

## **SIMSPARK: AN OBJECT-ORIENTED ENVIRONMENT TO PREDICT COUPLED HEAT AND MASS TRANSFERS IN BUILDINGS**

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### ABSTRACT

The non-uniform behavior of the air inside a room, which is important in comfort analysis, can be evaluated by zonal models. While not as fine-grained as CFD simulation, they do give useful information about temperature and moisture distributions that is not available from lumped-parameter models. Therefore, we have developed a tool, called SimSPARK, to automatically build dynamic zonal simulations of a building zone. Its model library includes different models to describe heat and moisture transfers across the building zone envelope, with two of them taking into account moisture adsorption/desorption by building materials. In this work, we describe in details the SimSPARK architecture and, the current zonal model library. To illustrate the applicability of this tool, we compare two zonal models including adsorption and desorption processes with one that ignores these phenomena, in a ventilated room composed of 27 zones. The results indicate that adsorption/desorption by building materials does affect indoor air behavior in a hot and humid climate.

### INTRODUCTION

Thermal comfort assessment requires details in space and time of indoor air conditions. Computation Fluid Dynamics (CFD) methods can, in principle, provide these necessary details but cannot yet, practically, be applied to long-time period (e.g. seasonal or annual) analyses nor to large complex buildings.

An alternative method that may serve these needs is the zonal method (Inard et al., 1996; Wurtz et al., 1999). It involves subdividing rooms of a building into a small number of control volumes or zones, defining appropriate zone-to-zone flow relations, establishing intrazone pressure field assumption (e.g. hydrostatic condition) and applying macroscopic conservation principles to

these control volumes to characterize simultaneous heat and mass transfers in confined spaces.

The resulting set of non-linear coupled equations is solved simultaneously by the object-oriented simulation environment, SPARK<sup>1</sup> (Sowell and Haves, 2001). This environment allows the user to easily test new models and share his library with other modelers. However, for large problems, building a SPARK simulation can be long and error prone. Therefore, we have developed a tool, called SimSPARK, to automatically generate simulations of specific building zone geometry, select the physical models to be used, and visualize results.

In this paper, we describe in details the current zonal model library and, the SimSPARK architecture. Then, we apply SimSPARK to study the influence of different models of coupled heat and moisture transfers in walls, on indoor air behavior of a ventilated room composed of 27 zones. Finally, we show the temperature and moisture distributions obtained from the different models.

### APPROACH

To make easier the development of a zonal model to predict temperature and moisture fields in a building, the latter was divided into two different domains: the indoor air and the building envelope. The zonal model is therefore composed of two different sub-models that correspond to the two domains in that the building was divided.

#### **Indoor air sub-model**

In the indoor air sub-model, the room is subdivided into a number of control volumes or *cells* in which the moist air properties are assumed to be homogeneous. The only exception is pressure that varies hydrostatically. Mass and

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<sup>1</sup> Simulation Problem Analysis and Research Kernel

thermal energy balances are applied to each cell, with their physical characteristics being coupled by the perfect gas law. The inter-cell airflow due to the pressure difference between two adjacent cells is based on the orifice flow equation (issues related with this formulation are discussed in Mora et al., 2003), while diffusive water vapor flow is based on the Fick's law. Finally, the inter-cell thermal energy flow is determined by common convection and diffusion relationships between two adjacent cells. All equations concerning this sub-model are detailed in Mendonça et al. (2002).

### Building envelope sub-model

The building envelope can be modelised by four envelope sub-models, with different degrees of complexity.

#### No heat nor moisture transfer

This is the simplest envelope sub-model. It supposes that there is *no heat nor moisture transfer through the material envelope*. Hence, it just allows to impose constant temperature to the walls. This sub-model will not be employed in this paper.

#### Only heat transfer

This second sub-model *neglects moisture adsorption and desorption* by building materials. Consequently, it calculates only the heat that crosses the material envelope, using the well-known conduction equation.

#### Coupled heat and moisture transfers (moisture transport in vapor phase)

This sub-model is described by the "Evaporation and Condensation theory" (Kerestecioglu and Gu, 1990), which is *valid in the materials hygroscopic range (pendular state)*. Moisture is supposed to migrate through the porous material in its vapor phase, as shown in the mass balance equation:

$$\varepsilon \frac{\partial \rho_{wv,s}}{\partial \tau} + \rho_0 \frac{\partial U_s}{\partial \tau} = \varepsilon D_{wv,s} \frac{\partial^2 \rho_{wv,s}}{\partial x^2} \quad (1)$$

with the following boundary conditions:

$$-\varepsilon D_{wv,s} \left. \frac{\partial \rho_{wv,s}}{\partial x} \right|_{x=0,i} = h_{M,i} (\rho_{wv,i} - \rho_{wv,a}) \quad (2)$$

$$-\varepsilon D_{wv,s} \left. \frac{\partial \rho_{wv,s}}{\partial x} \right|_{x=L,e} = h_{M,e} (\rho_{wv,a} - \rho_{wv,e}) \quad (3)$$

The other governing equation, Eq. (4), states that the temporal variation of energy is equal to the net

amount of heat received/lost by conduction plus the energy liberated/consumed during the sorption phenomena.

$$\rho_{\text{eff}} C p_{\text{eff}} \frac{\partial T_s}{\partial \tau} = \lambda_{\text{eff}} \frac{\partial^2 T_s}{\partial x^2} + L v \rho_0 \frac{\partial U_s}{\partial \tau} \quad (4)$$

The boundary conditions corresponding to equation (4) are:

$$-\lambda_{\text{eff}} \left. \frac{\partial T_s}{\partial x} \right|_{x=0,i} = q_{\text{SWL},i} + q_{\text{LWL},i} + h_{T,i} (T_i - T_a) \quad (5)$$

$$-\lambda_{\text{eff}} \left. \frac{\partial T_s}{\partial x} \right|_{x=L,e} = q_{\text{SWL},e} + q_{\text{LWL},e} + h_{T,e} (T_a - T_e) \quad (6)$$

As thermodynamic equilibrium is assumed to hold, the state variables are coupled by the equilibrium sorption isotherm.

In this work, the effective properties  $\rho_{\text{eff}}$ ,  $C p_{\text{eff}}$  and  $\lambda_{\text{eff}}$  are supposed to be constant, while the vapor diffusivity of the material varies as follows:

$$D_{wv,s} = \left( \frac{D_{wv,ma}}{\tau_0} \right) \frac{P_{ma,s}}{P_{ma,s} - P_{wv,s}} \quad (7)$$

with,

$$D_{wv,a} = \left( \frac{9,26E-4}{P_{ma,s}} \right) \frac{T_s^{2.5}}{T_s + 245} \quad (8)$$

#### Coupled heat and moisture transfers (moisture transport in liquid and vapor phases)

The last envelope sub-model, based on Mendes' works (Mendes, 1997), considers that moisture migrates through the porous material in both liquid and vapor phases. Then, it is not limited to low moisture contents. In other words, it is *valid for porous materials in the pendular and funicular states*.

Liquid phase is supposed to move by capillary flow while vapor phase is supposed to be diffused due to partial pressure gradients. Considering these hypothesis, the governing moisture balance equation is given by:

$$\frac{\partial \theta_s}{\partial \tau} = \left( D_T \frac{\partial^2 T_s}{\partial x^2} + D_\theta \frac{\partial^2 \theta_s}{\partial x^2} \right) \quad (9)$$

The boundary conditions for this equation are given by:

$$-\rho_l \left( D_T \frac{\partial T_s}{\partial x} + D_\theta \frac{\partial \theta_s}{\partial x} \right) \Big|_{x=0,i} = h_{M,i} (\rho_{wv,i} - \rho_{wv,a}) \quad (10)$$

$$-\rho_l \left( D_T \frac{\partial T_s}{\partial x} + D_\theta \frac{\partial \theta_s}{\partial x} \right) \Big|_{x=L,e} = h_{M,e} (\rho_{wv,a} - \rho_{wv,e}) \quad (11)$$

The governing energy balance equation, states that the temporal variation of energy is due to the net amount of heat received/lost by conduction and the phase change within pores.

$$\rho_0 C p_{\text{eff}} \frac{\partial T_s}{\partial \tau} = \lambda_{\text{eff}} \frac{\partial^2 T_s}{\partial X^2} + L v \rho_1 \left( D_{T, \text{wv}} \frac{\partial^2 T_s}{\partial X^2} + D_{\theta, \text{wv}} \frac{\partial^2 \theta_s}{\partial X^2} \right) \quad (12)$$

with the following boundary conditions:

$$-\lambda_{\text{eff}} \frac{\partial T_s}{\partial X} - L v \rho_1 \left( D_{T, \text{wv}} \frac{\partial T_s}{\partial X} + D_{\theta, \text{wv}} \frac{\partial \theta_s}{\partial X} \right) \Big|_{x=0, i} = q_{\text{SWL}, i} + q_{\text{LWL}, i} + h_{T, i} (T_i - T_a) + L v \left[ h_{M, i} (\rho_{\text{wv}, i} - \rho_{\text{wv}, a}) \right] \quad (13)$$

$$-\lambda_{\text{eff}} \frac{\partial T}{\partial X} - L v \rho_1 \left( D_{T, \text{wv}} \frac{\partial T}{\partial X} + D_{\theta, \text{wv}} \frac{\partial \theta}{\partial X} \right) \Big|_{x=L, e} = \dot{q}_{\text{SWL}, e} + \dot{q}_{\text{LWL}, e} + h_{T, e} (T_a - T_e) + L v \left[ h_{M, e} (\rho_{\text{wv}, a} - \rho_{\text{wv}, e}) \right] \quad (14)$$

The equilibrium sorption isotherm closes the system of equations.

Similar to the third sub-model, the effective properties ( $Cp_e$  and  $\lambda_e$ ) are considered to be constant, as well as, all transport coefficients ( $D_T$ ,  $D_\theta$ ,  $D_{T, \text{wv}}$  and  $D_{\theta, \text{wv}}$ ).

We note that the three envelope sub-models expressed as partial differential equations were discretized using a finite difference method.

We also note that, the short ( $q_{\text{SWL}}$ ) and long wave radiation ( $q_{\text{LWL}}$ ) exchanged among inside building surfaces are calculated using the “fictive enclosure method” (Walton, 1980). In general, this method considers that each surface of the room envelope (in our case, each zone face adjacent to the building envelope) exchanges radiation only with a second surface that is the equivalent of all other surfaces of the envelope.

All these sub-models (indoor air + envelope) have been implemented in the simulation environment SPARK described in the next section

### SIMSPARK: A SPARK PROBLEM DRIVER

SimSPARK is an intuitive interface to automatically build a dynamic zonal simulation of a building zone including convective and radiant exchanges at surfaces, coupled heat and moisture transfers through the envelope and moisture adsorption/desorption by envelope materials.

This tool has been built as a preprocessor of the simulation environment SPARK

### **The object-oriented simulation environment: SPARK**

SPARK is a general simulation environment that supports the definition of simulation models and solution of these models via a robust and efficient differential/algebraic equation solver (Sowell and Haves, 2001). In SPARK, the modeler describes the set of equations defining a model as equation-based objects. At the lowest level, an atomic object characterizes one equation and its variables. Then, macroscopic objects can be created as an assembly of various atomic or macroscopic objects. The entire model is built by connecting the different necessary objects. If one class of objects needs to be reused, it can be instantiated as many times as required, without any additional effort.

At this stage, it is necessary to observe that the model is input/output free. The particular problem to be solved is then described by imposing the adequate input data (boundary and initial conditions) and by specifying the variables to be solved. So in this environment it is not necessary to order the equations or to express them as assignments statements (algorithms) in opposition to conventional modular environments such as Matlab/Simulink (Mendes et al., 2001) or TRNSYS (Hiller et al., 2001).

SPARK uses a mathematical graph of the model to decompose it as strong components to be solved independently. Within each component, SPARK finds the appropriate function call sequence to get the solution. If no direct sequence is possible, as evidence by a cyclic problem graph, a small “cut set” is determined so as to minimize the number of variables involved in the Newton-like iterative numerical solution process. As a result, this decreases the size of the Jacobian matrix involved in the Newton iteration within the component. Consequently, the way SPARK handles the solution of coupled nonlinear equations makes it a fast solver for building energy simulation problems.

Since the “cut sets” of variables have been identified, the problem specification file is converted into a C++ program which is then compiled, linked and executed to solve the problem for given boundary and initial conditions.

We use SPARK to implement the solution of zonal models using the models presented in the previous section. The corresponding set of equations consists of a class library that has been organized using hierarchical relations between the different classes. In the next two subsections we'll describe the organization of this library, and then the procedure to build a specific problem from this library by using SPARK.

### Our zonal model class library

In the first section, we presented the different equations involved in the zonal modeling approach to predict temperature and moisture fields in a building zone. As said earlier, the model to be simulated within SPARK is built by assembling various atomic and macroscopic objects, each one describing a part of the overall set of equations.

Figure 1 presents the directory tree of the class library that implements the different models presented in the previous section. The HVAC components won't be presented since they are not used in these paper simulations. The interest of this hierarchical ordering is to make easier the maintenance of a large number of classes and to enable the storage of elementary model classes at a unique place. This feature is important for model selection. Before going deeper in the description of SimSPARK, we introduce, through a simple example, the way we build a simulation of a building zone using the zonal approach.

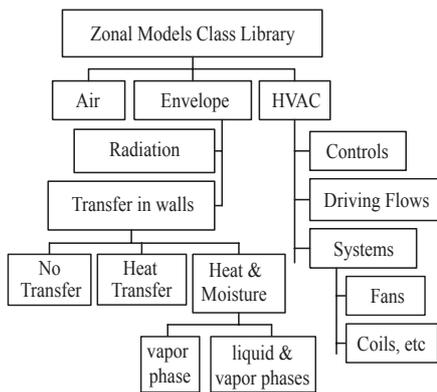


Figure 1 Class library diagram

### How we build a zonal model in SPARK

We chose a simple two-dimensional problem to illustrate the construction of a dynamic building zone simulation using SPARK. The problem geometry is described in figure 2. It consists of a

2-dimensional room with two openings, partitioned in four cells.

The simulation construction consists of declaring the model classes to be used and constructing the links between their data structures. Figure 3 presents a two-dimensional view of the different classes and the connections required for the specification of this problem geometry. The four cells are separated by four objects called interfaces and connected to the external environment through wall and opening elements. As we can see, two connection levels are necessary. The first one provide connections between adjacent cell and wall elements for convective and conductive modeling, while the second level connects the different wall surfaces for the modeling of radiant exchanges within the building zone (the radiant heat transfer model is represented in dotted line in figure 3).

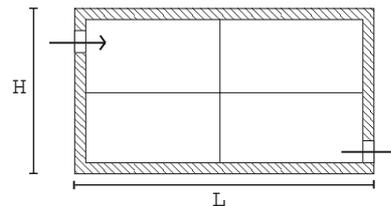


Figure 2 Example geometry

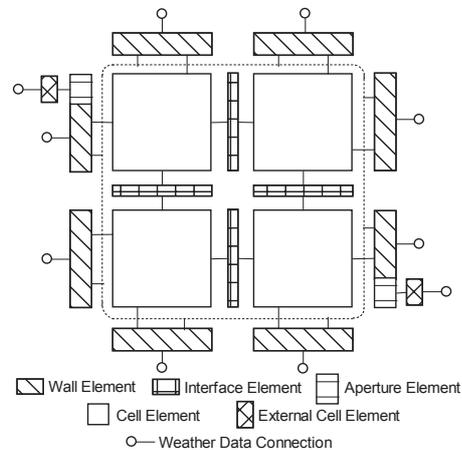


Figure 3 A 2D view of the object assembly

In the case of small openings, the aperture model is aggregated to a conventional wall element since the opening covers only partly the geometrical section of the element, then they compose a new kind of classes that inherits all standard wall elements characteristics. Figure 4 presents this new kind of classes compared with the standard wall element class. The standard wall element is composed of two faces bounding the multilayer core element. The inner face class implements the

heat mass convection model. The outer one embeds the same model, augmented by the external radiant heat transfer model.

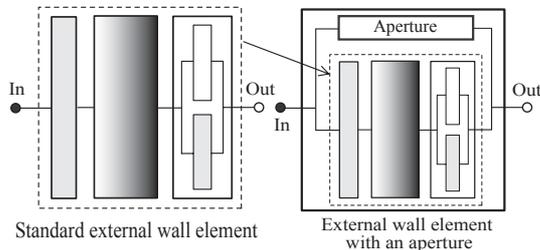


Figure 4 Two wall element classes

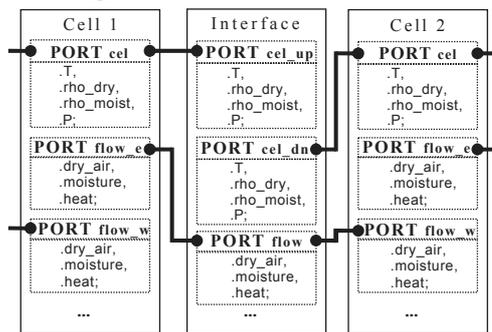


Figure 5 interface/cells example links

The connections between the different objects are made via fixed data interfaces that can be seen as vector data structures. A cell is characterized by the state variables of air such as pressure, temperature, air and moisture densities, etc. The *interface* class computes flow data such as mass flow rates, heat flux based on the data of the two cells it separates. Finally, a wall element determines the same flow variables based on some external conditions, and the values of its adjacent cell.

Figure 5 presents the fixed data interfaces as well as their connections in the case of two *cells* separated by a vertical *interface*. This mechanism is then generalized to the whole simulation domain so as to provide the connections between the different objects used including wall elements.

Since all object data structures are connected and the input/unknown variables specified, the problem description is set up. Then SPARK analyses the problem to identify the function call sequence to get the solution, compiles the atomic class functions, and implements a C++ file to be linked with the solver and class libraries to build the executable aimed at computing the solution.

However, as the number of objects used to describe the problem increases dramatically with the domain mesh density, the problem description

process can be error prone. So we developed a problem generator to automate this process. The next subsection describes this SPARK problem driver.

## SimSPARK

SimSPARK, as mentioned earlier is a SPARK simulation driver. It is able to generate the zonal room model with some selected specific models (e.g. coupled heat and mass transfers through wall materials), to pre-process weather data files and to post-process the results. These different features are discussed in this subsection.

### Problem generation automation

The problem generation consists of automating the generation of the SPARK problem specification file based on its conceptual description. The latter specifies the grid density on each direction, the grid dimensions, the types of building elements used and their location in the simulation domain (e.g. apertures, ventilation inlets/outlets, glazing etc.). All these data are stored in a structured data tree based on the XML<sup>2</sup> language. This language is powerful since many tools are developed around it. Our main interest here is to make the conceptual description easy to share between different computer codes with low implementation efforts. And in our opinion this can bring many advantages in long term developments, such as exchanging data through the web.

### Model selection

As shown in the previous subsection, all major elements of the simulation domain (*cells*, *interfaces*, and *wall* classes) have the same fixed data interface whatever is the model implemented in the class. That way, we are able to interchange models without changing the problem description file. So the model selection is only made by giving to SimSPARK the corresponding set of directories of classes. Then this information is stored in the conceptual description of the problem.

This model selection mechanism has proven to be very powerful for new model development and validation. To do so, one can develop his new particular model satisfying the data interface standard, integrate it to the library, and then select it to build the coupled simulation.

<sup>2</sup> eXtensible Markup Language

### Input data generation

In the previous simple simulation example, a 2x1x2 mesh using the envelope model with heat transfer only, the number of unknowns is 808 while the number of input data is 285. So it can be complex to manage so many input data when the domain grid is denser. To overcome this problem, we developed an input data preprocessor, so that all input variables can be set in a flexible way. All dynamic values related with the external environment are computed from a weather data file.

### Run and solver controls

The different run parameters as well as the solver settings are prescribed for each simulation. We also developed a mechanism to generate data used by SPARK to initialize dynamic variables as well as their derivatives.

### Front-end for pre- and post-processing

Figure 6 presents the SimSPARK's graphical user interface (GUI) aimed at giving some high level functions to quickly setup the main parameters of the simulation (the room partitionning, the models and corresponding library directories used for the envelope modeling, the names of the classes used from these directories) and then build and run the simulation. The GUI for post-processing is also linked to the last tab. SimSPARK is highly configurable, so that new elementary models can immediately be tested and coupled to the overall zonal model library.

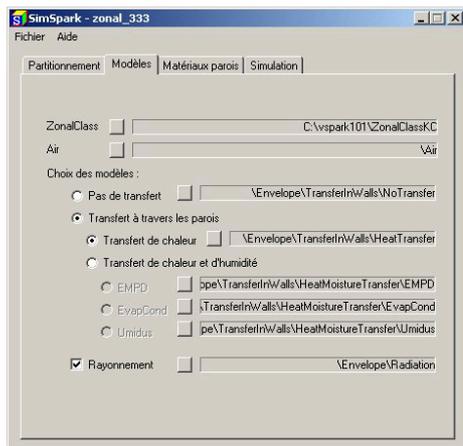


Figure 6 SimSpark GUI

## APPLICATION

With the double objective of showing the applicability of SimSPARK and studying the influence of hypothesis of different envelope models on indoor air behavior, we employed

SimSPARK to simulate a single room using three different zonal models.

These models, called Model 1, Model 2 and Model 3, are composed of the indoor air sub-model and an envelope sub-model as shown in table 1.

Table 1. Models description

	Envelope
Model 1	Only heat transfer
Model 2	Coupled heat and moisture transfers (moisture transport in vapor phase)
Model 3	Coupled heat and moisture transfers (moisture transport in liquid and vapor phases)

### Studied case

In this studied case, we tried to represent, in an idealized and simple way, an office in which one of its façades is surrounded by a hot and humid environment while the others are in contact with conditioned spaces.

The figure 7 shows a sketch of this office with the dimensions of the 27 zones in that it was divided and, the outdoor environment conditions. As we can see, the room is ventilated by an opening at the top of the West side and another at the bottom of the opposite side.

Initially, indoor, outdoor environment and conditioned spaces are in equilibrium at  $t = 24^\circ\text{C}$  and  $\phi = 50\%$  ( $\rho_{wv} = 0,011 \text{ kg/m}^3$ ), as well as the room envelope. All conditioned spaces are maintained at  $t = 24^\circ\text{C}$  and  $\phi = 50\%$  during the 44 hours of simulation. In the other hand, the outdoor environment follows the temperature and relative humidity distributions given in figure 7.

Air enters the room at 1 ACH by the West opening at outdoor air conditions. However, the ventilation is cut at time  $\tau = 12\text{h}$ .

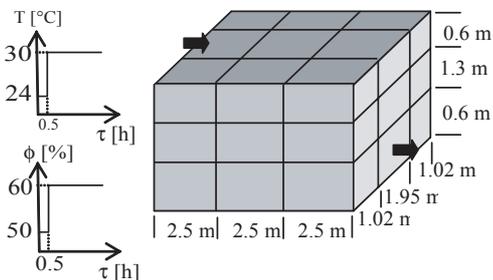


Figure 7 Sketch of the studied room.

To give emphasis to sorption processes, the room envelope (thickness = 10 cm) is constituted of a high hygroscopic material (Mortar) with the dry-basis properties given in table 2.

Additionally, in this case we don't take into account external and internal radiation exchanges. The convective heat and mass transfer coefficients are respectively 5.0 W/m<sup>2</sup>K and 0.005 m/s, for both external and internal surfaces.

Table 2. Dry-basis material properties for Mortar

Property	Cp <sub>0</sub>	ρ <sub>0</sub>	λ <sub>0</sub>	ε
Unity	J/kgK	Kg/m <sup>3</sup>	W/mK	%
Value	932	2050	1.92	18

## Results

Figures 8, 9 and 10 show respectively the calculated temperature, water vapor density and relative humidity distribution vs. time in the zone at the center of the room, for the models with or without moisture adsorption/desorption effects.

The temperature distribution obtained from models taking into account adsorption/desorption by the room envelope, are identical and higher than that provided by the other model. This difference is due to the higher temperature of the room envelope in models 2 and 3, as a result of the energy liberated during the adsorption process.

In the other hand, the model that neglects sorptive phenomena provided much higher water vapor density and relative humidity distributions than the other two models. In this case, the net amount of moisture that gets the room by the openings is accumulated in the room air, while in the other models an important amount of this moisture is adsorbed by the porous material of the envelope.

In the period where the room is not ventilated, we observe a slight difference between the profiles of water vapor density and relative humidity predicted by models 2 and 3. Because model 2 doesn't consider the liquid transport of moisture across the envelope, it provides higher moisture concentrations in the solid surface than model 3. Consequently, in model 2, an inferior amount of moisture can migrate from air to solid, and it predicts higher levels of water vapor density and relative humidity inside the room than model 3.

The results indicate that moisture adsorption/desorption by building material does affect the moisture field in confined spaces. They also indicate that, in this case with indoor low/middle moisture levels, the model valid in the material hygroscopic range gives similar indoor air behavior than the more complete model (not limited to the material hygroscopic range).

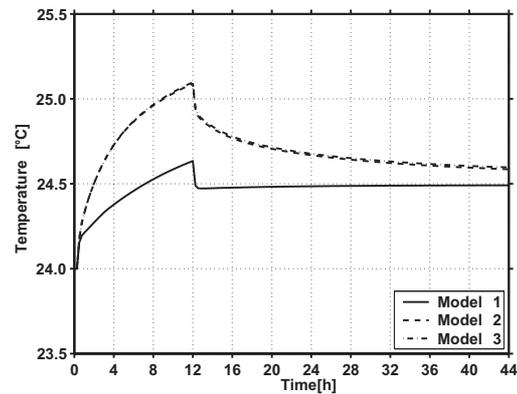


Figure 8 Temperature distribution

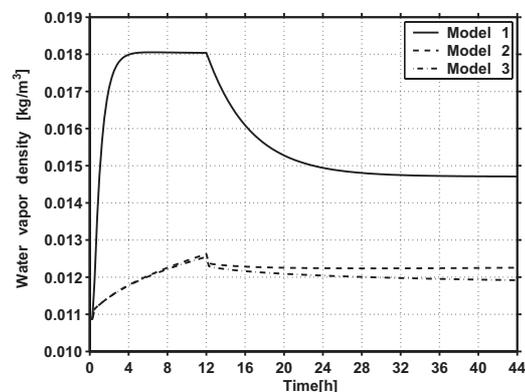


Figure 9 Water vapor density.

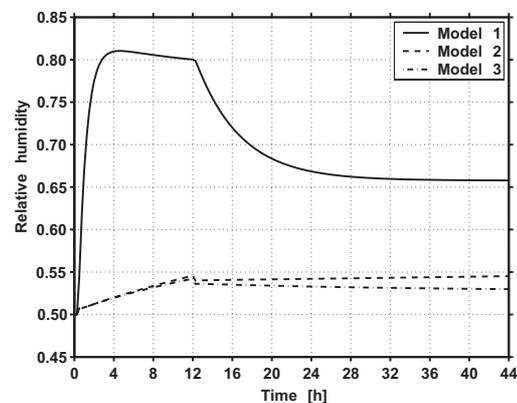


Figure 10 Relative humidity distribution.

## CONCLUSIONS

A tool to automatically build dynamic zonal simulation of a building zone, including a model library with different models to predict coupled heat and moisture transfers across the material envelope, has been proposed. This tool is especially well adapted to test different models due to its modular structure. We made use of this particular ability to compare two zonal models

taking into account adsorption and desorption processes with one that ignores these phenomena. The results indicated that moisture adsorption and desorption by building materials do affect dynamic moisture and temperature fields of a building zone in a hot and humid climate.

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## NOMENCLATURE

$C_p$	specific heat [J/kg°C]
$D_T$	mass transport (liquid plus vapor) coefficient associated with a temperature gradient [ $m^2/sK$ ]
$D_{Tv}$	vapor phase transport coefficient associated with a temperature gradient [ $m^2/sK$ ]
$D_{wv}$	water vapor diffusivity [ $m^2/s$ ]
$D_\theta$	mass transport coefficient associated with a moisture content gradient [ $m^2/s$ ]
$D_{\theta v}$	coefficient associated with a moisture content gradient [ $m^2/s$ ]
$h_M$	convective mass transfer [ $m/s$ ]
$h_T$	convective heat transfer [ $W/m^2K$ ]
$L$	length [m]
$L_v$	heat of vaporization [J/kg]
$P_{ma}$	total pressure of moist air [Pa]
$P_{wv}$	partial water vapor pressure [Pa]
$q$	radiant heat flow density [ $W/m^2$ ]
$T$	temperature [K]
$U$	moisture content [kg/kg]
$x$	distance [m]
$\varepsilon$	porosity
$\lambda$	thermal conductivity [W/mK]
$\rho$	density [ $kg/m^3$ ]
$\theta$	moisture volumetric content [ $m^3/m^3$ ]
$\phi$	relative humidity [%]
$\tau$	time [s]
$\tau_0$	tortuosity

### **Subscripts**

a	air
e	external surface
eff	effective
i	internal surface
l	liquid
ma	moist air
s	solid
LWL	long wave length
SWL	short wave length
wv	water vapor
0	dry porous material