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Analysis of IAQ based on modeling of building envelope coupled with CFD&HT room airflow.

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ABSTRACT

Buildings represent a major part of the world energy requirement. The simulation of combined heat, air and moisture (HAM) and pollutant transfer in this context is important to predict the indoor air quality (IAQ), along with the thermal comfort inside the buildings. Moreover, it is important to have appropriate levels of indoor humidity along with the room temperature as movement of water vapor through the building envelope causes a lot of harm to the building structure and reduces the quality of its thermal insulation leading to higher energy demand. In modern houses people is exposed to a big amount of building materials, many of which release pollutants, many of them are volatile organic compounds (VOCs) that degrade the IAQ. The knowledge of the peak loads, temperatures, humidity levels, pollutant dispersion can help to optimize the design of new buildings or existing buildings that need to be refurbished and therefore results in energy efficient buildings.

In this work a modular object-oriented building simulation tool (NEST) with CFD&HT code Termofluids, capable of coupling different levels of simulation models, allowing the simulation of heat, air, moisture and pollutant distribution (multizone model, envelope model, room analysis and HVAC system) and VOC is presented. The modular approach gives flexibility of choosing a model for each element and to have different levels of modeling for different elements in the system. Special attention has been focused on: the large eddy simulation turbulence models used for the room air dynamics and pollutants distribution transport and high performance parallel software. Parallelization of the building simulation is necessary if some critical processes/zones need to be modeled with more detail for reducing computational time. The main focus of this article is to couple the HAM and pollutants models for the building envelope with CFD&HT models with heat, moisture and pollutant transfer models for room airflow. An analysis of the effect of different materials on the IAQ of the buildings will be performed.

1. INTRODUCTION

The aim of this paper is to contribute towards the progress in the numerical simulation of the thermal and fluid flow processes within and around buildings. Buildings account to about 40% of the global CO₂ emissions which are directly related to the energy consumed for maintaining the building usability (European Commission, 2002). Building energy consumption has increased from 20% to 40% in developed countries exceeding the industrial and transportation (Pérez-Lombard *et al.*, 2008). It is estimated that almost 50% of the global energy demand is due to

buildings. Hence, energy conscious architecture is the need of current times. This involves the use of eco-friendly and less energy intensive building materials, incorporation of passive solar principles in building design, operation including day-lighting features, conservation of water, waste water recycling, rainfall harvesting, integration of renewable energy technologies and use of energy efficient appliances in buildings.

Energy simulations are important for the study of energy efficiency of buildings for optimizing the different processes involved, considering the building as a thermal system interacting with the surroundings through heat transfer and fluid flow processes. This numerical approach not only helps in saving the full scale experiment time and cost, but also helps in optimizing the governing parameters for the efficient functioning of the entire system. It can give vital information of the peak loads during the heating and cooling season, room temperatures and velocity distributions for maintaining an adequate IAQ, and overall energy demands during a year. This information can be used to reduce the energy costs with a good architectural and HVAC (Heating Ventilating, Air-Conditioning) design.

The prediction of the physical phenomena involved in buildings is difficult due to the large and complex geometry involved, changing boundary conditions, airflows due to natural convection, stack and wind effects, infiltration of ambient air and mechanical ventilation, and the mixture of free and forced convection flows which are often turbulent. In that sense, the present paper is focused on two main aspects: the combined Heat and Air Moisture transfer modeling (HAM) and the Computational Fluid Dynamics (CFD) air distribution analysis coupling with building energy modeling.

Many authors have studied heat and moisture transfer through building envelope. H.M. Kunzel (1995) presented a comprehensive study of the combined heat and moisture transfer mechanisms along with numerical and experimental studies. Methodology of heat air moisture transfer modelling was numerically detailed benchmark cases for one dimensional way (Hagentoft, 2002 and Hagentoft et al. 2005). The state of the art and the different programs for heat air moisture simulation in buildings and overview of the different approaches in heat and moisture transfer modelling are referenced in Woloszyn and Rode (2008) and Woloszyn *et al.* (2009). Recently, Tariku *et al.*, (2010) presented a transient model for coupled HAM through multilayered porous media.

On the other hand, several studies of airflow in buildings due to ventilation are referenced in the technical literature, available in different numerical codes. J. Axley (2007) presented a comprehensive study of the multizone airflow modelling where some models are described: LBL model (ASHRAE, 1989) for single zone buildings; CONTAM (Walton, 1977) for multizone modelling; AIRGLAZE (Voeltzel et al., 2001) modelling large highly-glazed spaces, or COwZ (Stewart and Ren, 2006) that divides the zones into sub-zones. Recently, Q. Chen (2009) has summarized the different methods for the ventilation performance for buildings and suggests that the use of subzonal models is not easy because of the special cells (with boundary layers, jets, etc.) and that they are not much superior to coarse grid CFD & HT simulations. Finally, Van Belleghem et al. (2011) are the one that have published benchmark experiments for moisture transfer modelling in air and porous materials along with the state of the art and CFD coupling.

In the IAQ, indoor air pollution plays a very important role since indoor air pollution has been recognized as one of the top environmental risks worldwide (World Health Organization, 1989). Two different factors can degrade the indoor environments: the synthetic building materials, which may emit a wide variety of pollutants such as volatile organic compounds (VOCs), and the air tightness of buildings. Ventilation, with appropriate air-handling processes, is used to create an indoor environment with acceptable air temperature, humidity, air velocity and remove pollutants, i.e. good thermal comfort and IAQ (Yang *et al.* 2004). Selection and design of appropriate HVAC require detailed knowledge of pollutant dispersion, which may depend on type and location of pollutant sources. Numerical simulation can help on the modellization of pollutant emission and dispersion.

In conclusion, the numerical simulation implies mathematical modelling and coding of the different physical processes occurring in different elements that constitute the building thermal system. In that sense, the models implemented in the numerical code presented could be from simple zero dimensional expressions relating the unknown variable, one dimensional model based upon experimental correlations, to two or three dimensional analysis with turbulence models or direct numerical simulations (DNS) for detailed resolution of fluid flow and heat transfer, where the level of modelling a given process may be different depending upon the nature of the process, resources available and the accuracy of the desired result. Thus, a modular object-oriented program can be very useful for the simulation of building processes. The modular methodology (Damle, et al. 2011), the description of the elements developed and the global resolution algorithm of the NEST program explaining the coupling of HAM models for the building envelope (Damle, et al. 2012a) with CFD&HT models (Damle, et al. 2012b) with heat, moisture and pollutant transfer models for room airflow, along with different case studies, are presented in the following sections.

2. MODULAR FRAMEWORK

In this work a building or a structure is modeled as a collection of basic elements (walls, rooms, windows, outdoor, etc.) as shown in Figure 1.

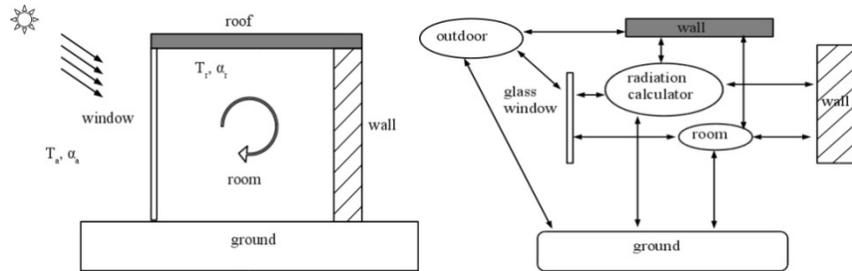


Fig. 1: A simple building diagram and group of elements structure equivalent.

MPI (Message Passing Interface) is used for the parallelization of the software and a given system is split into partitions (groups of elements) to be run on different processors. These elements/objects are capable of solving themselves when subjected to boundary conditions which are taken from the neighbouring elements. In each iteration, inputs (e.g., pressure, temperature, etc.) are taken from neighbours. Governing equations of the element are solved and the outputs (e.g., pressure, temperature, etc.) are set as boundary conditions for the resolution of the neighbour elements. Iterations continue until convergence is reached at a given time step and then the next time step calculation starts after updating the variables. The advantage of such a modular approach, as can be seen from Figure 2, is that each element can be represented in any form as long as it can exchange the necessary boundary information from the rest of the elements in the system.

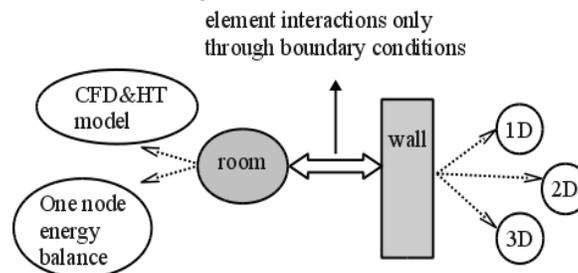


Fig. 2: Flexibility in choosing individual element models.

For instance, in a building with many rooms some rooms can be modelled with a detailed CFD & HT calculation while other rooms could be modelled using a global single CV energy balance. Also, new models can be implemented for a given element without changing the entire program.

3. WALL TREATMENT

The mathematical model for heat, air and moisture transfer implemented in the general building program, is described in this section. Both building walls and rooms are considered.

3.1 Moisture transfer

The moisture transfer equation (Künzel, 1995 and Tariku *et al.*, 2010) obtained by applying the Fick's law for vapor diffusion and Darcy's law for liquid transport, in terms of relative humidity ϕ and temperature T is written as:

$$\theta \frac{\partial \phi}{\partial t} = \nabla \cdot (D_{\phi} \nabla \phi + D_T \nabla T) - \nabla \cdot (D_l \rho_w \vec{g} + \rho_a \vec{V} \omega) \quad (1)$$

where $D_{\phi} = \delta_v p_{sat} + D_l \frac{\rho_w R T}{M \phi}$, $D_T = \delta_v \phi \frac{\partial p_{sat}}{\partial T} + D_l \frac{\rho_w R \ln \phi}{M}$

3.2 Heat transfer

The conservation equation of energy for a moist porous material, by taking into account condensation/evaporation within the material (Hagentoft, 2002 and Tariku *et al.*, 2010), can be written as:

$$\rho_0 C \frac{\partial T}{\partial t} + \nabla \cdot \rho_a V (C p_a + \omega C p_v) T = \nabla \cdot (\lambda \nabla T) + h_{fg} \dot{m}_{ce} + \dot{m}_{ce} T (C p_v - C p_l) \quad (2)$$

where $\dot{m}_{ce} = \nabla \cdot (\delta_v \nabla p) - (\rho_a V \nabla \omega)$

The equations (1) and (2) are solved simultaneously to resolve heat and moisture transfer in building walls with single or multiple material layers.

3.3 Air flow momentum balance

The air flow is governed by the Darcy equation that relates the flow rate with pressure gradient and air characteristics of the media.

$$-\nabla \cdot \left(\rho_a \frac{k_a}{\mu} \nabla P \right) = 0 \quad (3)$$

3.4. VOC

The modeling of VOC pollutants is done by considering the diffusion of the concerned species which may be emitted by the building materials. Concentration gradient is the driving force for VOC transport in the material with no chemical reaction inside. The transient VOC diffusion is given by

$$\frac{\partial C_m}{\partial t} = D_m \nabla^2 C_m \quad (4)$$

A partition coefficient $K_p = C_{mb}/C_{as}$ (Huang and Haghghat, 2002) is assumed to relate the VOC concentration at the boundary C_{mb} of the material to the concentration in the immediate vicinity of the boundary (C_{as}).

4. INDOOR ROOM MATHEMATICAL MODEL

On one hand, thermal and humidity room conditions can be predicted by means of heat and moisture balances using a single node energy balance. On the other hand, rooms can also be modeled by means of detailed CFD&HT calculations (Damle *et al.* 2011). The following section details numerical balances of a single node, while CFD&HT used within NEST code is referenced and detailed in Lehmkuhl *et al.* (2007).

4.1 Humidity balance

The moisture balance equation for a single well mixed zone room can be written as:

$$\rho_a \tilde{V} \frac{d\omega}{dt} = \sum_{j=1}^n \dot{m}_{wj} + \dot{m}_g + \dot{m}_e (\omega_e - \omega_r) \quad (5)$$

where the left hand side term represents moisture accumulation while the right hand side terms represent moisture transfer from room walls ($\dot{m}_{wj} = \beta_j A_j (p_j - p_r)$), internal moisture generation and moisture transported by the infiltrating ambient air respectively.

4.2 Energy balance

The general energy heat transfer equation in terms of enthalpy can be written as:

$$\rho_a \tilde{V} \frac{d}{dt} ((C p_a + \omega C p_v) T) = \sum_{j=1}^n \alpha_j A_j (T_{wj} - T_r) + \dot{m}_e C p_a (T_e - T_r) + \quad (6)$$

$$\dot{m}_e C p_a (\omega_e T_e - \omega_r T_r) + \sum_{j=1}^n \dot{m}_{wj} C p_v T_{sj} + \dot{m}_g C p_v T_g$$

where, the left hand side term represents accumulation of enthalpy while the right hand side terms represent convective heat from walls, heat brought by ambient air, heat added/removed by moisture coming from or going into the room walls ($\dot{m}_{w,j}$) at temperature $T_{sj} = T_w$ and $T_{sj} = T_r$ respectively, and heat added due to moisture generation (\dot{m}_g) at temperature T_g .

4.3. VOC balance

The conservation equation for each VOC emitted by the wall materials is written by considering a transient mass balance over the well-mixed room as:

$$\tilde{V} \frac{\partial C_r}{\partial t} = \dot{Q}_{ven}(C_{in} - C_r) + h_m A(C_r - C_{as}) + C_g \quad (7)$$

5. VERIFICATION AND VALIDATION

To verify the working of the aforementioned model equations for building rooms and walls, some benchmark cases are worked out.

5.1 Isothermal moisture transfer in a wall

The HAMSTAD benchmark exercise #2 (Hagentoft, 2002) is a one dimensional case with isothermal moisture transfer in a single layer exposed to air with relative humidity of 65% on one side and 45% on the other side, while the temperature is held constant at 25°C. Figure 3 shows how the numerical model is able to predict very well the transient moisture diffusion in the wall with the relative differences below 1.2 %.

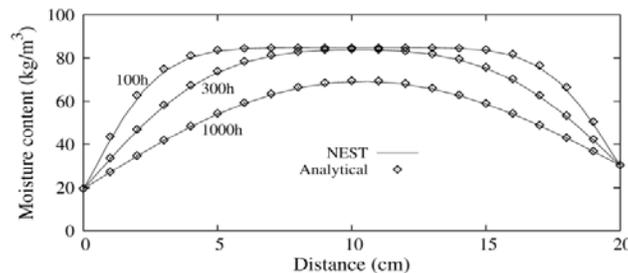


Fig. 3. Moisture distribution along the wall with time.

5.2 Air transfer in a “lightweight wall”

The HAMSTAD benchmark exercise #3 (Hagentoft, 2002) is a one dimensional case with air transfer through single 200 mm thick layer. Moisture transfer is caused mainly by airflow, but also by the moisture and temperature gradients across the layer. During 100 days of simulation, initial and boundary temperature is 20°C, with 70% and 80% of indoor outdoor humidity, respectively. During the first 20 days there is air exfiltration that changes within day 20 and 21 to air infiltration until the end of the period, both effects due to change of pressure distribution. Fig. 4 shows the temperature and moisture distribution in time in the middle of the layer. NEST results agree very well with the other four numerical solutions referenced in (Hagentoft, 2002).

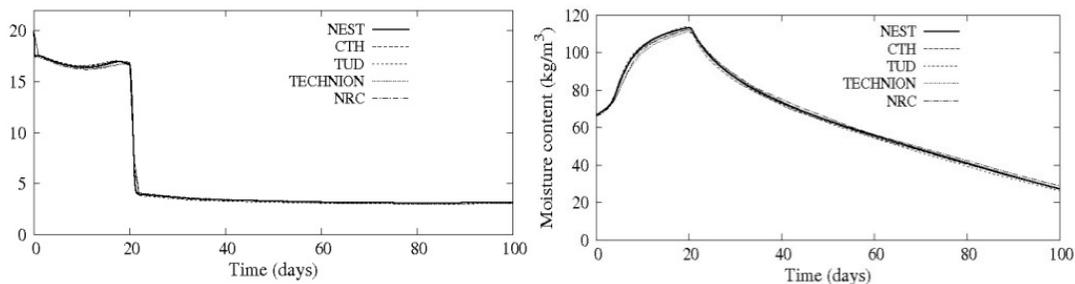


Fig. 4 Temperature and Moisture distribution in the middle of the layer with time.

5.3 Non-isothermal moisture transfer in a composite wall

Results for the benchmark exercise #4 (Hagentoft, 2002) with heat and moisture transfer in a two layer wall having a hygroscopic finish are presented. The wall is subjected to changes in heat and moisture loads at its surfaces. Severe climatic load is imposed for having different phenomena of heat and moisture transfer generated by heating, cooling, alternating drying and wetting due to rain load along with fast liquid transfer properties of the first layer. These conditions allow a very good case for checking the heat and moisture transfer model. Fig 5 shows interior and exterior moisture surface variation, while Fig 6 shows interior and exterior temperature surface variation. All comparative results show a very good agreement as compared with other programs.

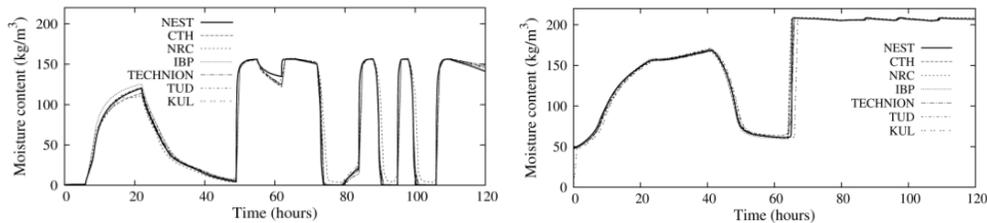


Fig. 5 External and internal moisture surface variation.

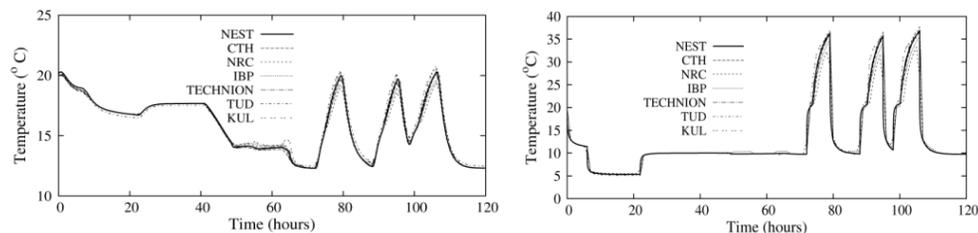


Fig. 6 External and internal temperature surface variation.

5.4 Room and wall moisture transfer

A simplified building (a rectangular box shape) is presented for verification purpose (Bednar and Hagentoft, 2005) with walls made monolithic layer (150mm) of aerated concrete is tested under isothermal conditions, but with moisture transfer until cyclic steady state is reached. The single zone envelope exchanges moisture with outdoor with an internal moisture generation of 500 g/h between 9:00h and 17:00h. Two different cases are studied: (a) vapor tight interior and exterior wall surfaces of the building (case 0A); b) only exterior surfaces vapor tight with absorption and desorption at interior wall surfaces (case 0B). Initial and boundary temperature is 20°C, while relative humidity is 30%, during the simulation period. Fig. 7 shows the relative humidity over the length of the day for case 0A and case 0B, respectively. Good agreement with analytical solution with a maximum relative difference of 1.0573% and 1.42065 % for case 0A and case 0B is observed.

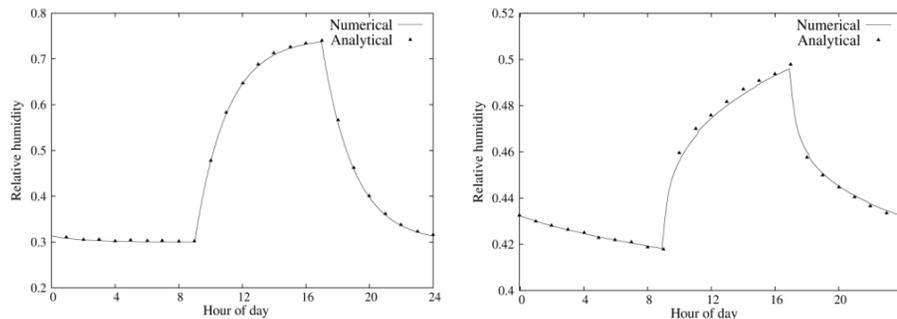


Fig. 7 Relative humidity variation of the room in case 0A and 0B, respectively.

5.5 Room and wall VOC transfer

The implemented models for the VOC transfer through walls and rooms is validated with experiment data of Yang *et al.* 2001. This is a case of a small chamber having a volume of 50 liters (0.212x0.212x0.0159m) with a pollutant emitting panel material inside. The VOCs in this case, TVOC (Total Volatile Organic Compound), are hexanal, α -

pinene, camphene and limonene. Two different particleboards PB1 and PB2 are tested. The initial concentration of the TVOC in these two particleboards is $5.28 \cdot 10^7 \mu\text{g}/\text{cm}^3$ and $9.86 \cdot 10^7 \mu\text{g}/\text{cm}^3$, respectively, while the initial concentration in the room is zero. For both particleboards the diffusion coefficient for TVOC is $7.65 \cdot 10^{-11}$ and the partition coefficient is 3289. Air exchange rate of 1h^{-1} is maintained during the tests. Figure 8 shows the evolution of the pollutant concentration in the chamber with time with both particleboards. It can be seen that, after the first few hours, the numerical values show a good agreement with the measured values for both the particleboards under consideration. The initial period corresponds to the high emission rate initially due to the high concentration of the VOC near surface and zero in the room air. Beyond the initial period the material dries and diffusion of VOC play a more significant role and the model compares well with the measured data.

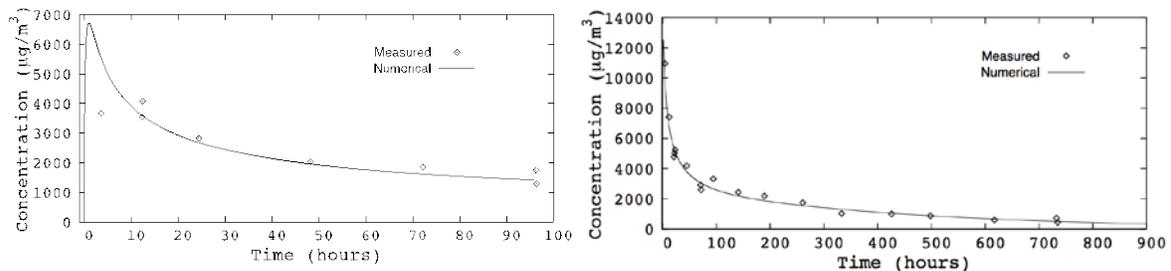


Fig. 8. Evolution of the pollutant concentration in the chamber with time with two particle boards: (left) PB1 and (right) PB2.

6. ILLUSTRATIVE RESULTS CASE

In order to show the possibilities that this modular and object oriented tool presents can offers, and illustrative test case is proposed as Figure 8 shows. Here, the channel is resolved with a CFD&HT model while the room is modeled with a global single well-mixed zone model. The channel which needs more computational resources for CFD&HT analysis is resolved with processors 1, 2 and 3, while the other objects like openings and the room are resolved on processor 4 as shown in the same Figure 9.

$T_{\text{hot}}=301\text{K}$ and $T_{\text{cold}}=296\text{K}$ are cold and hot temperatures channel sides, while the rest of the surfaces are adiabatic. $Ra=1.04 \times 10^{10}$ and $Pr=0.71$ are the non-dimensional parameters. The inflow at the bottom of the channel and the outflow at the top of the channel is put as the boundary condition for the room which adjusts itself to both the mass flow rates. The room model assumes a single well mixed zone. A compressible flow large eddy simulation (LES) model is used for the air flow movement in the channel.

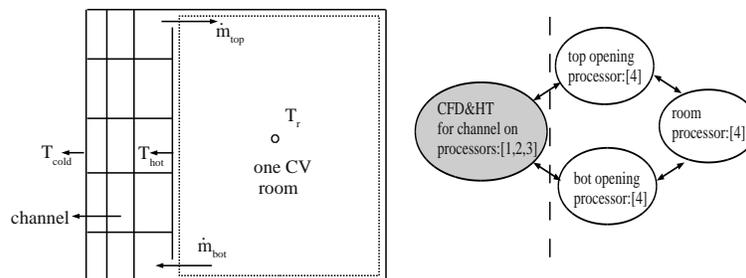


Fig. 9 Schematics of the solved case. Processors distribution of the case.

Figure 10 shows the evolution of the temperature in the room. All temperature values are non-dimension respect to the highest temperature 301K. Figure 11 shows the evolution of the temperature field with time. It can be seen how the air near the hot wall starts rising and the flow develops over the entire channel with time.

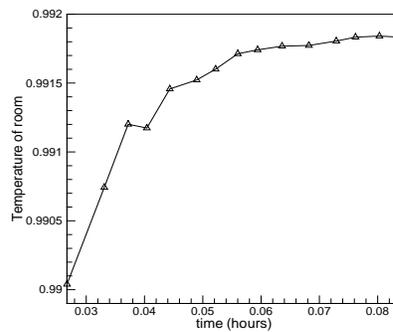


Fig. 10 CV room temperature evolution.

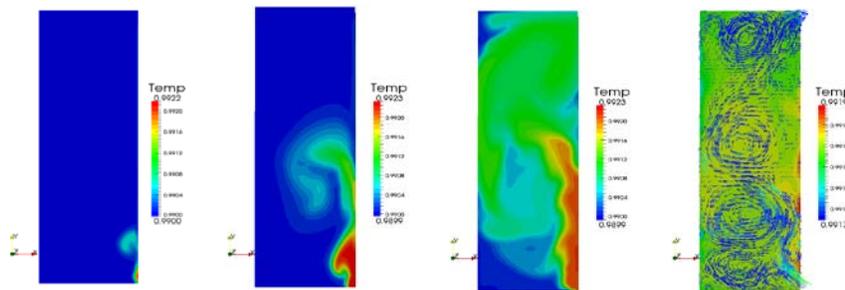


Fig. 11 Temperature maps after 40, 80, 120 and 300 seconds, respectively.

7. CONCLUSIONS

A modular object-oriented tool with parallel infrastructure has been presented for the simulation of buildings which also has the possibility to integrate CFD & HT models for required elements of a building system. The simulation of the Heat, Air and Moisture and VOC is taken into account coupling different levels of modelization. Verification and validation of the numerical platform is presented. Finally, an illustrative case is presented in order to show the possibilities that this tool offers.

NOMENCLATURE

A	area	(m ²)
C	bulk heat capacity	(J/kg K)
C _m	VOC concentration in the material	(kg/m ³)
C _{mb}	VOC concentration at the material boundary	(kg/m ³)
C _{as}	VOC concentration in the near material surface air	(kg/m ³)
C _g	generation of VOC in the room	(kg/m ³ s)?
C _{p,a}	heat capacity of dry air	(J/kg K)
C _{p,v}	heat capacity of water vapor	(J/kg K)
CFD	computational fluid dynamics	
C _r	VOC room concentration	(kg/m ³)
D _l	liquid conductivity	(s)
D _m	VOC diffusion coefficient of the material	(m ² /s)
h _{fg}	latent heat of condensation/evaporation	(J/kg)
h _m	mass transfer coefficient	(m/s)
K _p	material/air partition coefficient	
m _e	mass flow rate of dry air	(kg/s)
m _p	moisture production rate	(kg/s)
m _w	moisture from wall surfaces	(kg/s)
M	molecular weight of water	(kg/mol)

p	partial pressure	(N/m ²)
p _{sat}	saturation pressure	(N/m ²)
Q _{ven}	ventilation rate	(m ³ /s)?
R	universal gas constant	(J/mol K)
R _v	specific gas constant for water vapor	(J/kg K)
T	temperature	(°C)
t	time	(s)
dt	time step	(s)
V	volume	(m ³)
w	water content	(kg/m ³)

Subscripts

amb	ambient temperature
e	external/outdoor air flow rate
r	room
w	wall surface
g	moisture generation

Greek letters

α	heat transfer coefficient	(W/m ² K)
β	moisture transfer coefficient	(s/m)
δ	vapor permeability	(s)
λ	thermal conductivity	(W/mK)
ø	relative humidity	
ρ	density of dry air	(kg/m ³)
ρ _w	density of water	(kg/m ³)
ρ ₀	density of dry material	(kg/m ³)
θ	sorption capacity $\partial w / \partial \theta$	(kg/m ³)

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