# NUMERICAL SIMULATION OF MOISTURE DIFFUSION IN CONCRETE

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## ABSTRACT

Moisture content of concrete decreases due to moisture diffusion when concrete exposed to dry ambient air. Therefore, drying shrinkage is developed and damage is initiated; at the same time, the diffusion process in concrete is accelerated by the induced damage and micro-cracks. In this paper, a fully coupled hygromechanical model to simulate these phenomena is used, where the solution of a parabolic type and second order partial differential equation (PDE) of the moisture diffusion process is required. The numerical computation is done by using two different methods: finite element and finite difference. Numerical results from both methods were compared with the exact solution of a simple problem. Also, the obtained numerical results were compared with available experimental results of concrete specimens and showed good agreement. Finally, the results for simulation of a bridge deck slab subjected to uniform environmental drying were presented. This numerical study is part of an effort to develop an integrated computer program that simulates concrete structures degradation under different environmental conditions. This simulation is very important for durability and service life predictions of reinforced concrete structures.

## KEY WORDS

concrete, diffusion, finite element, finite difference, damage.

## INTRODUCTION

Environmental degradations of concrete structures are mainly attributed to heat transfer and transport of fluids and deleterious chemicals into concrete. These processes are diffusion-controlled, derived based on Fick's laws and described by nonlinear partial differential equations (PDEs) of a parabolic type.

In the last few years, several numerical models were developed using the finite element method to simulate real structures under different environmental conditions. Kim and Lee (1998) simulated a concrete slab under differential drying shrinkage. Isgor and Razaqpur (2004) developed a computer program to simulate the coupled heat transfer, moisture transport and carbonation processes in concrete structures. Witasse et al. (2002) and

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Benboudjema et al. (2005 a, b) investigated the effect of drying shrinkage and creep on concrete cracking. All the previous research calculations did not consider the influence of mechanical response on the diffusion process. Meschke and Grasberger (2003) analyzed concrete structures with a coupled hygromechanical model; in their simulation, they assumed only the capillary pressure as the driving force for the diffusion process. A numerical simulation which includes the coupling between the moisture diffusion and the induced damage is required to give more accurate simulations and to predict the structure life.

The application of hygromechanical analysis models of concrete structures is presented including the coupling effect between damage due to drying shrinkage and concrete moisture diffusion. The simulation is done using two different methods: finite element and finite difference. A comparison between both methods is presented; also a comparison between numerical and experiential results is shown, and finally a bridge deck slab simulation is presented.

## MODELING MOISTURE DIFFUSION IN CONCRETE

The moisture transport in concrete can be expressed in terms of the relative humidity, $H$, and Fick's first law which defines the moisture flux as:

$$J = -D_H \, grad(H) \tag{1}$$

where $D_H$ is the moisture diffusion coefficient (diffusivity), and $H$ is the internal relative humidity. Under unsteady state condition, where the driving force changes with time, $t$, the mass conservation law gives:

$$\frac{\partial w}{\partial t} = \frac{\partial w}{\partial H}\frac{\partial H}{\partial t} = -div\ (J) \tag{2}$$

where $w$ is the water content and $M_H=\partial w/\partial H$ is the moisture capacity. Substituting Eq. 1 into Eq. 2 yields:

$$M_H \frac{\partial H}{\partial t} = div\ (D_H \, grad(H))\,. \tag{3}$$

Eq. 3 describes the moisture distribution in time and space for concrete, and it is a nonlinear partial differential equation because both moisture diffusion parameters (moisture diffusivity and moisture capacity) are dependent on the relative humidity. The above equation will be solved using finite difference and finite element methods.

The initial condition can be written as follows:

$$H(x,y,z,t=0) = H_o(x,y,z) \tag{4}$$

where $H_o(x,y,z)$ is the initial distribution of relative humidity in the concrete body. The boundary conditions are imposed on the surface as follows:

$$J.\vec{n} = 0 \tag{5}$$

$$J.\vec{n} = \beta(H - H_{env}) \tag{6}$$

where $J$ is the humidity flux, $\vec{n}$ is a unit vector normal to the exposed surface and directed towards the exterior environment, $\beta$ is the surface moisture diffusion coefficient, $H$ is the unknown surface humidity and $H_{env}$ is the environmental relative humidity. Eq. 5 represents the case of no moisture exchange between the body and the environment on the surface of that body.

## NUMERICAL SOLUTION OF MOISTURE DIFFUSION

Since the partial differential equation (Eq. 3) which governs the moisture diffusion in concrete is nonlinear, it must be solved numerically. The numerical solution can be done either by finite element method or finite difference method. These solutions are becoming more effective with the advances in the computing technology. Both solutions are described in this section.

### FINITE ELEMENT METHOD SOLUTION

The moisture diffusion equation, Eq. 3, can be solved using the Galerkin finite element method as follows:

$$\int_\Omega N^T \left[ M_H \frac{\partial H}{\partial t} - \frac{\partial}{\partial x} \left(D_H \frac{\partial H}{\partial x}\right) \right] d\Omega = 0, \quad 0<x<L_d \tag{7}$$

where $\Omega$ is the total volume, $L_d$ is the total depth of the sample, and $N$ is the shape functions. By rearranging and applying boundary conditions, Eq. 7 becomes:

$$\int_\Omega N^T M_H \frac{\partial H}{\partial t} d\Omega + \int_\Gamma N^T \beta\left(H - H_{env}\right) d\Gamma + \int_\Omega \frac{\partial N^T}{\partial x} D_H \frac{\partial H}{\partial x} d\Omega = 0 \tag{8}$$

where $\Gamma$ is the surface area. The relative humidity at any point in an element can be determined using shape functions, $N$, as follows:

$$H(x,t) = \sum N_i(x)\overline{H}_i(t) \tag{9}$$

Substituting Eq. 9 into Eq. 8 and rearranging yields the following matrix form expression:

$$C\frac{\partial \overline{H}}{\partial t} + K\overline{H} = F_H \tag{10}$$

where $C$ is the moisture capacity matrix, $K$ is the moisture diffusion coefficient matrix, and $\boldsymbol{F_H}$ is the hygral load vector; these can be written as follows:

$$C = \int_\Omega N^T M_H N \; d\Omega \tag{11}$$

$$K = \int_\Omega \frac{\partial N^T}{\partial X} D_H \frac{\partial N}{\partial X} d\Omega + \int_\Gamma N^T \beta \; N \; d\Gamma \tag{12}$$

$$F_H = \int_\Gamma N^T \beta \; H_{env} d\Gamma \,. \tag{13}$$

Eq. 10 can be solved using one of the step-by-step integration schemes as follows (Logan 2002):

$$\left[I + \alpha \Delta t A\right]\overline{H}_{i+1} = \left[I - (1-\alpha)\Delta t A\right]\overline{H}_i + \Delta t(1-\alpha)P_i + \Delta t \alpha P_{i+1} \tag{14}$$

where

$$A = C^{-1}K \tag{15}$$
$$P = C^{-1}F_H \,. \tag{16}$$

The value of $\alpha$ should lie in the interval [0,1]; when $\alpha = 0$, This method is called Forward Euler (Explicit scheme); on the other hand, when $\alpha = 1$, 0.5, and 2/3,The methods are called Backward Euler, Trapezoidal and Galerkian, respectively (Implicit schemes).

## FINITE DIFFERNCE METHOD SOLUTION

The Crank-Nicolson scheme which is one of the powerful schemes of finite difference method (Allen and Isaacson 1997) can be employed to solve the moisture diffusion problem described in Eq. 3. The pore relative humidity (*H(x,t)* at different points of the mesh at different time intervals) is estimated as follows:

$$\delta_t^- M_H H_j^{n+1} - \frac{1}{2}\left(\delta_x D_H \delta_x H_j^{n+1} + \delta_x D_H \delta_x H_j^n\right) = 0 \tag{17}$$

where $\delta_t^-$ is the backward difference in time, $\delta_x$ is the central difference in space, $H_j^n$ is the value of relative humidity at point *j* and time *n*. Given the temporal grid as $\Delta t = k$, and the spatial grid $\Delta x = h$, Eq. 17 is rewritten as follows:

$$\begin{aligned} &-(1/2)\Gamma D_{j-1/2}^{n+1} H_{j-1}^{n+1} + (M_j^{n+1} + (1/2)\Gamma(D_{j-1/2}^{n+1} + D_{j+1/2}^{n+1}))H_j^{n+1} - (1/2)\Gamma D_{j+1/2}^{n+1} H_{j+1}^{n+1} = \\ &(1/2)\Gamma D_{j-1/2}^{n} H_{j-1}^{n} + (M_j^{n} + (1/2)\Gamma(D_{j-1/2}^{n} + D_{j+1/2}^{n}))H_j^{n} - (1/2)\Gamma D_{j+1/2}^{n} H_{j+1}^{n} \end{aligned} \tag{18}$$

where $\Gamma = k/h^2$ is the grid ratio.

Handling boundary condition in Eq. 6, which is known as Robin boundary condition, is done by assuming the difference equation holds at each of the boundary nodes. Then Eq. 6 can apply between the inner surface node (*j*=2) and a fictitious node at *j*=0 (knowing that the surface node is *j*=1) with the central difference in space $\delta_x$ as following:

$$\frac{D_H}{2h}(H_2 - H_0) = \beta(H_2 - H_{env}) \,. \tag{19}$$

Rearranging Eq. 19 gives:

$$H_0 = \gamma_1 H_2 + \gamma_2$$

where $\gamma_1 = 1 - 2h\beta / D_H$, *and* $\gamma_2 = 2h\beta H_{env} / D_H$ . (20)

Also, the boundary condition of Eq. 5 can be similarly done with the above steps and will give $\gamma_1 = 1$ and $\gamma_2 = 0$, which means no moisture exchange at that boundary.

Because of the coupling of the unknown $H$ associated with time step $n+1$ in Eq. 18, the following nonlinear system must be solved at each time step:

$$L_m H^{n+1} + L_v = R_m H^{n+1} + R_v \tag{21}$$

where

$$L_m = \begin{bmatrix} M_1^{n+1} + \frac{\Gamma}{2}(D_{0.5}^{n+1} + D_{1.5}^{n+1}) & -\frac{\Gamma}{2} D_{1.5}^{n+1}(1+\gamma_1) & & & \\ -\frac{\Gamma}{2} D_{1.5}^{n+1} & M_2^{n+1} + \frac{\Gamma}{2}(D_{1.5}^{n+1} + D_{2.5}^{n+1}) & -\frac{\Gamma}{2} D_{2.5}^{n+1} & & \\ & -\frac{\Gamma}{2} D_{2.5}^{n+1} & M_3^{n+1} + \frac{\Gamma}{2}(D_{2.5}^{n+1} + D_{3.5}^{n+1}) & -\frac{\Gamma}{2} D_{3.5}^{n+1} & \\ & \ddots & \ddots & & \\ & & -\frac{\Gamma}{2} D_{j-.5}^{n+1} + \gamma_1 & M_j^{n+1} + \frac{\Gamma}{2}(D_{j-.5}^{n+1} + D_{j+.5}^{n+1}) \end{bmatrix}$$

$$R_m = \begin{bmatrix} M_1^{n} - \frac{\Gamma}{2}(D_{0.5}^{n} + D_{1.5}^{n}) & \frac{\Gamma}{2} D_{1.5}^{n}(1+\gamma_1) & & & \\ \frac{\Gamma}{2} D_{1.5}^{n} & M_2^{n} - \frac{\Gamma}{2}(D_{1.5}^{n} + D_{2.5}^{n}) & \frac{\Gamma}{2} D_{2.5}^{n} & & \\ & \frac{\Gamma}{2} D_{2.5}^{n} & M_3^{n} - \frac{\Gamma}{2}(D_{2.5}^{n} + D_{3.5}^{n}) & \frac{\Gamma}{2} D_{3.5}^{n} & \\ & \ddots & \ddots & & \\ & & \frac{\Gamma}{2} D_{j-.5}^{n}(1+\gamma_1) & M_j^{n} - \frac{\Gamma}{2}(D_{j-.5}^{n} + D_{j+.5}^{n}) \end{bmatrix}$$

$$L_v = \begin{Bmatrix} \Gamma D_{.5}^{n+1}\gamma_2 \\ \vdots \\ \Gamma D_{.j+5}^{n+1}\gamma_2 \end{Bmatrix}$$

$$R_v = \begin{Bmatrix} \Gamma D_{.5}^{n}\gamma_2 \\ \vdots \\ \Gamma D_{j+.5}^{n}\gamma_2 \end{Bmatrix}.$$

## NUMERICAL APPLICATION

The results of hygromechanical simulations of concrete structures are presented in this section; three numerical examples are discussed in detail. First, the performance of the finite element and finite difference methods is studied. Then, a comparison between experimental and numerical results is shown. Finally, a full hygromechanical simulation of a bridge deck slab is presented. In the following examples, the environmental relative humidity, $H_{env}$, is assumed to be 0.5, and the value of surface moisture diffusion coefficient, $\beta$, is assumed to be 0.5 mm/day (Witasse et al. 2002).

## COMPARISON WITH THE EXACT SOLUTION

In order to study the performance of the two methods to solve Eq. 3, their results are compared to an exact solution. In this example, a constant moisture diffusion coefficient, $D_H$, and moisture capacity, $M_H$, are assumed to get an exact analytical solution of Eq. 3 as follows:

$$H(x,t) = A\exp(-D_H \lambda^2 t / M_H)\cos(\lambda(x - L_d)) + H_{env} \quad (22)$$

where $L_d$ is the depth of the slab. The moisture exchange occurs at $x$=0 and there is no diffusion occurs at $x$=$L_d$. $A$ is any arbitrary constant. Also, $\lambda$ is a constant which is required to satisfy the boundary condition of Eq. 6 at $x$=0, and it is defined as follows:

$$\lambda \tan(\lambda L_d) - \beta / D_H = 0 \,. \quad (23)$$

The above equation can be solved using Newton_Raphson scheme to find the constant λ. Figure 1 shows the results of the relative humidity profiles with $L_d$= 10 cm, $\lambda$= 0.1397, $D_H$=0.63, $M_H$=1.0 and $A$=0.5. With the number of elements equal to 10 (10 divisions), the finite element simulation gives better results than finite difference. However, as the number of divisions increase the finite difference shows better convergence to the exact solution.

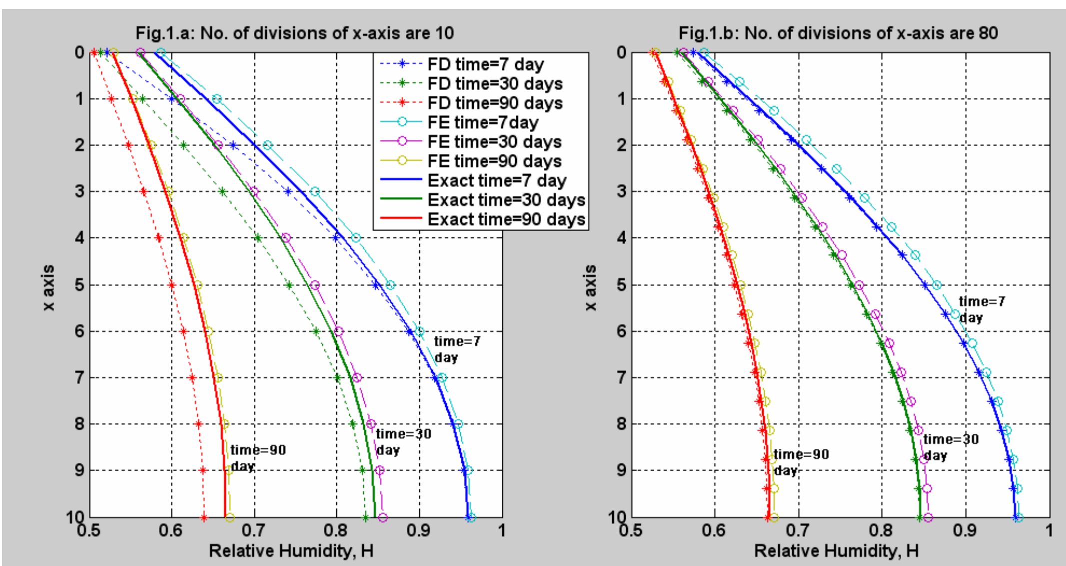


Figure 1: The comparison of realtive humidity profiles among exact solution, finite element and finite difference methods.

Also, Table1 shows the percentage of error to the exact solution for both methods at different time and position. It is clear that the finite difference with Crank_Nicolson scheme has a convergence rate with a first order. On other hand, the finite element method gives lower percentage of error than finite difference with ten elements, but it does not show any convergence.

Table 1: The comparison of the percentage of error to the exact solution for both finite element and finite difference methods.

| No. of divisions | Time= 50 days | | | | | | Time = 100 days | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Depth=3 cm | | Depth=5 cm | | Depth=8 cm | | Depth=3 cm | | Depth=5 cm | | Depth=8 cm | |
| | FD | FE | FD | FE | FD | FE | FD | FE | FD | FE | FD | FE |
| 10 | 4.8 | 0.7 | 3.8 | 0.9 | 2.9 | 1.0 | 4.2 | 0.4 | 4.2 | 0.6 | 4.2 | 0.7 |
| 20 | 2.3 | 0.7 | 1.8 | 0.9 | 1.3 | 1.0 | 2.1 | 0.4 | 2.1 | 0.6 | 2.0 | 0.7 |
| 40 | 1.1 | 0.7 | 0.9 | 0.9 | 0.6 | 1.0 | 1.1 | 0.4 | 1.0 | 0.6 | 1.0 | 0.7 |
| 80 | 0.6 | 0.7 | 0.4 | 0.9 | 0.3 | 1.0 | 0.5 | 0.4 | 0.5 | 0.6 | 0.5 | 0.7 |
| 160 | 0.3 | 0.7 | 0.2 | 0.9 | 0.2 | 1.0 | 0.3 | 0.4 | 0.3 | 0.6 | 0.3 | 0.7 |
| 320 | 0.1 | 0.7 | 0.1 | 0.9 | 0.1 | 1.0 | 0.1 | 0.4 | 0.1 | 0.6 | 0.1 | 0.7 |

## COMPARISON WITH EXPERIMENTAL DATA

Drying shrinkage due to ambient conditions can initiate damage in concrete structures. Drying shrinkage induced-damage accelerates the moisture diffusion of concrete by affecting the diffusion parameters.

The moisture capacity is defined as the derivative of the moisture content with respect to the relative humidity in pores. The BSB adsorption isotherm model is used to relate the moisture content with relative humidity (Brunauer et al. 1969) as follows:

$$w = \frac{C_0 \; k \; V_m \; H}{(1 - kH)[1 + (C - 1)kH]} \qquad (24)$$

where $V_m$ is the monolayer capacity which is the mass of adsorbate required to cover the adsorbent with a single molecular layer, $C_0$ is the net heat of adsorption, which is a function of temperature, and $k$ determines the degree of saturation of the pores. The moisture capacity, $M_H$, can be obtained by deriving the adsorption isotherm with respect to $H$ (more details in Xi et al. 1994 a, b). Bazant and Raftshol (1982) stated that the new surface area formed due to damage and cracks is small and cannot appreciably influence the internal surface area and thus the moisture capacity of concrete. Therefore, no effect of the damage on the moisture capacity is assumed in this study.

A moisture diffusivity model using S-shaped curves was developed by Bazant and Najjar (1972). Later this model was modified by others, e.g., Sakata (1983) and CEP_FIP (90). A modified version of Bazant and Najjar model is used in this study:

$$D(H) = D_1 \left( \alpha_0 + \frac{1 - \alpha_0}{1 + \left( \frac{1 - H}{1 - H_c} \right)^e} \right) \qquad (25)$$

where $D_1$ is the maximum of $D(H)$ for $H$ =1.0, $\alpha_0 = D_0/D_1$, $D_0$ is the minimum of $D(H)$ for $H$=0, $H_c$ is the pore relative humidity at $D(H)$ = 1/2 $D_1$, and $e$ is a constant  The constants in Eq. 25 were calibrated for best fits between experimental and numerical results. In addition, Ababneh et al. (2005) presented a model to incorporate the effect of damage on moisture diffusivity, and that model is used in this study.

Kim and Lee (1998) presented experimental data for concrete specimens with water-cement (w/c) ratio equal to 0.68; specimen dimensions were 10 X 10 cm exposed area with 20 cm in depth. Specimens were sealed from five sides to ensure one-direction moisture diffusion. Relative humidity probes were used to measure the relative humidity at 3, 7 and 12 cm from the exposed surface; the results are shown in Figure 2, and more details of the experiment and concrete mix design can be found in Kim and Lee (1998).

Because of the result from the comparison with the exact solution above, only the finite element method is used, and its results are compared with experimental results. By using the hygromechanical models developed in Ababneh et al. (2005), the numerical simulation is able to approximate the experimental results quite well. Figure 2 shows the experimental and numerical results using moisture diffusion coefficient in Eq. 25 with $D_1$= 0.6168 cm$^2$/day, $H_c$=0.85, $\alpha_0$ = *0.12*, and $e$= 3. As shown in Figure 2.a, the numerical results are in good agreement with the experimental data. Also, Figure 2.b shows the numerical results of the relative humidity profiles with different times.

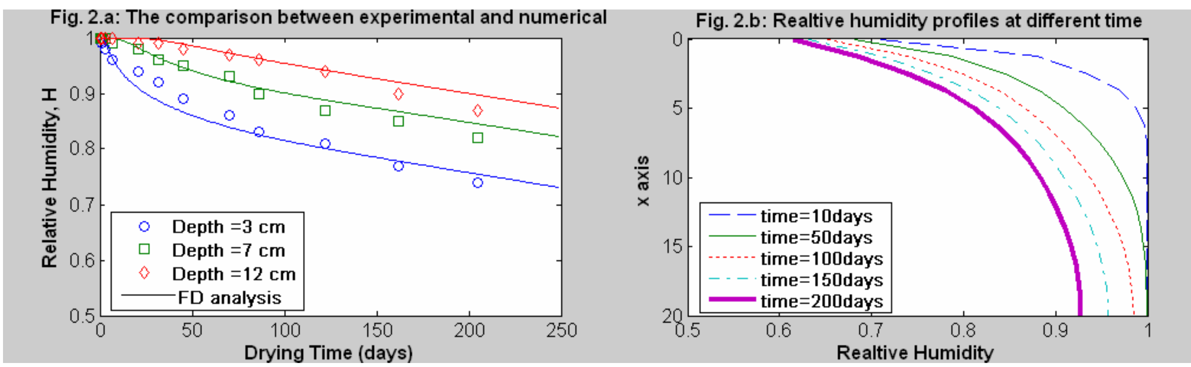


Figure 2 : Relative humidity verses drying time and depth.

### SIMULATION OF BRIDGE DECK SLAB

A concrete slab, 20 cm in depth, is simulated by the fully coupled hygromechanical model mentioned above. The concrete has an average compressive strength of 34 MPa and is moist cured for 28 days before drying. The slab, which is initially saturated ($H_{ini}$=100%), is exposed to drying on the top surface ($H_{env}$= 50 %) after curing. The effect of micro-cracking due to drying shrinkage is taken into account through the damage parameter, $d$; the mechanical analysis is done within the framework of continuum damage theory (Ababneh et al. 2005).

Figure 3 shows result comparisons of the slab simulation for two cases: case I, when the effect of damage on moisture diffusivity is ignored and only Eq. 25 is applied, case II, when full coupling between damage and moisture diffusion is considered. In this case, the drying process generates damage in concrete, which accelerates the drying process; this is clear in Figure 3.a, at 50 days. However, at 10 days, the difference in relative humidity profiles starts only near the top surface (exposed to drying). Then, the difference in relative humidity profiles between both cases increases with time. Figure 3.b shows that the damage in concrete is accelerated and reached higher values in case II, which means ignoring the coupling effect between damage and moisture diffusion can lower the estimation of the drying process and damage.

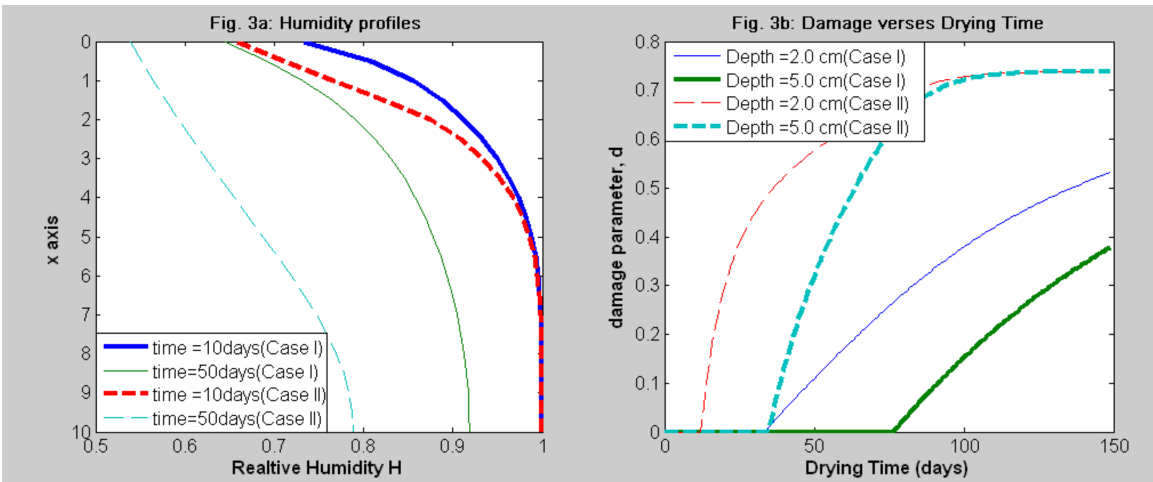


Figure 3 : The relative humidity profiles and the damage parameter verses drying time for the bridge deck slab.

## CONCLUSIONS

Two numerical methods, finite element and finite difference, were described to simulate the moisture diffusion in concrete including the coupling between the diffusion and the induced damage. Numerical solutions were obtained for simple problem with known exact solution, concrete specimen with available experimental data, and bridge deck slab simulation.

Based on the numerical results presented in this paper, the following conclusions can be drawn:

1. Both finite element and finite difference provided reasonable predication of the drying process and damage propagation in concrete.

2. The finite element solution gave better predictions for the drying process with less number of elements.

3. The simulation also showed that ignoring the effect of damage on the moisture diffusion process yields an overestimation of the relative humidity in concrete.

4. This model can be used on to analyze different types of concrete structures, and with some modification can be used for durability and service life predictions of reinforced concrete structures.

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