Simulation Of Chloride Ingress Into Unsaturated Concrete Exposed To Tidal Areas

Van Quan Tran, Hoang Long Nguyen, Huu Nam Nguyen, Quang Hung Nguyen

Abstract*: The paper focuses on establishanumerical model to simulate penetration of chloride ions in unsaturated concrete exposed to tidal areas. The model will be set up based on two mechanisms of fluid flow and ion diffusion. The first part of the paper will present the equations of fluid flow in unsaturated pore milieu and ion ingress into concrete. The numerical model will be compared with the experimental results from literature, the numerical model. A full model of chloride ion ingress into unsaturated concrete can be established. The model will be validated by comparison with the experimental results from literature. The results show that the prediction of numerical model is relatively accurate in the chloridepenetration in ordinary concrete.

***Keywords*: Unsaturated concrete, chloride, tidal areas, Imbibition/Drying**

I. INTRODUCTION

The service life of a reinforced concrete structure is strongly linked to the sustainability of the association concrete / reinforcement, in other words, the ability to withstand physico-chemical attacks leading to the failure of materials and therefore of structure. Three families of concrete degradation can be distinguished[1]. The first corresponds to the corrosion of armatures. Corrosion is induced by carbonation and chloride penetration. The expansion of the corrosion products leads to the bursting of the coating concrete. The second family refers to the mechanism of dissolution of hydrates which leads to the loss of alkalinity and to the decline of the resistance. The phenomenon mainly concerns concrete structures in contact with fresh water. The third family is associated with swelling phenomena, such as alkali-granular reactions and internal sulfuric reactions, which also lead to the expansion and bursting of concrete. These phenomena are encountered in works of art in the last 20 years. During the life of a reinforced concrete structure degraded by corrosion, we can distinguish two periods: an initiation period and a propagation period[2]. The duration of the first period is determined by the rate of neutralization of the asphalt concrete or the speed of penetration of aggressive substances such as chloride ions through the coating. When theconcentration of chloride ions at the steel bar is sufficiently large oraccording to several authors, we say that "the critical threshold is reached" [3].The period of propagationbegins, then the steel corrodes to the point that the steel section is less than a valueacceptable. On the other hand, Ueli Angst[4] shows that the critical threshold is unreliable to evaluateinitialization of corrosion, this problem is discussed in the other chapter. The life of thestructure is defined as the period between the commissioning of the structure and the incubation ofcorrosion of reinforcement. With regard to chloride-induced corrosion, the aimof research is to develop a numerical model of initiation of corrosion allowingin particular to determine the time required for the reinforcement corrosion to appear.The penetration of aggressive agents in concrete in situ (structures exposed to the tides,splash and de-icing salts) is usually a combined process of diffusion andadvection. Indeed, aggressive agents can be transported to the surface by advectionwhen drying concrete surfaces. They accumulate there because of the evaporation of the water. In addition, the imbibition / drying cycles can increase the corrosion rate of the reinforcements.On the other hand, when the chloride threshold is reached at the reinforcement level, the drying of the concrete facilitates the availability of oxygen required for priming steel corrosion.

Some parts of the work are constantly submerged. In this case, the diffusion phenomenon is, as a first approximation, the only transport process. However, it is recognized that it is not the parties that are degrading the fastest. They are not the objective of the article. The tidal zone is the most problematic [5]. In fact, the imbibition-drying cycles involve penetration of the aggressive agents followed by a corrosion rate 20 times greater than during exposure under saturated conditions [6]. We will focus on these aspects in this paper although they are more complex to model: several phases during fluid flow, several chemical species to take into account.

II. MODEL APPROACH

A. Fluid flow

The transport of aggressive agents in unsaturated concretes is characterized by a combined process of diffusion and advection. The advection phenomenon is generated by the velocity of the fluid resulting from the hydrodynamic process. The flow of water takes two forms: liquid and gas. The transport of moisture in the porous materials is subjected to different mechanisms simultaneously or not. Two types of models are commonly used: unsaturated flow theory (simple model) [7]and multiphase transfer models (reference model) [8]. In this part, we recall the model of water transfer resulting from the theory of unsaturated flows. The equations governing

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multiphase flows are described in Mainguy's thesis[9] for example. From the work of Celia et al [7], we present the simple model. In this model we assume that the gas pressure p_g is constant and uniform and is equal to the atmospheric pressure p_{atm}.

$$p_g = const = p_{atm} \quad (1)$$

Then we use the Richards equation which constitutes the general equation of the flows in unsaturated medium:

$$q = -K(\theta(h))\nabla h \quad (2)$$

Where q is debit, K is hydraulic conductivity, θ is water content depending on the elevation of water h. The following continuity equation is then obtained taking into account the variation of the water content over time:

$$\frac{\partial\theta(h)}{\partial t} + \mathrm{div}q = 0 \quad (3)$$

Richard's equation is presented in the form:

$$-\nabla\left(K(\theta(h))\nabla h\right) + \frac{\partial\theta(h)}{\partial t} = 0 \quad (4)$$

With

$$K(h) = k_s k_r(h) \quad (5)$$

Richards equation assumes that: the effect of air on the movement of the liquid phase (air is present at atmospheric pressure), as well as the dynamic effects [10], [11] and hysteresis on the relations between hydraulic conductivity - matrix pressure and water content are neglected. Permeability K represents the ability of the porous medium to "drive" water. In saturated water, all the pores are filled with water and participate in the flow, the permeability is then maximum. Its value is called absolute permeability which is noted k_s [m²].

Models based on a physical representation of the structure of the poral network make it possible to describe the curve of evolution of the permeability as a function of the water content. They are based on an integration of the capillarity models and are valid at the macroscopic scale, since the porous medium can be considered as homogeneous. The most commonly used models are the relations of Van Genuchten[12] and Brooks and Corey [13] making it possible to describe well the curve K(θ) [14]. They use the parameters obtained by the water retention curve h(θ), generally easier to obtain experimentally, as well as the value of ks, to predict the evolution of the permeability as a function of the water content. Brooks and Corey's relationship is based on the equation:

$$K(h) = k_s S_e^{\frac{2}{\lambda}+l+2}(h) \quad (6)$$

where l is the tortuosity factor which can be equal to 0.5 [15] in most cases and $\lambda = m\times n$; S_e effective saturation. If one chooses the van Genuchten model to describe the water retention curve.

We use van Genuchten's relationship here:

$$K(h) = k_s S_e^l\left[1-\left(1-S_e^{\frac{1}{m}}\right)^m\right]^2 \quad (7)$$

This relation is obtained by combining the expression of the capillary pressure -saturation relationship with the expression of the hydraulic conductivity of the material based on the porous distribution of Mualem [18], the expression of the capillary pressure resulting from the expression following:

$$p_l - p_g = p_c \quad (8)$$

The value of the parameter l = 0.5, in van Genuchten's relationship, was originally used for soils. Savage at Janssen has shown that it can also be applied to cementitious materials [16]. According to Van Genuchten, the relations between S_e; θ; h are expressed as:

$$\theta = \theta_r + S_e(\theta_s - \theta_r) \quad (9)$$

$$S_e = \frac{1}{(1+|\alpha h|^n)^m} \quad (10)$$

$$m = 1 - \frac{1}{n} \quad (11)$$

The Van Genuchten model is the most widely used in the literature to describe the water retention curve and applies to cementitious material. The Brooks and Corey model is validated over a limited range of capillary pressure (for $p \geq p_i$) and is well adapted to the data obtained for coarse, reworked soils with a narrow pore size distribution, it does not allow a good representation of the retention near saturation conditions.

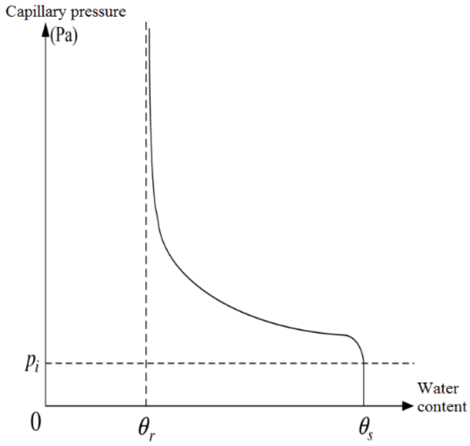


Fig.1: Representation of a water retention curve

B. Ion transport model

In order to evaluate the durability of a material and predict the life of a structure, models describing the transport phenomena of aggressive agents are necessary. The ion transfer in a porous medium such as concrete can be described mathematically by partial differential equations in space and time. As in unsaturated conditions, transport is multi-phasic (gas, liquid), we must add the water balance between water vapor and liquid water [3]. The previous part allows us to consider the constant gas pressure. The generalized Darcy's law (Richards equation) is used to describe the advection of the liquid phase. The ion transport (in liquid phase) is described from the advection-diffusion equation.

$$\frac{\partial c}{\partial t} - \mathrm{div}(D\nabla c - cu) = 0 \quad (12)$$

Where velocity uis the solution of equation (2), c is the chloride concentration.

The penetration of chlorides depends on the characteristics of the material and the climatic conditions undergone (frequency of humification/drying cycles, their amplitude, temperature, etc.). In a saturated environment (in the case of structures immersed in seawater), chloride ions penetrate the concrete by diffusion, under a concentration gradient [19]. When the concrete structure is subjected to humification / drying cycles (tidal zone, exposure to spray or deglaze salts), the chlorides can penetrate into the concrete by capillary absorption and migrate through the liquid phase by advection within the area concerned by the cycles [24]. In this case, the ion transport is coupled with the transport of moisture. On the one hand, the penetration of chloride ions is greatly accelerated by convection of the liquid phases. Humidification of a partially saturated material with saline solution during a day can penetrate chlorides more deeply than would be the case several months later in saturated media [20]. On the other hand, the transport of ions in the interstitial solution can change the activity of water [14] and change the balance between liquid water and water vapor. This affects the water transfer. Chlorides can occur in different states in the internal structure of concrete [22]:

- Chemical chloride binding (Friedel's salt for example) and physical chloride binding adsorption on C-S-H (ion exchange between OH- and Cl- ions).
- Free chloride (in ionic form and unreacted with the cement matrix) in the interstitial solution of the pores. The total amount of chloride (c_t in [mol/m^3 of concrete]) is expressed as the sum of the amount of chloride binding (c_b [mol/m^3 of concrete]) in the solid phases and the amount of free chlorides in the pore solution (c_f [mol/m^3 of the solution]):

$$c_t = c_b + \phi c_s \quad (13)$$

Where ϕ is the accessible porosity

Equation (12) can be written:

$$\frac{\partial c}{\partial t} - \mathrm{div}\left(D\nabla c_f - c_f u\right) = 0 \quad (14)$$

Or

$$\left(\phi + \frac{\partial c_b}{\partial c_f}\right)\frac{\partial c_f}{\partial t} - \mathrm{div}(D\nabla c_f - c_f u) = 0 \quad (15)$$

There are several models to describe the adsorption isotherm, but we introduce that the Freundlich adsorption isotherm which is used in the work of Amor [17]:

$$c_b = \tau c_f^{\beta} \quad (16)$$

α,βare empirical coefficients.

III. COMPARISONS OF EXPERIMENTAL RESULTS AND NUMERICAL RESULTS USING COMSOL

A. Materials and the necessary parameters

Thanks to the parameters determined in the work of Amor[17], we realize the simulation with two types of materials, ordinary concrete: B45 and B45L. The cylindrical specimen measuring 5 centimeters in diameter and 11 centimeters in height. We assume an isotropic behavior of the material in all the planes perpendicular to the axis of the cylinder. The contours and the surface at the top of the specimens were protected from water transfer by two layers of epoxy resin, therefore, the flow in the concrete is unidirectional. (see Fig.2). Table 1 summarizes the parameters used.

Table 1: Parameter of Richard equation and isothermal Freundlich

Material	B45	B45L
W/C	0.48	0.48
Permeability k_s	1.06×10^{-19}	0.23×10^{-19}
n	1.78	1.78
m	0.44	0.44
l	0.5	0.5
α	0.054	0.054
β	0.82	0.67
Φ	0.102	0.097
Coefficient of apparentdiffusion (m^2/s)	5×10^{-11}	3.5×10^{-11}

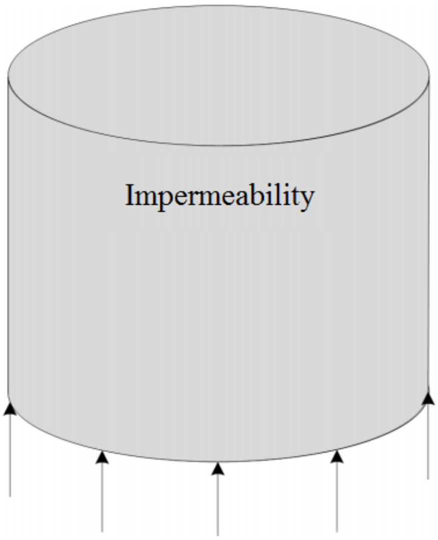


Fig.2: Model geometry

B. Boundary and initial conditions

The objective is to compare the results of the model with experimental results [5]. We use the same initial condition as in the work of Amor. He considers that the temperature and the effective saturation are uniform throughout the concrete, that the cycles are realized when the equilibrium of the temperature and the relative humidity between the concrete and the laboratory are reached. We carry out 2 cycles, 6 cycles, 20 cycles, 60 cycles of drying / imbibition equivalent to 1 day, 3 days, 10 days and 30 days. The duration of a cycle is 12 hours including 6h of imbibition/6h of drying. NaCl solution 30g/l, c_{Cl^-}= 513 mol/m^3

It is considered that the temperature of the concrete is equal to the ambient temperature 20°C. Two simulations with two types of concrete, two different relative humidity (75% and 90%) are realized. Thanks to the compositions of the concretes used in Amor work, which are identical to those used in Mainguy work, we allow ourselves to use the Van Genuchten parameters and absolute permeability previously used (see Table 1). From equation 17, we give the summary table of boundary conditions or initial condition used in our simulation models. In order to make the connection between capillary pressure and relative humidity, we use, from equation 8, the following Kelvin-Laplace relation:

$$p_c = \rho_l \frac{RT}{M_\upsilon} \ln h_r \qquad (12)$$

As part of equation 12, the parameters given in Table 2 and van Genuchten model parameters in the work V. Baroghel-Bouny [4], we find the following boundaryand initial condition (see Table 5):

Table 2: Physical parameter of drying model

Masse of water volume ρ	Perfect gas constant R	Molar mass of water M_υ	Temperature
1000 kg/m^3	8.3147 $J.K^{-1}.mol^{-1}$	0.018 $Kg.mol^{-1}$	293 K

Therefore, boundary and initial conditions: concentration and capillary pressure of imbibition /drying are summarized in table 3

Table 2: Boundary and initial conditions used in the numerical model

Material			B45(B45L)	
Relative humidity (%)			75%	90%
Initial condition		Capillary pressure (MPa)	39	14
		Concentration (mol/m^3)	513	513
Boundary condition	Imbibition	Capillary pressure (MPa)	39	14
	Drying	Concentration (mol/m^3)	0	0

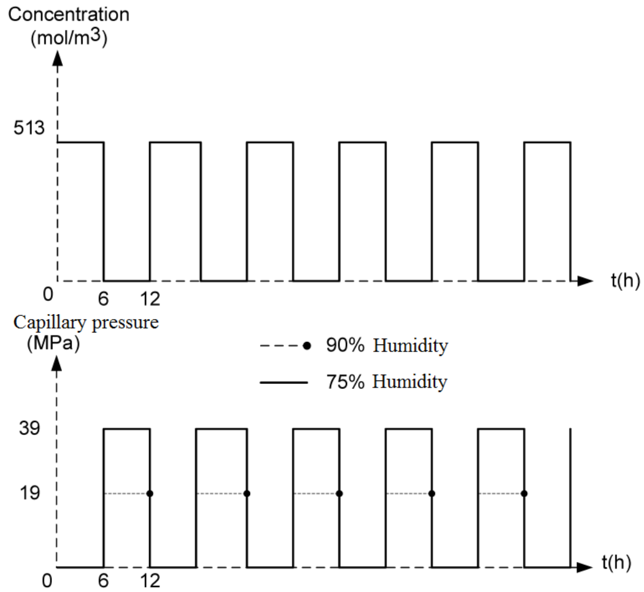
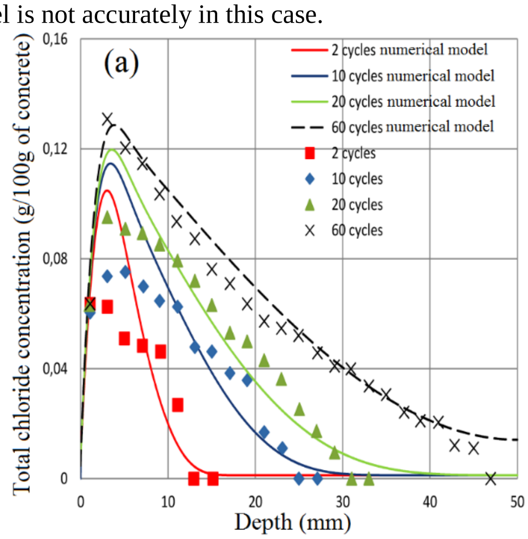


Fig.3: Evolution boundary conditions during the imbibition/drying cycle

C. Results and discussions

Fig. 4 and Fig. 5 show total chloride concentration over depth of B45 and B45L, respectively. Numerical resultsare relatively consistent with the experimental results. Therefore, the model can predict relatively accurately chloride concentration of ordinary concrete exposed to tidal areas. That helps to estimate initial time of corrosion in reinforced concrete. However, numerical results are not really identical with experimental results for the short time 2, 10 and 20 cycles, in particular case B45L 90% humidity. In the B45L, slag is used to replace partially Portland cement so that the model is not accurately in this case.



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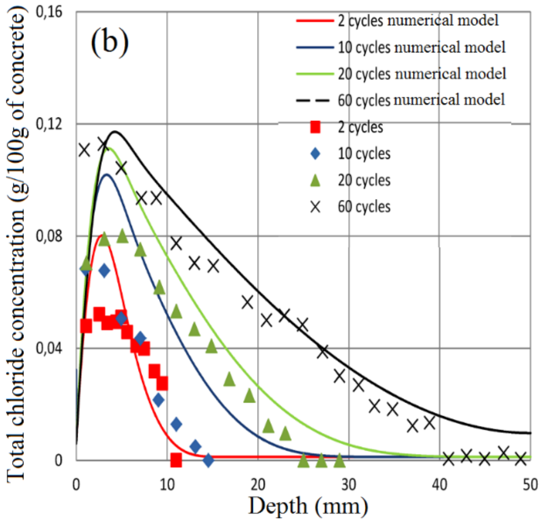
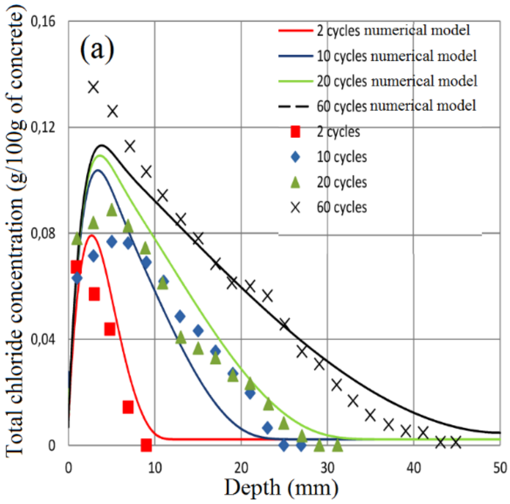


Fig.3: Comparison between numerical results and experimental results [17] of total chloride concentration over depth in different cycles a) B45-75% humidity b)B45-90% humidity



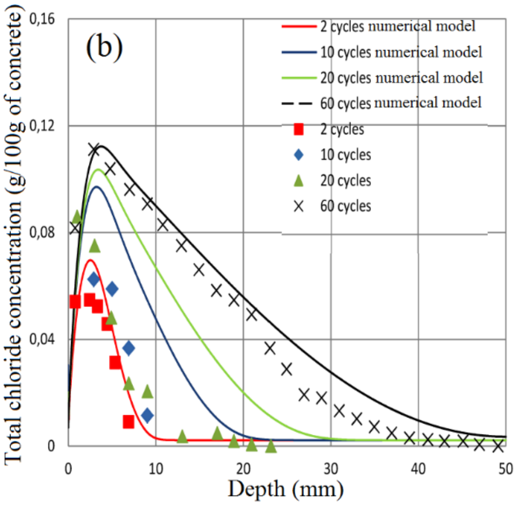


Fig.4: Comparison between numerical results and experimental results [17] of total chloride concentration over depth in different cycles a) B45L-75% humidity b)B45L-90% humidity

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