

# Modeling and Experimental Measurement of Mass Diffusion Coefficient in a Standard Cement Mortar under Isothermal Conditions

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## Abstract

The prevention of disease or assessment of the sustainability of building walls in a wet medium requires the study of the mass diffusivity in these walls. The aim of this work is to study the isothermal kinetics of a chemical space in a standard mortar. Water steam has already been the subject of multiple studies, the subject of this contribution is to model the mass diffusion of loaded free water, and the experimental determination of the apparent mass diffusion coefficient for different temperatures (20°C, 30°C and 40°C).

**Keywords:** Diffusion coefficient; modeling; cement mortar; isotherm.

## 1. Introduction

Damage to concrete structure walls in wet media is fundamentally due to the penetrating of aggressive agents in the porous network of the constitutive material. The water diffusion is a transport parameter on this spreading. Loaded water enters unsaturated concrete according to a diffusive process. The resulting multiform pathology (cracking, molds) affects not only the durability and

aesthetics of this material but also the environmental comfort of dwellers the occupants of these structures that are bounded by these walls.

The purpose of this paper is to establish an hygrothermal quantitative approach of climate threats (heat and water acting separately or together) [1] on the simple concrete walls (uncoated) with the aim of understanding the potential causes for rehabilitation, which are the origin of pathology, or in new works, which may give rise to the pathology to come in so far as sustainability [2] constructs is a concern economic and environmental front. The Economic Implications of repair or maintenance are substantial.

The computer codes used in the building walls design include the thermal diffusivity as a fundamental facture [3] while the mass transfer has also its importance in the analysis.

As determination of the diffusivity by conventional methods requires long and laborious steps, the conductivity method constitutes infact [4], a good alternative what requires less effort. With this method, the routine phase of the mass diffusion in this material is easily determined.

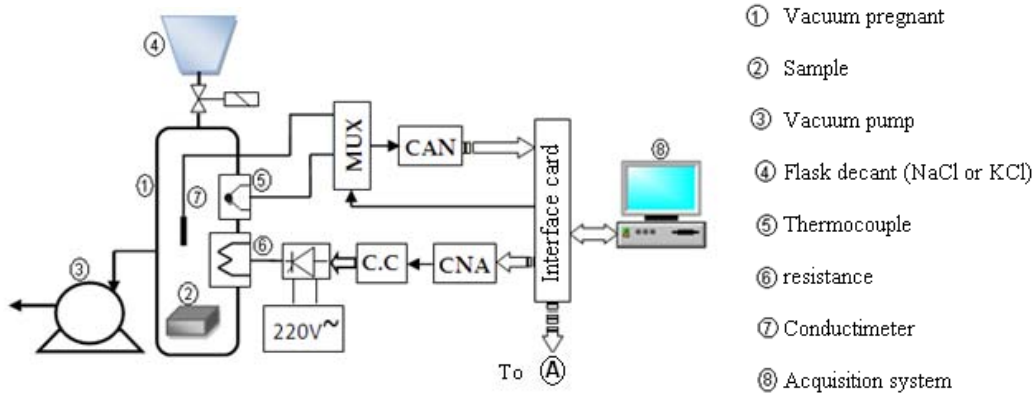
In this context we determine the apparent diffusion coefficient  $D_{app}$  of cementitious material by successive assessment starting from a mathematical model incorporating key entry as the reduced mass deduced from the experimental measurement of the conductivity of the solution permeating the porous material studied.

## 2. Material

The samples are of prismatic shape size (40x40x10) mm<sup>3</sup> mortar made up of standard-type composition similar to mortar 1 / 3 standard is 1350g using natural sand (0 / D: 0.315 to 1.25 mm. Standard EN 12620), 450g composed Portland cement (CPJ-CEM II Class 42.5) and 225g of mixing water free of impurities.

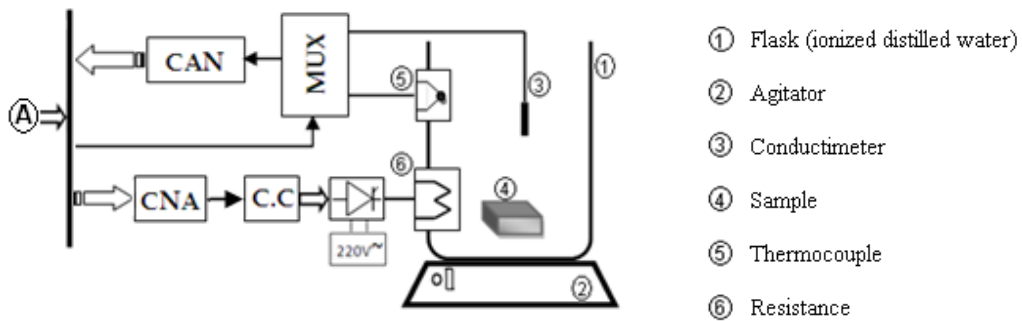
## 3. Procedure

The sample is successively weighed to determine its initial density, dried at a temperature of 105°, covered with resin to seal on its sides and impregnated under vacuum by a salt tracer KCl (0.2M) at a temperature  $T^\circ$  (Figure 1).



**Figure 1:** Illustration of the vacuum impregnation of the sample

The sample is immersed, with stirring at a speed of rotation  $\omega$  and temperature  $T$ , in the ionized distilled water which is withdrawn, the prior conductivity from a string of acquisitions. We measure the evolution over time, the conductivity of distilled water containing the sample through its free sides in a transient regime (Figure 2).



**Figure 2:** Illustration of the measurement concentration of desorption.

#### 4. Modeling

Water is present in concrete in two forms: free and bound. Free water is contained in the pores and depends on water retention in the walls of these voids. The retaining forces of the free water are lower than those applied on the bound water molecules. The diffusion causes the migration of chemical species through the pore walls. Thus a concentration difference is established between the different volumes. The water moves following the concentration gradient.

Our model is based on the mass balance of chemical species diffusing through an elementary volume of the composite. The general transfer equation governing the distribution for various geometries of the composite can be put in the following expression:

$$\left( \text{Accumulation term} \right) - \left( \text{Diffusion term} \right) \pm \left( \text{Production term} \right) + \left( \text{Convection term} \right) = 0 \quad (1)$$

The model is based on the fact that the composite has an initial concentration ( $c_0$ ) and is in a turbulent environment concentration ( $c_\infty$ ). The coefficient of mass transfer surface ( $k$ ) is very important as the surface concentration ( $c_s$ ) remains constant and is equal to ( $c^*$ ) at the beginning of the process ( $c^* = kp \cdot c_\infty$ ). It thus determines, during desorption, the concentration distributions inside the composite finite simple geometry. This consideration can be explained as following dimensionless equation (2).

$$\frac{\partial C_i(X_j, Fo_j)}{\partial Fo_j} - D_{iapp} \left[ \frac{\partial^2 C_i(X_j, Fo_j)}{\partial X_j^2} - \frac{\beta}{X_j} \cdot \frac{\partial C_i(X_j, Fo_j)}{\partial X_j} \right] \pm \frac{\xi^2 \cdot R_i}{D_{iapp}(c_{ip} - c_{i0})} + \frac{\xi}{D_i} \frac{\partial [C_i(X_j, Fo_j) \cdot U_c]}{\partial \zeta} = 0 \quad (2)$$

In our case we work in the absence of terms of production and convection, and we have:

$$\frac{\partial C_i(X_j, Fo_j)}{\partial Fo_j} - D_{iapp} \left[ \frac{\partial^2 C_i(X_j, Fo_j)}{\partial X_j^2} - \frac{\beta}{X_j} \cdot \frac{\partial C_i(X_j, Fo_j)}{\partial X_j} \right] = 0 \quad (3)$$

With:  $C_i$  reduced concentration  $\{C_i = (c_i - c_{i0}) / (c_{ip} - c_{i0})\}$ ,  $X_j = \zeta/\zeta$  the size reduced  $\{X_j = X_l = x / L$ : for the longitudinal direction and  $X_j = X_l = r / R$ : radial direction  $\}$  and  $(Fo)_j = (D_{iapp} \cdot t) / \zeta^2$   $\{(Fo)_l = (D_{iapp} t / L^2)\}$  for the Fourier number of mass longitudinal and  $\{(Fo)_r = (D_i \cdot t) / R^2$  for the number of Fourier radial mass  $\}$ .

The system to be solved by simplifying assumptions, the boundary conditions and initial condition take the following form [4]:

$$\left. \begin{aligned} D_{i\text{app}} \frac{\partial^2 c_i(x,t)}{\partial x^2} - \frac{\partial c_i(x,t)}{\partial t} &= 0 \\ c_i(x,t) \Big|_{t=0}^{x>0} &= c_{i0} \\ c_i(x,t) \Big|_{t>0}^{x=l} &= c_{ip} \\ \frac{\partial c_i(x,t)}{\partial x} \Big|_{t>0}^{x=0} &= 0 \end{aligned} \right\} \quad (4)$$

The kinetics of desorption of solute immersing the mortar towards the outside environment (distilled water) is well modeled and the mass equation is solved using Laplace transform and simplifying assumptions adopted. A resolution will be made simpler by using the method of separation of variables.

Similarly it will be possible to achieve the quantity of the substance released experimentally at time  $t$   $(m_t)_{\text{exp}}$  from the instantaneous concentration  $(c_t)_{\text{exp}}$  measured by the conductimeter:

$$(m_t)_{\text{exp}} = (c_t)_{\text{exp}} \cdot v_{\text{sol}} \quad (5)$$

With:  $m_t$  the mass of the substance released at time  $t$ ,  $m_\infty$  the mass of the substance transferred after complete desorption of the sample at infinite time;  $v_{\text{sol}}$  the volume of the liquid solution (by  $l$ ) immersing the object.

Solving the previous system is:

$$\frac{m_t}{m_\infty} = 1 - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \left\{ \frac{1}{(2n+1)^2} \cdot \exp \left( - \frac{(2n+1)^2 \cdot \pi^2 \cdot D_{i\text{app}} \cdot t}{4l^2} \right) \right\} \quad (6)$$

The coefficient of mass diffusion of our mortar is inferred indirectly from experimental measurements of the conductivity of water (initially distilled) instantaneous concentration  $C_i$ .

The concentration of solute  $C_{\text{KCl}}$  (mM) during desorption (equation 7) is calculated from the limiting equivalent conductivity  $\lambda_x$  ( $\lambda_{\text{K}^+}(T)$  or  $\lambda_{\text{Cl}^-}(T)$ ) (extrapolated to infinite dilution) ions solutions used at temperature  $T$  ( $^\circ\text{C}$ ) [5].

$$c_{KCl} (mM) = \frac{\Lambda_{KCl}}{[\lambda_{K^+}(T) + \lambda_{Cl^-}(T)]} \quad (7)$$

$$= \frac{(\Lambda_{KCl})_t - (\Lambda_{KCl})_{t=0}}{[\lambda_+^\infty + a_+(T-25) + b_+(T-25)^2 + c_+(T-25)^3] + [\lambda_-^\infty + a_-(T-25) + b_-(T-25)^2 + c_-(T-25)^3]}$$

With:  $\Lambda_{KCl}$  The conductivity of the fluid indicated by the meter as a function of time.

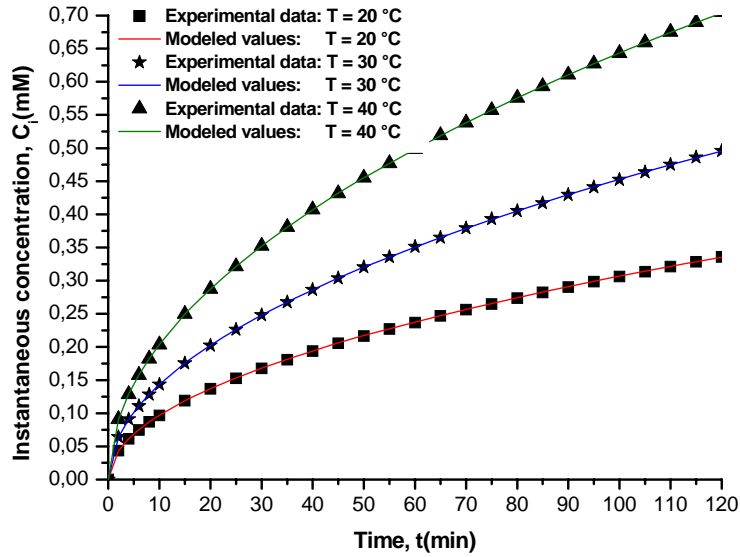
## 5. Results and Discussion

The figure 3 shows the evolution of solute concentration over time (Vial 1 in Figure 2). This concentration is related to the reduced mass in equation (5). The concentration will thus be directly calculated from equation (7) according to the conductivity measured.

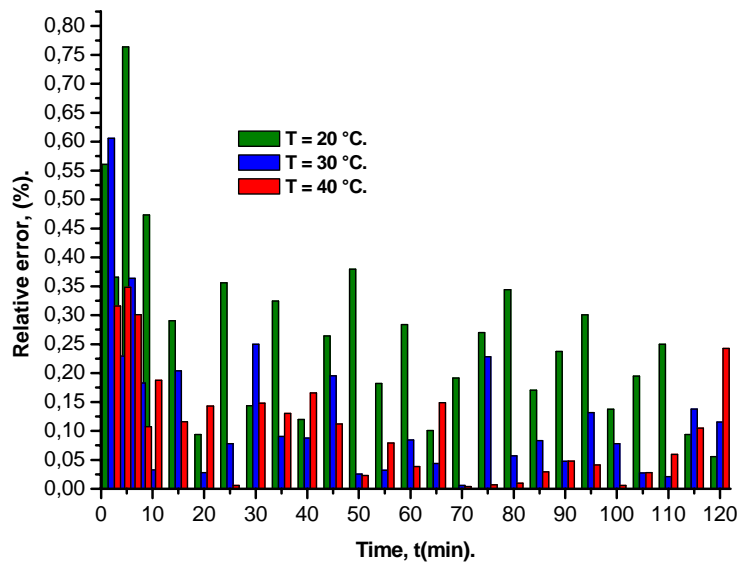
The mass diffusion coefficient is deduced after fitting our model with experimental results (Figure 3) with an error not exceeding 0.8% (Figure 4) which confirms the reliability of our model.

Note that this coefficient is about  $10^{-11}$  (Table 1) which is in perfect accordance with the Halamickova result [6] and [7] in terms of composition (sand, cement, water) from our mortar.

Furthermore this coefficient increases with temperature, which induces dilation of the pores of our material and an increase in the water entropy: these two factors contribute to strong mass diffusion [8] and [9].



**Figure 3:** Model Validation: Effect of temperature on the evolution of the external concentration over time.



**Figure 4:** Percentage of error on the values of the reduced masses measured and modeled for different temperatures studied.

**Table 1:** Values of the apparent diffusion coefficient for three temperatures. Mortar soaked in KCl (0.2M).

Interval time (min)	$D_{app} \cdot 10^{11}$ (m <sup>2</sup> /s)	Temperature (°C)
[0 – 120]	1,300	20
[0 – 120]	2,850	30
[0 – 120]	6,300	40

## 6. Conclusion

The results can be useful for modeling the mass distribution in the standard mortar and concrete eventually. Their review would be useful for predicting the behavior of hygroscopic porous material to efficiently identify multiple pathology and durability in a humid environment so aggressive. For healing, this study may be useful in a numerical simulation of water transfer in the outer casing damaged a building exposed to treatment by a layer of cement mortar, characterized by mass diffusion evaluated.

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