T)}{dt} = \frac{d}{dx_j}\left(\lambda \frac{dT}{dx_j} - \left[c_{p,w} g_{w,j} + c_{p,v} g_{v,\mathrm{j}} \right] T - h_v g_{v,\mathrm{j}} \right) \quad (4)$$

where

$$c_{p,eff} = \left(c_{p,s} + \frac{w_w}{\rho_s} c_{p,\mathrm{w}} \right)$$

3. Benchmarks

3.1. Description of the Hamstad #1 benchmark

In the Hamstad benchmark #1 two material layers, which share an interface that experience condensation when the surrounding conditions call for it, are involved in a long term drying process of one of the material layers. The benchmark shall resemble a roof structure, as seen in figure 1a, where a loadbearing material is insulated by another material layer on the inside while having a water and vapour tight membrane layer on the exterior side. The loadbearing material layer, with a thickness of 100 mm, has an initial moisture content of 145 kg /m^3 ($\approx$99 % RH) while the insulating material layer, with a thickness of 50 mm, has an initial moisture content of 0.065 kg /m^3 ($\approx$56 % RH). Initial temperature is 20 °C for both layers, and 20 °C is also the constant value of the interior temperature. The interior vapour pressure as well as the exterior temperature is given by a table which gives varying values for a whole year. Although the benchmark covers 5 years, it uses the same boundary conditions for all the years. Exterior vapour pressure is also given, but the values are irrelevant due to the vapour tight exterior surface. Heat transfer coefficients for the interior and exterior are given as 7 W/(m^{2}K) and 25 W/(m^{2}K) respectively, and the interior vapour transfer coefficient is given as 2·10-8 s/m. Material properties for the two materials and more detailed description of the benchmark are given by [10].

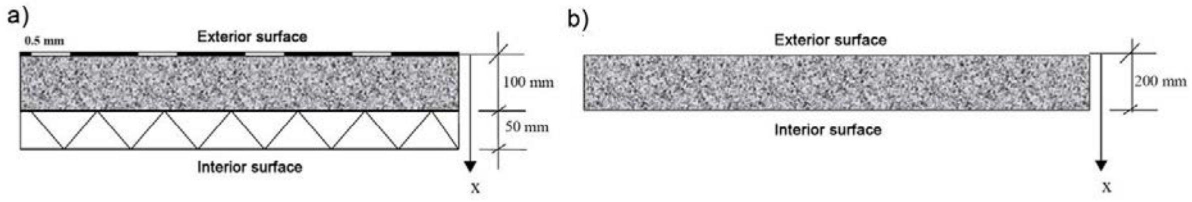

Fig. 1. (a) Benchmark #1, a two layer roof structure [10]; (b) Benchmark #2, a single material layer [10].

3.2. Description of the Hamstad #2 benchmark

The Hamstad benchmark #2 is a test which looks at the redistribution of moisture as the external and internal relative humidity, are suddenly changed from the initial situation, all while behaving as an isothermal case. An analytical solution exists for this test, assuming isothermal behavior [6]. The geometry consists of a single, perfectly airtight, 200 mm material layer, as seen in figure 1b. Initial conditions of the material include a relative humidity of 95 % and a temperature of 20 °C. When time starts running, boundary conditions of 45 % RH external and 65 % RH internal are imposed. As the benchmark case is isothermal, the boundary temperature is 20 °C. However, in order to keep the material temperature more or less constant at 20 °C the latent heat of evaporation has been set to 56.8 J/kg, which is considerably less than the usual value of 2500000 J/kg. The heat and vapour transfer coefficients at both surfaces are 25 W/(m^2K) and 1·10-3 s/m respectively. Material properties for the two materials and more detailed description of the benchmark are given by [10].

3.3. Methodology of benchmark implementation in COMSOL

The COMSOL model is built up around the PDEs for moisture and heat transport. These PDEs have been user defined in COMSOL, to become equal to equation (3) and (4), by using the so-called *coefficient form PDE* from the physics interface available in the software. A 3D geometry of the benchmark cases has been built as shown in figure 2, with dimension values in meters. Benchmark #1 and #2 are respectively having the x shown in figure 1 as a vertical and horizontal directional variable, i.e. z and x directions respectively in the PDEs. Each material layer is defined as a domain. The PDEs automatically call up the material properties of the material for the domain in question during the numerical solving. Meshes are generated as seen in figure 2, with eight layered boundary layers on surfaces and internal interfaces.

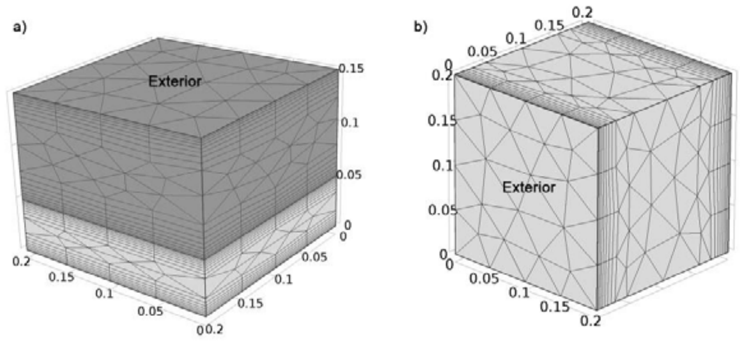

Fig. 2. The benchmark geometry and mesh including boundary layers at all interfaces. Values in meters. (a) Benchmark #1; (b) Benchmark #2.

The results from benchmark #1 are given as the hourly average of the moisture content in the loadbearing material. As shown in figure 3 and 4 the results for the first and fifth of a total of five years of benchmark #1 shows a rather good correlation to the benchmark solutions. The results are seen in the figures to more or less follow the benchmark solution given by Technion. However, the results also show more hourly fluctuations compared to the benchmark solutions. It has not been established whether this is caused by the 3D dimensionality of the model, the integration technique which was used to get average values, or some other aspect of the model.

The results of benchmark #2 can be seen in figure 5a and b, which show a very good fit with the benchmark solutions. It should be mentioned that the lines marked "results from Hamstad" on figure 5 consist of several lines lying more or less on top of each other. For more details on the results supplied by the Hamstad benchmark refer to [10].

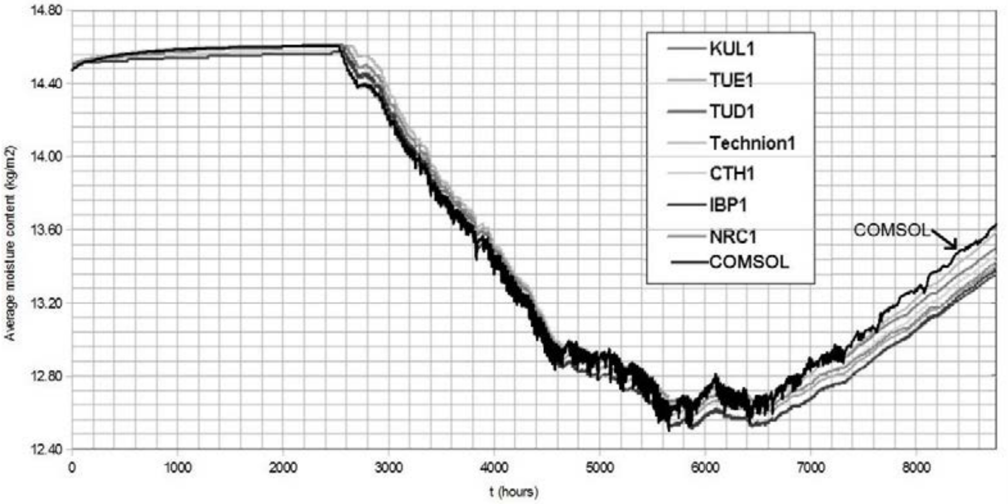

Fig. 3. Benchmark #1, superposition of average moisture content, COMSOL result, over solutions from [10] for year 1 of the benchmark.

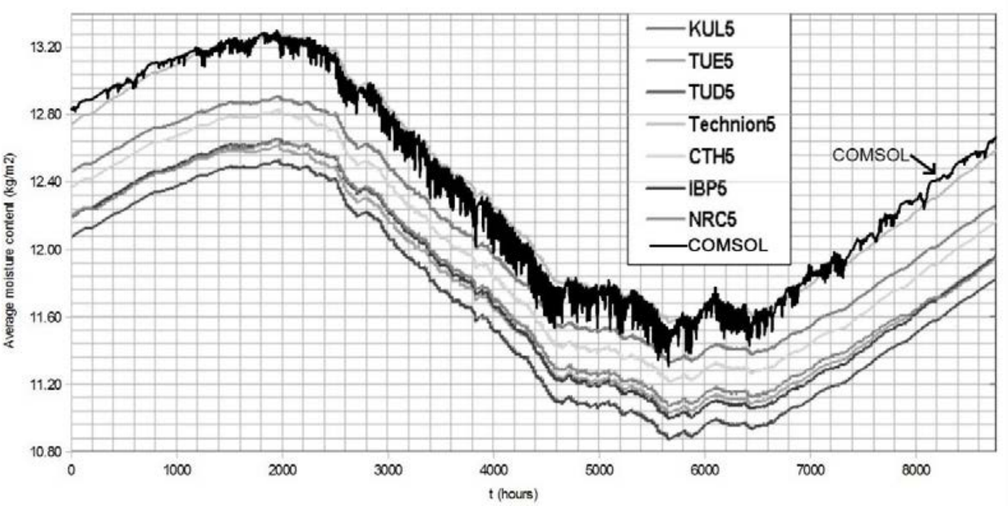

Fig. 4. Benchmark #1, superposition of average moisture content, COMSOL result, over solutions from [10] for year 5 of the benchmark.

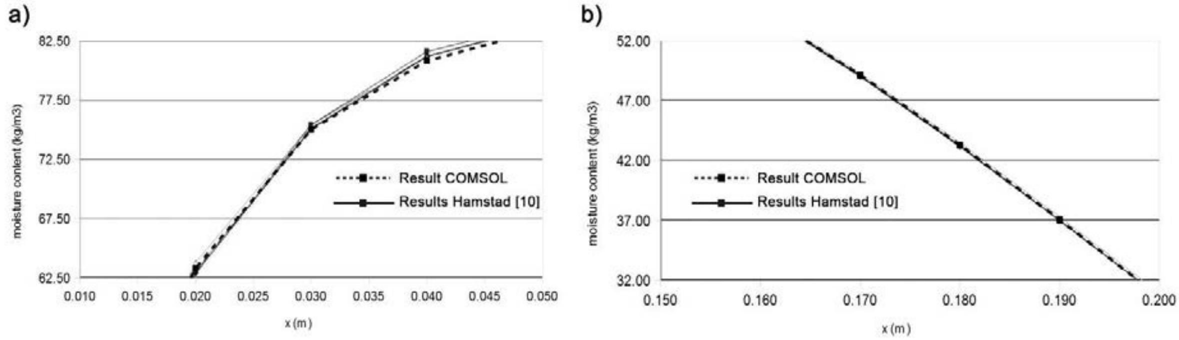

Fig. 5. Benchmark #2, superposition of COMSOL moisture content result over solutions from [10] at x(m); (a) 100 hours; (b) 1000hours.

4. Conclusion

The application of COMSOL for 3D hygrothermal simulation seems promising after running through Hamstad benchmark #1 and #2, where the results showed good agreement with the benchmark solutions. However, these two benchmarks only include moisture and heat transport where the only boundary exposure is varying vapour pressure and temperature. Further benchmarking is needed to be done on benchmarks including air transport and liquid water uptake, in order to evaluate the applicability, as well as the full functionality and performance, of COMSOL for 3D hygrothermal simulation.

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