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Numerical Simulation of Influence of Pores Sizes on Water Migration Dynamic in Concrete Building Walls

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Abstract

The sometimes extreme hydro-climatic stresses that buildings undergo can lead to significant deterioration which can lead to their collapse. The concern to realize durable works and ensuring a comfortable framework for the life of the occupants leads to seek effective solutions, as well for the new construction as for the renovation of old construction, answering the sempiternal problem of harmful action of water on buildings materials. This paper proposes a numerical simulation of moisture migration in concrete building walls, the aim being to highlight the influence of pore size on the kinetics of moisture migration, and its gradient in the wall. A mathematical model taking into account the mechanisms of moisture migration due to liquid moisture gradient and by vapor diffusion is proposed; the discrete formulation of the equation by the numerical scheme of Crank Nicolson is then carried out, and results from computer modeling using Matlab software version 7.10.0.499 (R2010a), show that pore size is a key parameter that influences the dynamics of moisture migration in the wall. Indeed, this parameter qualitatively and quantitatively influences the kinetics of moisture migration, as well as it gradient in the concrete wall.

Keywords: Mathematical modelling • Migration • Moisture • Numerical simulation • Pore size

Introduction

Construction materials are mostly parous media, and therefore subject to almost permanent moisture exchange with the environment around them. Among these construction materials, concrete is the most widely used in the world, and its water content due to its porous character, is an important parameter in terms durability of concrete structures. The influence of this porosity on the dynamics of moisture migration in concrete has been the subject of several publications. Thus, several authors have conducted research on the dynamics of water migration in concrete, going as far as modifying the porous structure of concrete thanks to various additives, in order to highlight the influence of these additives on the kinetics of migration and the moisture gradient in concrete. Ivan Lukic [1] shows that mineral additives increase the porosity of concrete, leading to high capillary absorption; Nilforoushan, and Reza [2] show that micro silica modifies pore size distribution and permeability of type V cement concrete; in fact, they show that the permeability of concrete with addition of micro silica decrease due to modification in pore size distribution. Similarly, Zineb Bajja [3] studied the microstructure of paste, mortars and concrete based on cement (CEM I), with silica addition, and shows that this addition modifies the microstructure and then influences the moisture transport properties. Moussa and others [4] show that the replacement of cement by iron powder improve the porosity and influence the water absorption of hardened concrete, especially the water absorption of the hardened concrete increase when the percent content of iron powder increase. Further on, Oltulu and Sahin [5], Mohseni and others [6] highlight the combined effects of nano-particles: nano- SiO_2, nano-Al_2O_3, nano- Fe_2O_3, nano- TiO_2 powder on the water absorption dynamic. Djima and others [7] show the increasing of water absorption of concrete as the lime treated palm kernel shell and sugarcane bogasse ash increase in the concrete mixture. Malab and others [8] made comparative study of the drying kinetics of self-compacting concrete with those of an ordinary concrete and sand concrete, and show the first one with macropores has lower drying kinetics than the second with mesopores; these conclusions are also confirmed by Goual and others results [9], who show that the presence of macropores considerably attenuates moisture transport of civil engineering materials in general. Similarly, according to Suchorab and others [10], laboratory experiment and computer modeling confirm strong capillary properties of aerated concrete. Some authors have carried out research on the composition parameters of concrete and their influence on the porous structure and the moisture transport properties in concrete; thus Ghashghali and Hassani [11] show that characteristics such as water permeability and porosity present a clear dependence on the size of aggregate and mix design parameters; in fact the porosity and consequently water permeability coefficient decrease when the constant water to cement ratio (W/C) of pervious concrete increase. Suchorab [12] shows that the impregnation of building materials in hydrophobic solutions modifies their porosity leading to decreasing in dynamics of capillary moisture migration. However, even if these works take into account the porosity of materials, they do not explicitly highlight the pore size influence in the moisture migration; in other words, they studies carried out are sometimes contradictory and do not clearly present the role of pore size on the moisture migration dynamic in porous material. This work is part of the overall objective of highlighting the influence of pore sizes on the moisture migration dynamics specifically to show the influence of pore size on migration kinetics and moisture gradient in the wall. So, this paper first presents a mathematical modeling of moisture migration in a single layer wall; then, the results of numerical simulation are analyzed.

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Material and Methods

To study the water migration in based of buildings, a mathematical model is proposed and then the numerical simulations are done with Matlab software. The method is based on finite differences and consists in defining an optimal geometry, space and time discretization, initial and boundary conditions.

Mathematical modelling

The model is based on the Philip and De Vries equations; moisture moves in the liquid and vapor state, with the moisture potential as the common potential. In this approach, the scale is assumed to be macroscopic, where the parous medium is considered to be an equivalent fictitious continuous medium; transfers are unsteady and one-dimensional; the different states (liquid and vapor) are in thermal equilibrium at any point in the parous medium; the capillary pores are assumed to be parallel and cylindrical. The liquid and vapor moisture flows are given according to Philip and De Vries [13] respectively by Equation (1) and Equation (2) while neglecting the gravity flow:

$$J_l = -D_l\overrightarrow{grad}(RH) - D_{lT}\overrightarrow{grad}(T) \tag{1}$$

$$J_v = -D_v\overrightarrow{grad}(RH) - D_{vT}\overrightarrow{grad}(RH) \tag{2}$$

J_1 and J_V represent the liquid and vapor moisture flow respectively, D_1 and D_V respectively the liquid and vapor moisture diffusion coefficients. D_{1T} and D_{VT} respectively the liquid and vapor moisture diffusion coefficients due to temperature gradient. T the temperature and RH moisture content (relative humidity).

At the liquid-gas thermodynamic equilibrium, Thomson's equation [14] gives the relationship between relative humidity, temperature and pore radius as presented in Equation (3), and transformed to get Equation (4):

$$P_v / P_{0v} = RH = esp\left[(-2\times T_s \times \gamma_w \cos\beta)/(r\times R\times T)\right] \tag{3}$$

$$T = \left(-2\times T_s \times \lambda_w \times \cos\beta\right)/\left(r\times R\times \ln RH\right) \tag{4}$$

P_V and P_{0V} are respectively the vapor pressure and the saturated vapor pressure; Ts the surface tension; Y_W the molar volume of water; r the pore radius; R the perfect gas constant and β the water contact angle.

A coupling of Equation (1), Equation (2), and Equation (4) lead to Equation (5):

$$(\partial RH/\partial t) = F_1(RH)\times\left(\partial^2 RH/\partial x^2\right) + F_2(RH)\times(\partial RH/\partial x)^2 \tag{5}$$

With F_1 (RH) and F_2 (RH) the moisture migration coefficients, function of the moisture RH and given by the Equation (6) and Equation (7):

$$F_1(RH) = D_w - (D_T/T_0)\times\left(a/RH\times(\ln RH)^2\right) \tag{6}$$

$$F_2(RH) = (D_T/T_0)\times\left[\left(a\times(2+\ln RH)\right)/\left(RH^2\times(\ln RH)^3\right)\right] \tag{7}$$

Where a is a coefficient defined to simplify writing. D_W the moisture diffusion coefficients due to water content gradient. And D_T the moisture diffusion coefficients due to temperature gradient [13].

$$a = (-2\times T_s\times\gamma_w\times\cos\beta)/(r\times R) \tag{8}$$

$$D_w = D_l + D_v \tag{9}$$

$$D_T = D_{lT} + D_{vT} \tag{10}$$

Linearization

The computational of the homogeneous and nonlinear Equation (5) by the finite difference method requires to linearize it. An approximation is therefore made on the coefficients and, they are discrete and supposed known at time j and abscissa i. we then obtain Equation (11) and Equation (12):

$$F_1\left(RH_i^j\right) = D_w - (D_T/T_0)\times\left[a/\left(RH_i^j\times\left(\ln RH_i^j\right)^2\right)\right] \tag{11}$$

$$F_2\left(RH_i^j\right) = (D_T/T_0)\times\left[a\times\left(\ln RH_i^j+2\right)/\left(\left(RH_i^j\right)^2\left(\ln RH_i^j\right)^3\right)\right] \tag{12}$$

Geometry and discretization

The diagram in Figure 1 illustrates the spatial and temporal discretization of the studied geometry.

The progressive finite differences method is used to discretize moisture flow, given by Equation (13); and the centered finite differences method discretize the moisture gradient, given by Equation (14)

$$\partial RH(x,t)/\partial t = \left(RH_i^{j+1} - RH_i^j\right)/T_2 \tag{13}$$

$$\partial^2 RH(x,t)/\partial t = \left(1/h^2\right)\times\left(RH_{i+1}^j - 2RH_i^j + RH_{i-1}^j\right) \tag{14}$$

With T_2 and h respectively the temporal and spatial discretization rates, defined by Equations (15) and Equation (16):

$$T_2 = t_{max}/N_2 \tag{15}$$

$$h = e/N_1 \tag{16}$$

e is the wall thickness, t_{max} the duration of moisture migration, N_1 and N_2 respectively the number of space and time steps.

Discrete formulation of the equation by Crank Nicolson scheme

For the discrete formulation of Equation (5), the second coefficient F_2 (Θ) is

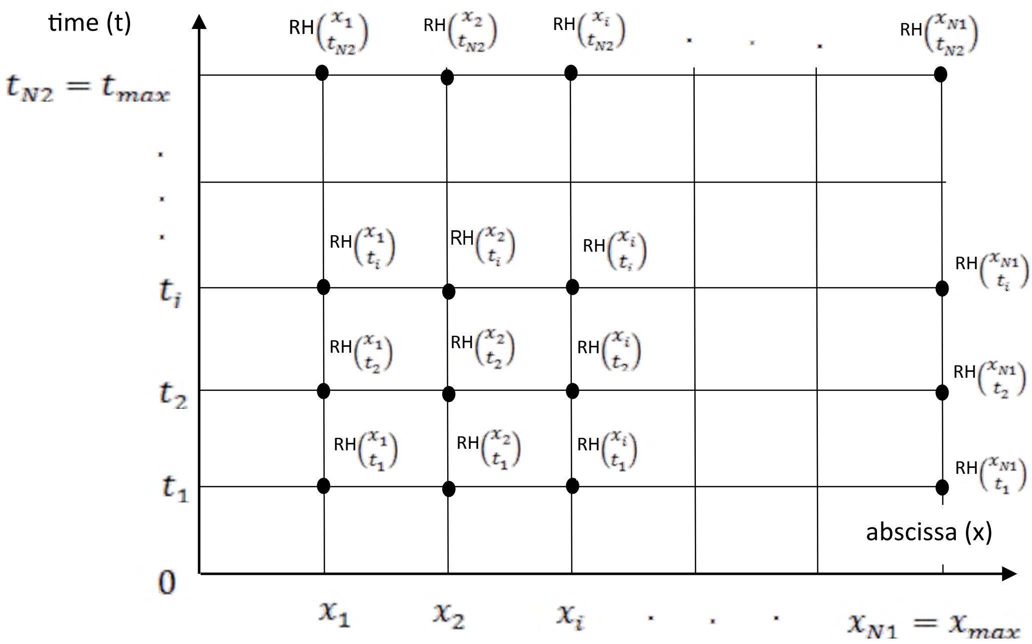

Figure 1. Spatial and temporal discretization.

excluded because its influence on the migration dynamics is negligible. Thus, the discrete scheme of Crank Nicolson, of Equation (17) leads to the algebraic equation system, Equation (18):

$$\left(\partial RH / \partial t\right) = F_1\left(RH\right)\times\left(\partial^2 RH / \partial x^2\right) \quad (17)$$

$$\left[M_2\right]\left\{RH^{j+1}\right\}+\left\{N_{ak}\right\}=\left[M_1\right]\left\{RH^{j}\right\}+\left\{N_{al}\right\} \quad (18)$$

$[M_1]$ and $[M_2]$ are the material characteristics matrix. The matrix of boundaries conditions are given at time j and j+1 respectively by $\{N_{al}\}$ and $\{N_{ak}\}$

Initial and boundaries conditions, calculation parameters

The initial conditions and the boundaries conditions in moisture, applied to the geometry are defined as follows:

$$\text{For } x=0,\ RH(0,t)=RH_0(t)\ \forall t\geq 0 \quad (19)$$

$$\text{For } x=\infty,\ RH(\infty,t)=RH_0(t)\ \forall t\geq 0 \quad (20)$$

$$\text{For } t=0,\ RH(x,0)=RH_i(t=0)\ \forall x \quad (21)$$

The numerical values of the parameters used in this simulation come from Bordachev's work on moisture calculation analysis and injection methods in brick masonry walls, where he shows that the revetment based on a material with high porosity or its injection into the wall basement, considerably limits the moisture migration in the wall [15]. Furthermore, some numerical values of parameters were taken from Kiwan's work, on the reliability of energy performance in buildings [16]. Simulations are performed using Matlab software (version 7.10.0.499 (R2010a)), varying the pore size.

Results and Discussion

To highlight the influence of the pore size on moisture migration dynamic in porous wall, the map of Figure 2 show the spatial and temporal moisture distribution in the wall; while graphs of Figure 3, Figure 4 and Figure 5 respectively present the spatial and temporal evolution curves of this moisture, for different pore sizes. These curves are qualitatively in agreement with Abahri et al's contribution to the analytical and numerical study of combine heat and moisture transfer in parous building materials [17]; Fitsum et al's work on the transient model for coupled heat, air and moisture transfer through multilayered parous media [18]; Ketelaar et al's results on the comparison of diffusion coefficients from moisture concentration profile and drying curve [19]; and Nytsch-Geusenet et al's work on the object oriented language 'Modelica' for the monitoring of heat and moisture in the building [20]. The observed deviations can be justified by the boundary conditions and the moisture diffusion coefficient of the materials.

Moisture mapping in the geometry

The maps of Figure 2 show on the one hand a low diffusivity in the center of the wall, this independently of pores sizes; and on the other hand a moisture concentration attenuated over time, for smaller pores radius. This can be explained by the fact that the capillary pressure which leads to the moisture migration in the wall increases as the capillary radius decreases. Thus, at the end of the migration (final state), at hygrometric equilibrium the moisture concentration gradient in the wall is less important; and the migration kinetics leading to this equilibrium is increasing when the pore size decreases.

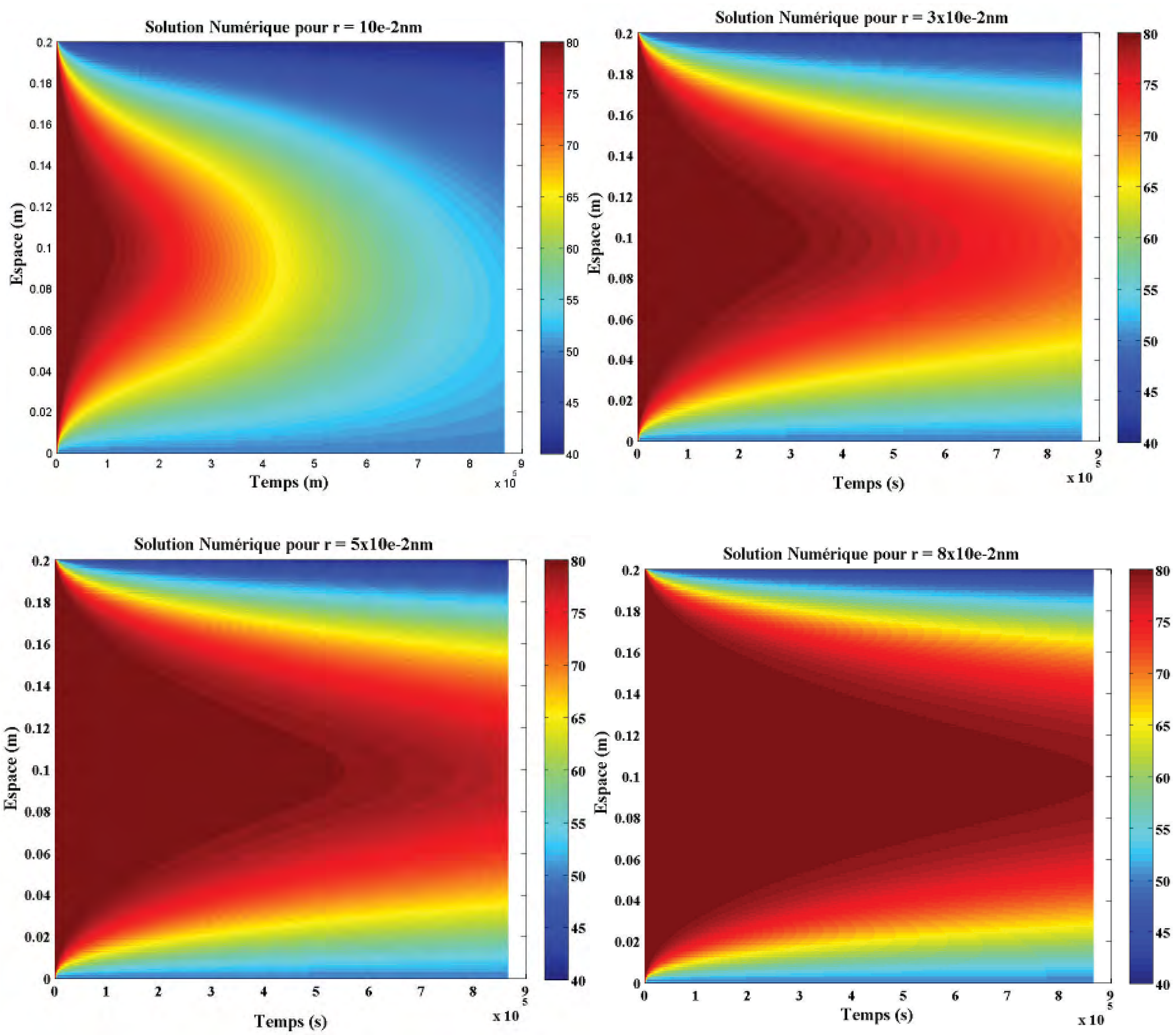

Figure 2. Moisture mapping for different pores sizes.

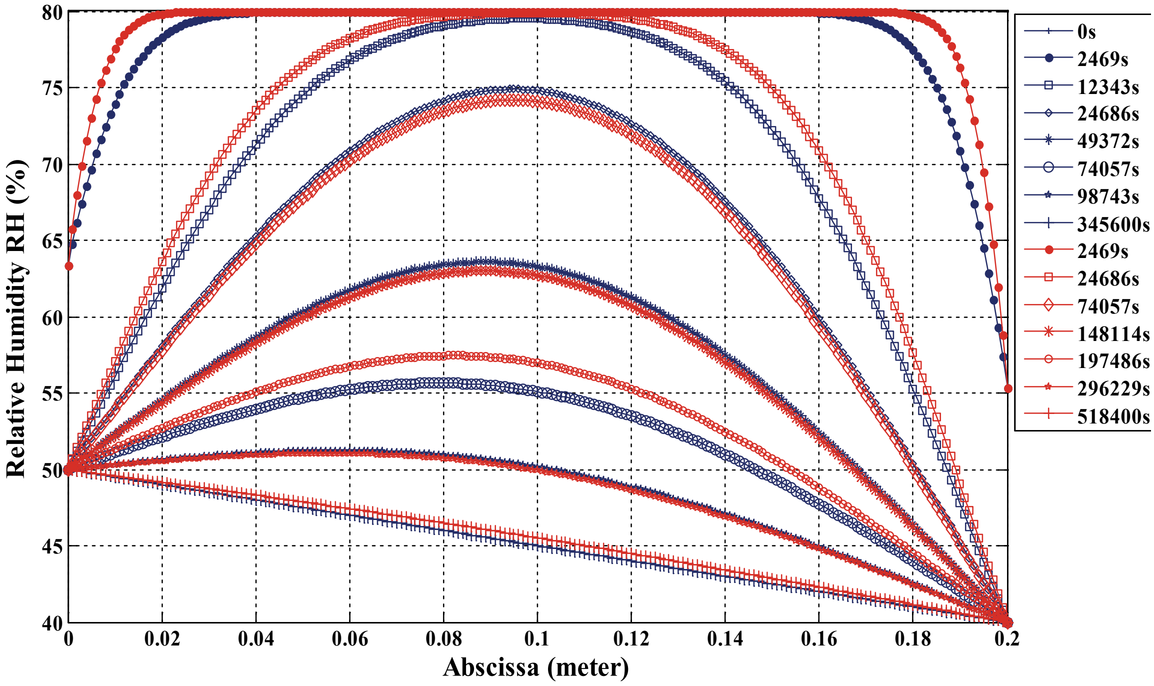

Figure 3. Spatial evolution of moisture at different times of simulation, for different pores sizes: 0.003 nm (red curves), 0.001 nm (blue curves).

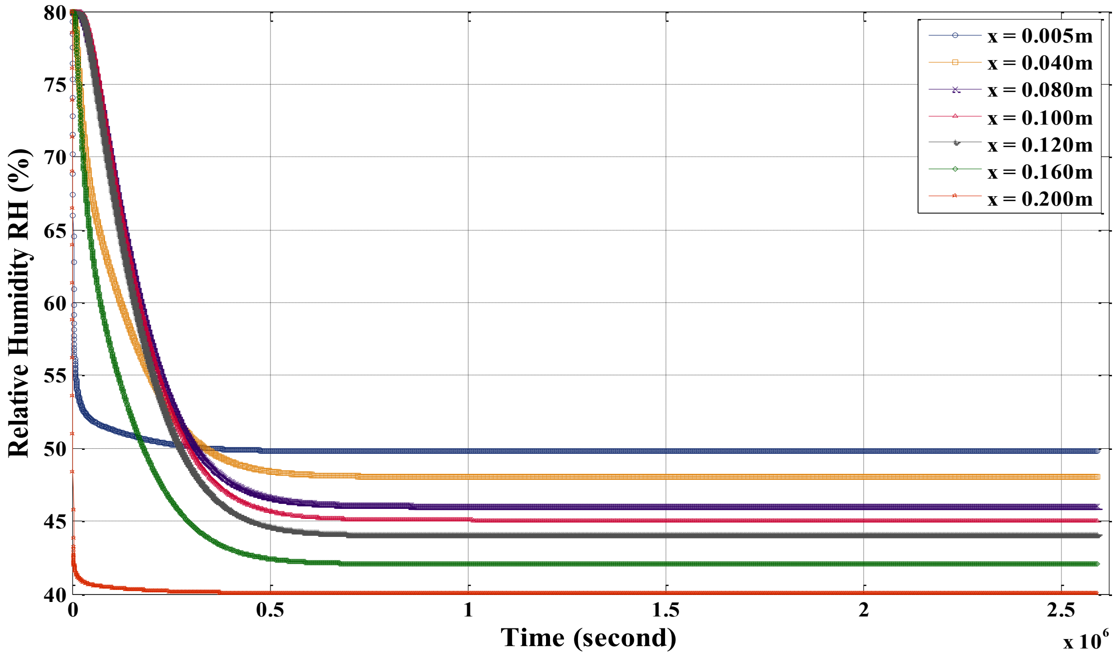

Figure 4. Temporal evolution of moisture at different abscissa of the wall for a pore radius of 0.001 nm.

Spatial evolution of moisture

The curves in Figure 3 illustrate for each time of simulation, the evolution of moisture content in the wall made of two different pores radius. The red curves correspond to the largest pore radius 0.003 nm, while the blue curves correspond to the smallest pore radius 0.001 nm. It appears a faster migration for the smallest pore radius; indeed, for this pore size, the moisture balance is reached after 345600s, against 518400s for largest pore radius. This result explicitly highlights the influence of pore size on the spatial evolution of moisture in the wall.

Temporal evolution of moisture

The result of Figure 4 presents the temporal evolution of moisture at different abscissa of the wall, for a pore radius 0.003 nm. The general shape of the curves is the same for each variation on each abscissa; the curves decrease more or less quickly, and then evolve in level (almost stationary evolution in time). Furthermore the slopes of these curves are increasingly steep, for abscissa which move away from the middle of the wall (x=0.10 m), and the plateau is quickly reached for the abscissas located near from the edges of the wall. Indeed, the slopes of these curves materialize the kinetics with which the material reaches its hygrometric equilibrium at a given abscissa in the wall. The diffusion is therefore faster at the edges of the wall than towards the inside thereof. This can be explained by the fact that the edges of the wall during the simulation time are influenced by the boundary conditions; their hygrometric balance is thus quickly reached compared to that of the middle of the wall.

Figure 5 above presents the temporal evolution of the moisture in the

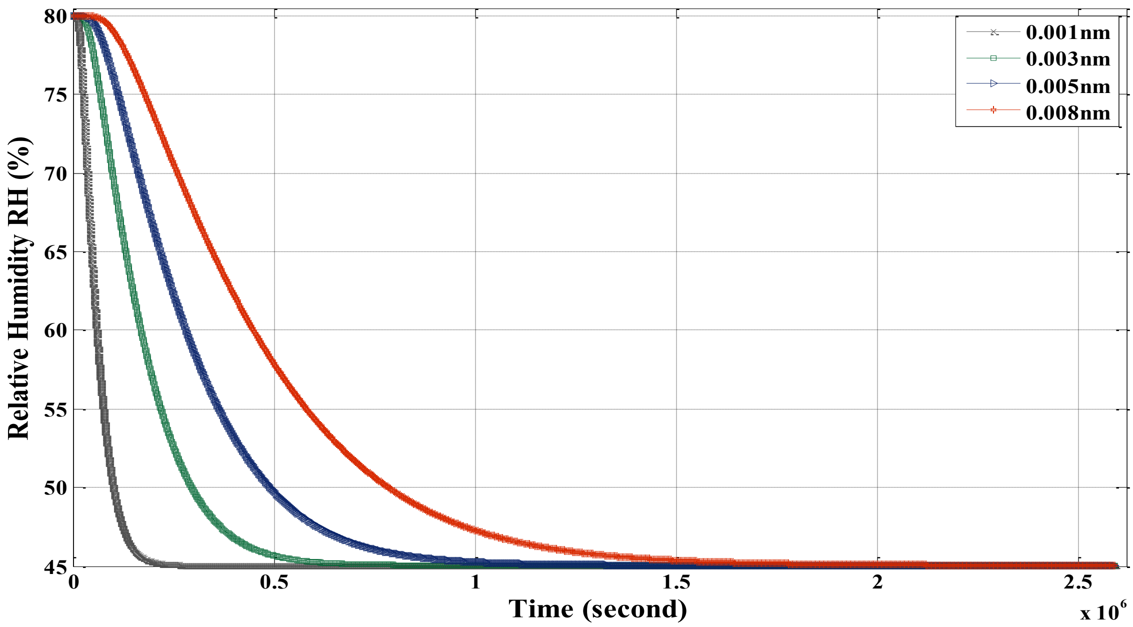

Figure 5. Temporal evolution of moisture in the middle of the wall, for different pores radius, 0.001 nm (black curve), 0.003 nm (green curve), 0.005 nm (blue curve) and 0.008 nm (red curve).

middle of the wall, for different pores sizes: 0.001 nm (black curve), 0.003 nm (green curve), 0.005 nm (blue curve) and 0.008 nm (red curve). The curves have the same decreasing appearance then evolve in level, reflecting a state of hygrometric equilibrium in the material. However, this state of equilibrium is quickly reached for the wall with the smallest pore size. Indeed around a duration of 250,000 s (72 h), this hygrometric balance is reached in the wall of porosity 0.001 nm; against a duration of 518,400 s (144 h) in the wall of pore size 0.003 nm, a duration greater than 1,875, 000 s (521 h) in the wall of pore size 0.005 nm, and a duration greater than 2 400 000 s (667 h) in the wall of pore size 0.008 nm.

The curves in Figure 5 illustrate the evolution over time, of the moisture in the wall, for different abscissas in the wall corresponding to two pores sizes. The curves in solid lines correspond to the largest pore size 0.003 nm, while the curves in dashed lines correspond to the smallest pore size 0.001 nm. These curves are qualitatively identical, decreasing in appearance and then evolving in level, reflecting a state of hygrometric equilibrium in the wall. However, regardless of the abscissa x, this equilibrium is reached quickly for the wall whose pore size is the smallest.

Conclusion

This paper presents a numerical simulation of moisture migration in concrete building walls, the influence of pore size on the dynamic of moisture migration has been highlighted, and it appears a low diffusivity in the center of the wall, this independently of pores sizes. Furthermore, a greater migration dynamic when the pores sizes decrease, means a greater kinetics of moisture migration and lower moisture gradient in the walls at the hygrometric equilibrium, for a decreasing pore size. These results find their applications in the choice of building materials their quality, their manufacture and their use for a better durability.

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