EFFECT OF THE TEMPERATURE ON THE WATER TRANSPORT BY CAPILLARITY INTO THE CONCRETE POROSITY

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Abstract

This paper presents a new 2D water transport model considering capillary suction to predict the water content evolution in the concrete porosity. The basic formulations of the model are illustrated, and a switching algorithm is introduced to simulated wet-drying effects. Two specific absorption tests are studied to validate this model. The first test conducted under room temperature allows to observe that capillary effects play an important role in the concrete material sorptivity and this phenomenon was well captured by the numerical model. The second test conducted under different temperatures highlight that temperature has significant effect on the capillary suction process and it has been considered in the model as an important input parameter.

Keywords: Capillary suction, concrete porosity, transport model, finite element method, absorption test

1. INTRODUCTION

Over the past decades, concrete structures have suffered from corrosion induced by chloride ions, decreasing both their durability and sustainability [1,2]. When the concrete is unsaturated and exposed to aggressive environment (tides, mist, splash), it is commonly admitted that the capillary suction of salt water will significantly accelerate the penetration of chloride ions in the concrete structure [3-6], compared to the speed of chloride diffusion. Many transport models using traditional Fick's diffusion law in the literature [7-9], however, failed to capture this physical nature and kinetics of capillarity. More elaborated multiphase transport models [10-12] can explain capillarity by introducing a "capillary pressure" on liquid-vapor interface in its formulation, yet applications of these models on water absorption tests have not been found. Water transport with presence of capillarity in concrete porosity is still poorly understood and modelled. To address this problem, the 1D FEM software TransChlor® [6,13] was developed considering the coupling between temperature [14], carbonation, water transport, ion diffusion and chloride isothermal adsorption [15] during the concrete corrosion process. Water and chloride diffusion equations from Bazant et al. [7] coupled with a kinetic term driven by

capillarity [6] were implemented in TransChlor®, to simulate water transport in porosity with capillary suction effect. Based on the simulation results from TransChlor®, Sanchez et al. [16] developed a new numerical model on a geochemical software PhreeqC [17, 18] and simulated the capillary suction impact on chloride transport at ambient temperature. However, few studies can be found about the impact of different temperatures, especially low temperature, on the capillary suction process in concrete, and till now, not many models exist. In addition, most of existing numerical models with capillarity effect are quite limited to a 1D framework [6, 12,13] and are only able to simulate tests with laboratory exposure conditions [17, 18] (constant temperature, fixed salt solution concentration, constant boundary relative humidity, 1D drying or wetting…). Higher dimensional transport simulations considering capillarity, with real environmental exposures as boundary conditions, are still absent in the literature.

The objective of this paper is then to present a better concrete pore water transport model that models the influence of the temperature on capillary process and that is developed in 2D to further consider real complex exposure conditions. This model (TransChlor2D®) was formulated by integrating the effect of vapor diffusion and liquid suction with Fick's and Darcy's law, respectively and was implemented in the architecture of TransChlor® (Fig. 1).

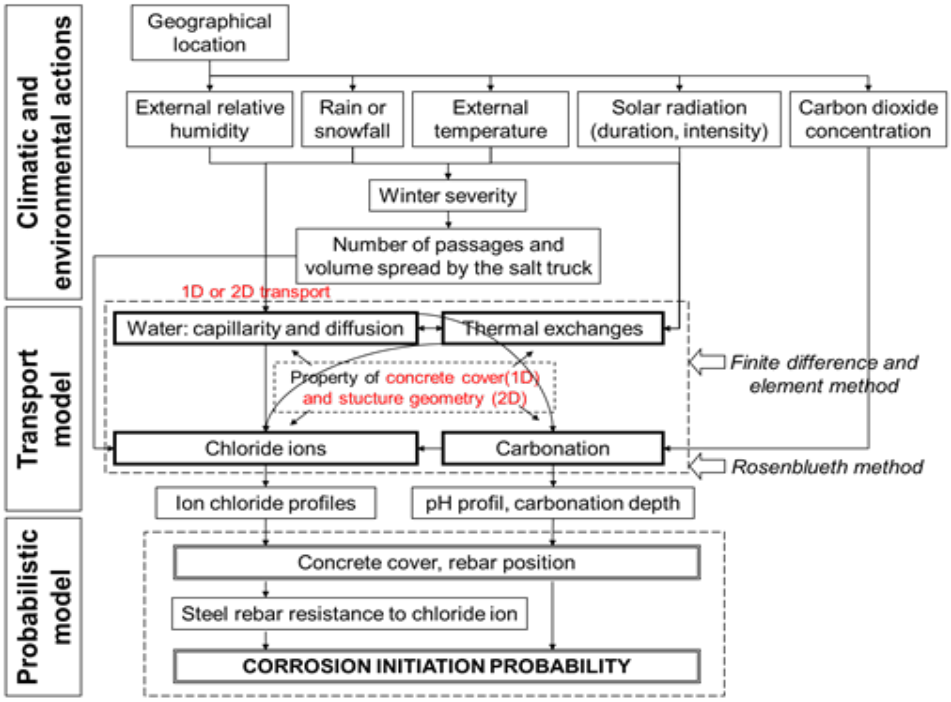

Figure 1: Implementation of a new 2D water transport module in the TransChlor® software architecture

A 2D Finite Element Method (FEM) algorithm was implemented to solve the nonlinear differential equations. The transport parameters in this new transport model were calibrated with various durability tests [19-22] while in this paper, only the simulation results on water absorption tests [20,21] were discussed since they are most relevant to capillary suction phenomenon.

2. MODELLING WATER TRANSPORT INTO CONCRETE POROSITY CONSIDERING CAPILLARY EFFECTS

Water movement in porous medium can be considered as a multiphase transport process.

Considering concrete as a homogeneous porous medium and no presence of liquid water inside, the whole water transport process can be generally represented by "vaporized water" diffusing through an interconnecting pore network [7]. In this case, the "Bazant-Najjar" diffusion model [8,9] is commonly used to represent the mass balance of non-wetting phase (water vapor + air). Using saturation degree as state variable and by introducing porosity, the expression of mass balance on water vapor yields to [8,9]:

$$\rho_{nw} \cdot \emptyset \cdot \frac{\partial S_{nw}}{\partial t} = -\nabla . \overrightarrow{J_{nw}} \tag{1}$$

ρ_l is the density of water vapor ($kg.m^{-3}$), $\emptyset$ is the porosity of medium and S_{nw} is the pore saturation of water vapor. The massive flux of water vapor $\overrightarrow{J_{nw}}$ ($kg.m^{-2}.s^{-1}$) is driven by saturation gradient in space with the massif water vapor diffusion coefficient D_{nw} ($kg.m^{-1}.s^{-1}$),

$$\overrightarrow{J_{nw}} = -D_{nw} \cdot \boldsymbol{\nabla} S_{nw} \tag{2}$$

The coefficient D_{nw} can be further modelled with a nonlinear "S-Shape" mathematical function [8] and coupled with an Arrhenius law [6]:

$$D_{nw} = \rho_{nw} \cdot D_{nw0} \cdot \left(\alpha_0 + \frac{1-\alpha_0}{1+\left(\frac{1-S_{nw}}{1-S_{cr}}\right)^n} \right) \cdot e^{\frac{Q}{R}\left(\frac{1}{T_0}-\frac{1}{T}\right)} \tag{3}$$

with D_{nw0} the asymptotic diffusion coefficient at 100% pore relative humidity, α_0 a minor non-zero constant, S_{cr} the turning point in $(D_{nw} - S_{nw})$ relationship and n governing the curvature of function curve. For vapor diffusion, the Arrhenius par Q refers to the activation energy (Q=32000 kJ/mol) and R refers to the gas constant (R=8.314) [7]. T_0 is the referential temperature (usual laboratory temperature, 293K) and T is the actual ambient temperature.

However, not only vaporized water engaged in water transport. With the presence of wetting phase (liquid) in concrete pores and contact surfaces, the capillary suction phenomenon comes from the capillary pressure difference on liquid-air interface on thermodynamic equilibrium state [12]. According to some research [11,12] and by neglecting the non-wetting phase (since liquid capillarity becomes dominant in transport process), the governing equation for wetting phase driven by capillary pressure can be expressed as simple as:

$$\rho_w \cdot \emptyset \cdot \frac{\partial S_w}{\partial t} = -\boldsymbol{\nabla} . (D_w(T, S_w) \cdot \boldsymbol{\nabla} S_w) \tag{4}$$

The transport coefficient of wetting phase D_w can be modelled with a Darcy's law [10] upon pressure gradient combined with an Arrhenius law of temperature variation:

$$D_w(T, S_w) = \left(\rho_w(T) \cdot \frac{\partial P_c(S_w)}{\partial S_w} \cdot \frac{K \cdot k_{rw}(S_w)}{\eta_w(T)} \cdot f_w(S, \emptyset) \right) \cdot e^{\frac{Q}{R}\left(\frac{1}{T_0}-\frac{1}{T}\right)} \tag{5}$$

where $P_c(S_w)$ is the capillary pressure (function of saturation) derived from material's main isotherm curves [23]. K is the intrinsic permeability of medium, k_{rw} is the pore relative

permeability to wetting phase, η_w is the viscosity of wetting phase and f_w is the tortuosity factor related to the complexity of pore microstructure.

To decide the appropriate D coefficient to use in different transport modes, a 'hybrid model' was introduced here. Let us introduce a general pore saturation degree S and the density ρ as state variable (may be different according to temperature), we can have one single equation for all scenarios:

$$\rho \cdot \emptyset \cdot \frac{\partial S}{\partial t} = -\nabla.(D \cdot \nabla S) \quad (6)$$

The 'hybrid model' interprets how to determinate the right equation to integrate with the correct transport coefficient by the following switching algorithm based on local element hygroscopic state. Whenever local material element is in contact with wetting front (on its adjacent position/element, water saturation changes with a positive rate ≥ 0 and saturation passes the liquification threshold level $S \geq 0.95$ [24]) (Fig. 2)

$$\begin{cases} S = S_w, \rho = \rho_w, D = D_w \; if \; \dot{S} \geq 0 \; and \; S \geq 0.95 \; (liquid \; capillary \; suction) \\ S = S_{nw}, \rho = \rho_{nw}, D = D_{nw} \; if \; \dot{S} < 0 \; or \; S < 0.95 \; (water \; vapor \; diffusion) \end{cases} \quad (7)$$

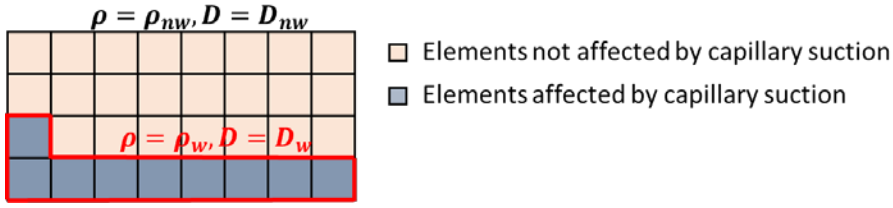

Figure 2: Numerical interpretation of the "Hybrid model"

The integrated form of Eq. (6) was then discretized and solved with a FEM computation program TransChlor2D ® [25] with given initial and boundary water saturation conditions.

3. SIMULATION RESULTS ON WATER ABSORPTION TEST AT AMBIANT TEMPERATURE

A unidimensional water absorption test from Lunk [20] was simulated in this paper to validate the performance of the implemented hybrid transport model algorithm.

Table 1 provides some important properties and transport parameters used for the simulation of the studied samples. Cement type used for all concrete samples were Portland CEM I 42.5R with properties and compositions in accordance with norm SN EN 197-1 [26].

Table 1: Water transport properties of the Lunk samples [20].

Properties	**A**	**B**	**C**
Cement type	CEM I 42.5	CEM I 42.5	CEM I 42.5
Cement (kg/m^3)	400	350	310
Water (kg/m^3)	160	175	186
Density (kg/m^3)	2445	2412	2388

Porosity	0.1024	0.119	0.133
D_{nw0} **(m²/s)**	5E-11	1.27E-10	1.7E-10
K **(m²)**	1.5E-21	3.7E-21	5.5E-21

The test consists in merging three different cuboid concrete samples with different formulation in brine container and measuring their water content evolution inside and alongside over time (2h, 24h, 72h), as shown in Fig. 3a). Samples were initially dried and kept at 75% RH and their lateral surfaces were sealed by resin. Only the bottom faces are immerged into a 3% NaCl solution. The chamber temperature was maintained at 20°C during the test.

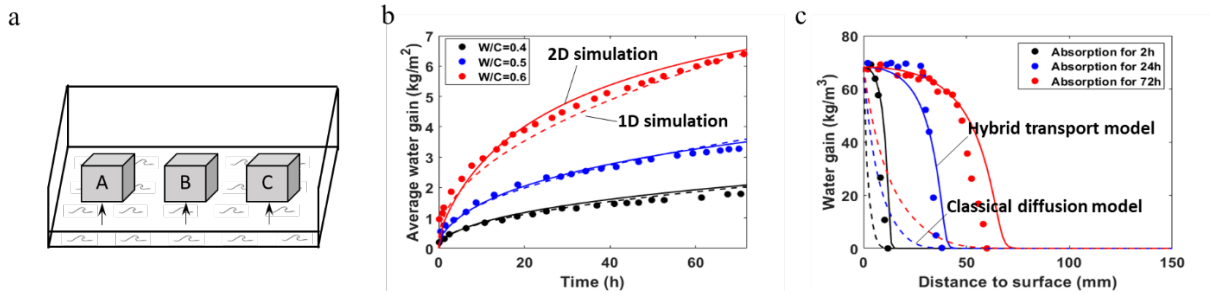

Figure 3: Simulation results on Lunk's water absorption test at 20°C (273K): a) test setup b) average mass water gain c) water gain distribution over height.

The numerical simulation results on average water gain in concrete porosity, with 2D implementation of transport equations, are compared with experimental data from all three concrete mixtures (Fig. 3b). A good correlation was observed between model prediction and real results. Additionally, the simulation results with 1D implementation of same equations were also compared, showing very similar tendency. The very little difference between 1D and 2D simulations should come from the different mesh densities and integration schemes (1D:2 Gauss points and 2D: 4 Gauss points) chosen for FEM computation.

In particular, the water saturation profiles at 2h, 24h, and 72h were extracted from simulated saturation field values and compared with results measured in laboratory (Fig. 3c). The simulated profile matches quite well the experimental data set and captures well the rapid water penetration into concrete especially during the first few hours of absorption. Then, a comparative transport model, with only diffusion equations, was also implemented and the simulation results are far from satisfying. By comparison we can tell it is impossible to obtain a concave water profile with only a diffusion law and calculation based on it will lead to signification underestimation in water content variation, whereas our implementation of capillarity part into the governing equation of TransChlor2D® compensated this systematical error successfully.

4. SIMULATION RESULTS ON WATER ABSORPTION TEST AT DIFFERENT TEMPERATURES (-20°C TO 10°C)

Experimental results from Conciatori [21] showed that the external temperature has a significant impact on the capillary suction process. One of the concrete mixtures casted

(referred by sample A in [21]) is composed with 375 kg/m^3 of cement CEM I 42.5 and 154 kg/m^3 of water. The density is 2450 kg/m^3, the porosity is 0.12, the diffusion coefficient D_{nw0} (m^2/s) is 6E-11 m^2/s and the permeability K is 8.5E-22 m^2. Cylindric concrete specimens were merged in a temperature and humidity-controlled basin filled with salt solution (27%) for 7 days (Fig. 4a). Lateral and top surfaces of cylinders were sealed by resin to have only 1D capillary suction along height. Four different temperatures were applied on each group of samples (-20°C, -10°C, 0°C, 10°C) and the mass samples were registered every 15 mins. Temperature dependent parameters of salt solution are given here in Table 2.

Table 2: Transport properties related to temperature impact.

Properties	**10°C**	**0°C**	**-10°C**	**-20°C**
ρ_w **(kg/m^3)**	1207	1208	1208	1208
Q (kJ/mol)	75216	5477.1	16804	-361840
Porosity ϕ	0.12	0.12	0.12	0.12/0.018*

* porosity after correction

Experimental results on samples A showed the significant impact of temperature on capillary suction process and our capillary model equipped with Arrhenius law correctly predicted it (Fig. 4b). Above -10°C, salt solution remains liquid and its movement into porosity obeys an ordinary Darcy's law. Higher external temperature leads to a higher transport coefficient thus a higher water suction rate, as observed from the simulated curves. At -20°C, however, a sharp decrease of the amount of water absorbed by capillarity was observed in experimental data points. This requires a correction factor applying on material's porosity since formation of freezing ice in pores will largely reduce porous space. An abnormal negative activation energy at this temperature was also observed. Comparing to real data, a slight overestimation on the amount of water absorbed can be also found in model prediction, this may be due to some minor effects neglected in numerical assumptions such as: 1) Cement hydration or other chemical reactions that consume water 2) Phase change of water (liquid to vapor, liquid to ice). Besides that, the new TransChlor2D® exhibits good performance in capturing the temperature impact while modelling capillary suction in the transport process.

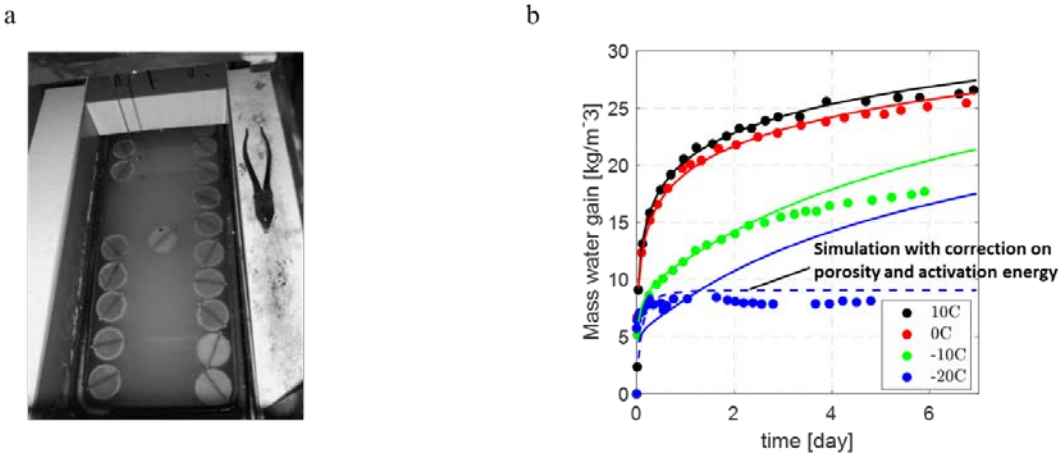

Figure 4: a) Experimental setup for capillary absorption test in temperature-controlled basin [10] b) results on water mass gain at different temperatures.

5. CONCLUSIONS

In this paper, a new FEM pore water transport model for unsaturated concrete was presented, as an extension to the previous chloride corrosion prediction computation program TransChlor ®. In this model, the wetting phase transport in concrete pore structure was modelled with a Darcy's law and the non-wetting phase transport was modelled with a classical Fick's law of diffusion. The combination of the two constitutive laws was realized with a switching algorithm, based on material's hygroscopic state (whether affected or not by capillary suction). Temperature effect on capillarity was modelled with an Arrhenius law.

Two water absorption tests were studied here to validate the model: one at room temperature and the other one at different temperatures. The model showed good overall performance in simulations and an excellent capacity in capturing the capillary suction as well as the temperature impact on it.

The following conclusions can be drawn from numerical analysis:

- Capillary suction happens quite faster than normal diffusion process. In transport model, capillary suction should be coupled with a traditional diffusion model and a switching algorithm.
- Compared to the Fick's law used in most transport models, Darcy's law better captures the capillary suction
- Temperature has an important impact on capillary suction. Higher temperature tends to accelerate the capillary suction process and this effect was considered with an Arrhenius law coupled with capillary transport coefficient. Specifically, at -20°C, the freezing effect in concrete pores will lead to a huge reduction in concrete's sorptivity. This effect was considered in capillary model by a reduction of the overall material porosity.
- The use of a 2D model allows to treat more ambitious exposure conditions, such as underground water, splash/tide zone and floating structures.

To improve the simulation results, further model refinement should be done to consider the chemical reactions, physical binding and phase change models involving the water participation. As the whole transport model presented in this paper was developed in a 2D framework, the

simulation of structures under more complex exposure conditions could be considered and simulated properly.

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