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NUMERICAL SOLUTION OF MASS TRANSPORT EQUATIONS IN CONCRETE STRUCTURES

by

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ABSTRACT

To calculate the service life of reinforced concrete (R.C.) structures, the process of reinforcement corrosion was modeled using a numerical formulation of the associated mass transport partial differential equations (PDE's). Migration of chlorides, moisture and heat transfer within concrete, resulting from seasonal variations in the surface conditions of the R.C. member, form a coupled boundary-value problem, which was solved in space using a finite element formulation and in time using a finite difference marching scheme. The stage of active corrosion was modeled by including in the numerical algorithm of the F.E. formulation the mass conservation equation that describes diffusion of oxygen in the concrete cover. The paper presents details of the F.E. formulation and computed results from selected case studies.

Keywords: Corrosion; far field boundary; finite elements; Galerkin formulation; heat transfer; mapped infinite elements; mass transport.

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DEFINITION OF THE ASSOCIATED PHYSICAL PROBLEM

The service life of reinforced concrete highway structures is often limited by chloride-induced corrosion of the reinforcement, due to exposure to marine environments or to de-icing salts that are routinely used in the winter. Corrosion leads to loss of reinforcement section, loss of steel-concrete bond and delamination of the concrete cover with detrimental consequences on the load carrying capacity of the structure.

In general, concrete protects embedded reinforcing steel against corrosion by providing a highly alkaline environment ($\text{pH} > 13.0$) that maintains the steel in a passive state. The concrete cover also serves as a physical barrier against the ingress of aggressive species that are necessary to initiate and sustain the process of corrosion. In the literature, corrosion of steel in concrete is usually idealized as a sequence of two separate phases: *initiation* and *propagation* of the chemical process (Fig. 1, [1]). During *initiation* chlorides migrate from the surface of the member through the concrete cover to the steel reinforcement. When their concentration exceeds a threshold value, the pH level is considered low enough that the oxidation of iron may take place, and this point is referred to as *depassivation*. (Note that steel dissolution is a process by which iron converts to ferrous and ferric oxides, and hence the presence of oxygen is required to sustain it). During the *propagation* stage corrosion takes place until an unacceptable level of steel loss occurs, or until the concrete cover spalls-off (the end of service life may be defined in terms of a mechanical index that characterizes unacceptable performance of the reinforced concrete member).

Migration or *transport* of the various species that participate in the mechanism of corrosion is facilitated by the network of interconnected pores in the material structure. Species diffuse through the pore water due to concentration gradients that exist between the exposed surface and the pore solution of the cement matrix in saturated concrete. Another transport mechanism is that of capillary sorption (or desorption) which occurs when concrete is partially saturated. As water flows from saturated to partially saturated areas, it carries along dissolved chlorides or oxygen that add to the total concentration.

The two main mechanisms of transport, i.e., diffusion and capillary sorption, are governed by considerations of mass conservation (modified version of Fick's 2nd law). Whether chloride ions (Cl^-) or oxygen (O_2) are considered, their transport by sorption is coupled with the movement of moisture (water) in concrete. Moisture diffusion is also governed by mass conservation

considerations (Fick's 2nd law), but it also depends on temperature, T , since the temperature affects both the state of pore water and the diffusivity characteristics of concrete.

Thus, in order to describe mathematically the process of corrosion, the transport equations of the following four coupled physical problems must be resolved simultaneously: (1) chloride transport, (2) moisture diffusion, (3) heat transfer, and (4) oxygen transport.

MATHEMATICAL DEFINITION OF THE PROBLEM

Based on conservation of mass (or energy in the case of heat transfer), the partial differential equations governing these four coupled boundary value – initial value problems all have the same general form, i.e.,

$$\kappa \frac{\partial \phi}{\partial t} + \underbrace{\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y}}_{\text{diffusion}} + \underbrace{\frac{\partial J'_x}{\partial x} + \frac{\partial J'_y}{\partial y}}_{\text{sorption}} = 0 \quad (1)$$

Table 1 shows the correspondence between Eqn. (1) and the different governing field equations. For the sake of completeness of the mathematical definition of the problem, the following physical aspects must also be considered in establishing the solution procedure:

(1) Depassivation and initiation of corrosion is due to the chloride ion (Cl^-) concentration in the pore solution (known as free chlorides, denoted in the remainder as C_{fc}). Apart from chlorides dissolved in the pore solution, some Cl^- in concrete may be physically or chemically bound to the cement hydrates. This binding capacity of the hydrates affects chloride ionic mobility, effectively reducing the diffusivity of Cl^- in concrete D_c (m^2/s) to an apparent value D_c^* (m^2/s). Figure 2 presents established models for the binding properties of cements in the form of binding isotherms [2]. Through those curves the concentration of bound chlorides, C_{bc} , is expressed in terms of the concentration of free chlorides, C_{fc} . The total concentration of Cl^- in concrete is $C_{tc} = C_{bc} + \omega_e C_{fc}$ (kg/m^3 of concrete), where ω_e is the evaporable water content (m^3 of pore solution/ m^3 of concrete) and C_{bc} and C_{fc} are given as kg/m^3 of concrete and kg/m^3 of pore solution, respectively.

(2) The apparent diffusion coefficient D_c^* is obtained from a reference value of diffusivity which is a characteristic of concrete, $D_{c,ref}$, by consideration of temperature, T , age, t , relative humidity, h , and chloride binding capacity of concrete, $\partial C_{bc} / \partial C_{fc}$, through pertinent mathematical expressions [3, 4]:

$$D_c^* = \frac{D_c}{1 + \frac{1}{\omega_e} \frac{\partial C_{bc}}{\partial C_{fc}}} \text{ (m}^2\text{/s)}; \quad D_c = D_{c,ref} \cdot F_1(T) \cdot F_2(t) \cdot F_3(h); \quad (2)$$

$$F_1(T) = \exp\left[\frac{U}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]; \quad F_2(t) = \left(\frac{t_{ref}}{t}\right)^m; \quad F_3(h) = \left[1 + \frac{(1-h)^4}{(1-h_c)^4}\right]^{-1}$$

where U is the activation energy of the chloride diffusion process (kJ/mol), reported as 41.8, 44.6 and 32 kJ/mol for water:cementitious ratios of 0.4, 0.5 and 0.6, respectively [5], R is the gas constant (8.314×10^{-3} kJ/K·mol), T_{ref} is the reference temperature at which the chloride diffusivity $D_{c,ref}$ has been measured (K), T is the actual absolute temperature in concrete (K), t_{ref} is the time of exposure at which $D_{c,ref}$ has been evaluated (s), t is the actual time of exposure (s), m is an age reduction factor, dependent on the concrete mix proportions, h is the concrete pore relative humidity, and h_c is the humidity level at which D_c drops halfway between its maximum and minimum values, taken as 0.75 [6].

(3) Similarly, the humidity diffusion coefficient is obtained from a reference value $D_{h,ref}$, which is determined at specified reference conditions, by considering the effect of pore relative humidity, temperature and age [4, 6, 7, 8]:

$$D_h = D_{h,ref} \cdot G_1(h) \cdot G_2(T) \cdot G_3(t_e);$$

$$G_1(h) = 0.05 + 0.95 \frac{1}{1 + \left(\frac{1-h}{1-h_c}\right)^n}; \quad G_2(T) = \exp\left[\frac{U}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]; \quad G_3(t_e) = 0.3 + \sqrt{\frac{13}{t_e}} \quad (3)$$

Here n is a parameter characterizing the spread of the drop in D_h (ranging from 6 to 16 [6, 7]), U is the activation energy of the moisture diffusion process (typical values for U/R range from 2700 K to 4700 K [3, 6]), and t_e is an equivalent hydration period of concrete (s).

(4) Parameters ρ_c , c_q , and λ in the equation of heat transfer (Eqn. 1.3, Table 1) are, respectively, the density (kg/m³), the specific heat capacity (J/kg·°C) and the thermal conductivity of concrete (W/m·°C). For simplicity they have been assumed constant and insensitive to changes in moisture content and temperature [9]. Temperature T in Eqn. 1.3, Table 1, is given in °C.

(5) Oxygen availability at the cathodic areas determines the rate of metal corrosion. In Eqn. 1.4, Table 1, C_o is the amount of oxygen dissolved in the concrete pore solution (kg/m³ of solution)

and D_o represents the oxygen diffusion coefficient (m^2/s) expressed as a function of the degree of water saturation in concrete [4].

MATHEMATICAL MODEL

From the preceding discussion it is evident that the process of corrosion in reinforced concrete is modeled through a set of four partial differential equations that describe chloride ingress into concrete, moisture and heat diffusion through concrete, and oxygen transport to the reinforcement. A closed-form solution of this system of equations is not possible due to the dependence of the various material properties and boundary conditions on the physical parameters of the concrete and the time level of exposure. In this paper a two-dimensional finite element formulation is developed to solve numerically the transport equations in space as a boundary-value problem and in time as an initial-value problem. Pertinent boundary conditions are enforced to simulate seasonal variations in exposure conditions. A time-step integration procedure (finite-difference scheme) is applied to determine the variation in time of the different variables in concrete [4].

During the initiation stage, the first three of the four transport equations are solved simultaneously in order to obtain variations in time t and space (x, y) of the concentration of chlorides in the pore solution, C_{fc} , the level of pore relative humidity, h , and the temperature distribution, T , within concrete. The concentration of total chlorides in concrete, C_{tc} , and the amount of evaporable water, ω_e , are determined by means of chloride binding relationships and adsorption isotherms, respectively. Once the concentration of chlorides in contact with the reinforcing steel reaches a specified threshold value, the oxygen-transport equation is added to the system of equations being solved to obtain the distribution of dissolved oxygen, C_o , in concrete. An estimate of the corrosion current is obtained from the concentration-polarization equation where the kinetics of the cathodic reaction are limited by depletion of oxygen at cathodic sites.

The derivation of the weak form of the governing differential equations and its numerical implementation are presented in the following sections.

F.E. FORMULATION OF GOVERNING DIFFERENTIAL EQUATIONS

Since all of the transport equations considered have a similar mathematical structure (Eqn. 1), a single numerical tool is required to solve any of them. Using the Galerkin weighted residual method on Eqn. (1) yields,

$$\int_{\Omega} W_i \left(\kappa \frac{\partial \phi}{\partial t} + \underbrace{\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y}}_{\text{diffusion}} + \underbrace{\frac{\partial J'_x}{\partial x} + \frac{\partial J'_y}{\partial y}}_{\text{sorption}} \right) d\Omega = 0 \quad (4)$$

In Eqn. (4) $W_i(x,y)$ is the weighting function and Ω is the domain of the problem. In a single element domain, the field variable ϕ is expressed in terms of the element nodal values, $\phi^{(e)} = [N]\{\Phi^{(e)}\}$, where $[N]$ is the row vector containing the element interpolation functions associated with each node and $\{\Phi^{(e)}\}$ is the vector of nodal degrees of freedom (unknowns). Using the shape functions as weighting functions (i.e., $W_i = N_i$, the subscript i referring to the corresponding node number) and expanding terms, the element residual takes the form,

$$\int_A [N]^T \left\{ \kappa \frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x} \left(D \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial y} \left(D \frac{\partial \phi}{\partial y} \right) - \frac{\partial \phi}{\partial x} D_h \frac{\partial h}{\partial x} - \frac{\partial \phi}{\partial y} D_h \frac{\partial h}{\partial y} - \right. \\ \left. \phi \left[\frac{\partial}{\partial x} \left(D_h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_h \frac{\partial h}{\partial y} \right) \right] \right\} dA = 0 \quad (5)$$

In Eqn. (5), A is the domain of a single element. Using the product-rule of differentiation and Green's theorem, the second-spatial derivatives are replaced by first-derivative terms:

$$\int_A \kappa [N]^T \frac{\partial \phi}{\partial t} dA - \oint [N]^T D \left(\frac{\partial \phi}{\partial x} \cos \gamma + \frac{\partial \phi}{\partial y} \sin \gamma \right) ds + \int_A D \left(\frac{\partial [N]^T}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial [N]^T}{\partial y} \frac{\partial \phi}{\partial y} \right) dA \\ - \int_A D_h [N]^T \left(\frac{\partial h}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial h}{\partial y} \frac{\partial \phi}{\partial y} \right) dA - \int_A [N]^T \frac{\partial \omega_e}{\partial h} \frac{\partial h}{\partial t} \phi dA = 0 \quad (6)$$

where s denotes the element boundary and γ is the angle of the outward normal with respect to the x -direction. Time derivatives of the field variable are related to time derivatives of the nodal variables using consistent formulation [10]:

$$\frac{\partial \phi^{(e)}}{\partial t} = [N]\{\dot{\Phi}^{(e)}\} \quad (7)$$

By substituting in Eqn. (6), the transport equation (1) is obtained in matrix form for the element as:

$$[c^{(e)}]\{\dot{\Phi}^{(e)}\} + \{I^{(e)}\} + [k^{(e)}]\{\Phi^{(e)}\} = 0 \quad (8)$$

where, $[c^{(e)}]$, known as the capacitance matrix, is given by:

$$[c^{(e)}] = \int_A \kappa [N]^T [N] dA \quad (9)$$

The inter-element vector, $\{I^{(e)}\}$ [10], is given by:

$$\{I^{(e)}\} = -\oint [N]^T D \left(\frac{\partial \phi}{\partial x} \cos \gamma + \frac{\partial \phi}{\partial y} \sin \gamma \right) ds \quad (10)$$

where integration is performed on the element boundary in a counterclockwise direction. Last, the element property matrix, $[k^{(e)}]$, is given by:

$$\begin{aligned} [k^{(e)}] = & \underbrace{\int_A D[B]^T [B] dA}_{[k_1^{(e)}]} - \underbrace{\int_A D_h [N]^T \left[\frac{\partial [N]}{\partial x} \{h^{(e)}\} \quad \frac{\partial [N]}{\partial y} \{h^{(e)}\} \right] [B] dA}_{[k_2^{(e)}]} \\ & - \underbrace{\int_A \frac{\partial \omega_e}{\partial h} [N]^T [N] \{\dot{h}^{(e)}\} [N] dA}_{[k_3^{(e)}]} \end{aligned} \quad (11)$$

From a mathematical perspective, matrix $[k^{(e)}]$ is similar to the element stiffness matrix in mechanics applications. Entries of matrix $[B]$ are the element interpolation gradient vectors, i.e.,

$$[B]^T = \begin{bmatrix} \frac{\partial [N]^T}{\partial x} & \frac{\partial [N]^T}{\partial y} \end{bmatrix} \quad (12)$$

Boundary conditions are enforced by specifying either the value of ϕ at the boundary or the flux across it. When fluxes across the boundary are specified, the boundary condition takes the following form:

$$-D \left(\frac{\partial \phi}{\partial x} \cos \gamma + \frac{\partial \phi}{\partial y} \sin \gamma \right) = L \phi_b - M \quad (13)$$

where ϕ_b represents the value of ϕ at the boundary (unknown quantity), and L and M are two constants. Equation (13) assumes the boundary flux going into the body. Substituting Eqn. (13) into the expression for the inter-element vector, Eqn. (10) takes the form:

$$\begin{aligned} \{I^{(e)}\} &= \oint [N]^T (L \phi_b - M) ds = \\ &= \oint [N]^T (L [N] \{\Phi^{(e)}\} - M) ds = \underbrace{\left(\oint L [N]^T [N] ds \right) \{\Phi^{(e)}\}}_{[k_4^{(e)}]} - \oint M [N]^T ds \end{aligned} \quad (14)$$

The term $\oint L [N]^T [N] ds$ which multiplies $\{\Phi^{(e)}\}$ adds to the element property matrix $[k^{(e)}]$, whereas the component $\oint M [N]^T ds$ constitutes the element environmental load vector, $\{f^{(e)}\}$, i.e.,

$$[k^{(e)}] = [k_1^{(e)}] - [k_2^{(e)}] - [k_3^{(e)}] + [k_4^{(e)}]; \quad \{f^{(e)}\} = \oint M [N]^T ds \quad (15)$$

Note that the integrals in Eqs. (14) and (15) are only evaluated at the element boundaries where fluxes are specified.

After element assembly for the entire mesh, a system of linear first-order differential equations in the time domain is obtained:

$$[C]\{\dot{\Phi}\} + [K]\{\Phi\} - \{F\} = 0 \quad (16)$$

This is integrated in time using a finite difference approximation, i.e., variables $\{\Phi\}^{t+\Delta t}$ at time $t+\Delta t$ are evaluated in terms of the solution $\{\Phi\}^t$ at time t using the following algorithm [10, 11]:

$$([C] + \theta \Delta t [K])\{\Phi\}^{t+\Delta t} = ([C] - (1-\theta)\Delta t [K])\{\Phi\}^t + \Delta t((1-\theta)\{F\}^t + \theta\{F\}^{t+\Delta t}) \quad (17)$$

where Δt denotes the time increment and θ is a parameter ranging from 0 to 1 (the Crank Nicolson method with asymptotic rate of convergence Δt^2 is obtained with $\theta = 0.5$).

BOUNDARY CONDITIONS

Initial values for C_{fc} , h , T and C_o in the concrete need be specified at time $t=0$. It is common practice to take $C_{fc}(t=0)=0$ unless chlorides have been externally added to the concrete mix. Boundary conditions simulating exposure conditions on the free surface of the concrete member are enforced by means of fluxes, which depend on the difference between the environmental and the concrete surface values. These are related by surface mass transfer coefficients, B_c , B_h , and B_T (for chlorides, m/s, moisture, m/s, and heat convection, $W/m^2 \cdot ^\circ C$).

Typical form of the boundary conditions considered is given by Eqn. (13). Table 2 gives the correspondence between L and M values in Eqn. (13) and the different boundary conditions associated with the diffusive and sorptive terms of the transport problems considered in this work. To define the environmental values for Cl , h , and T (i.e., C_{en} , h_{en} , and T_{en}) the idealized yearly distributions of Fig. 3 are considered. Exposure of reinforced concrete highway structures to de-icing salts occurs only during the wintertime and hence, application of chlorides to concrete is discontinuous. Assuming a step function for the amount of applied chlorides (Fig. 3(a)) enforces this environmental condition. To simulate the seasonal variation in temperature and humidity, a sinusoidal function is used to calculate the environmental values for temperature and humidity (Fig. 3(b), 3(c)).

DERIVATION OF ELEMENTS

The field variable ϕ was modeled as a linear function in x and y within the element, since only first order spatial derivatives of the element shape functions were required in Eqns. (9)-(14). The region of interest was discretized using linear triangular and bilinear rectangular finite elements as shown in Fig. 4. Note that for the transport problems considered, the area of primary interest

comprises the concrete cover to the steel reinforcement. This region is a small fraction of the entire cross section of the reinforced concrete member. To keep the problem size as well as the computational effort manageable, it is common practice to truncate the finite element model at an arbitrary distance that is sufficiently far from the region of interest. Far field boundary conditions need be imposed at this limiting edge. If this artificially created boundary lies on an axis of symmetry, then the condition imposed is zero normal flux (i.e., $\partial\phi/\partial n=0$); otherwise, the far field boundary condition corresponds to the initial condition of the problem. A difficulty that arises with simple truncation is the positioning of the remote boundary in order to obtain an accurate solution. This problem has been addressed in finite element formulations by treating the domain corresponding to the far field as infinite in extent and using what is known as “infinite elements”, which extend the domain of a finite element to infinity so that it remains unbounded [12]. Use of infinite elements in a finite element model allows for satisfactory results to be obtained from fewer elements than would otherwise be required [13]. To formulate the infinite element, the finite domain is mapped onto an infinite domain, with the infinite dimension in the direction of interest [12, 14, 15].

In the following sections the shape functions of the finite and infinite elements used in this formulation are listed. Values of the capacitance and property matrices and of the force vector for each element type, calculated with the respective shape functions, are given in Appendix I.

(a) Linear triangular element (3-noded with straight sides)

The field variable is approximated as $\phi=N_i\Phi_i$, $i=1,3$, where N_i is the shape function associated with node i , and Φ_i is the nodal value of ϕ . Note that:

$$N_i = \frac{1}{2A}(a_i + b_i x + c_i y); \quad \begin{pmatrix} a_i = & X_j Y_k - X_k Y_j \\ b_i = & Y_j - Y_k \\ c_i = & X_k - X_j \end{pmatrix}; \quad A = \frac{1}{2} \begin{vmatrix} 1 & X_i & Y_i \\ 1 & X_j & Y_j \\ 1 & X_k & Y_k \end{vmatrix} \quad (18)$$

where (X_i, Y_i) are the coordinates of node i and A is the area of the triangle.

(b) Bilinear rectangular element (4-noded with straight sides)

In the orthogonal local coordinate system $x'-y'$, which is centered on node i , the element is rectangular with sides $2b \times 2a$. The field variable is approximated as $\phi=N_j\Phi_j$, $j=1,4$, where N_j is the shape function associated with node j and Φ_j is the corresponding nodal value of ϕ . With reference to the system of axes $x'-y'$, the shape functions are given by:

$$N_i = (1 - \frac{x'}{2b})(1 - \frac{y'}{2a}); \quad N_j = \frac{x'}{2b}(1 - \frac{y'}{2a}); \quad N_k = \frac{x'y'}{4ab}; \quad N_l = \frac{y'}{2a}(1 - \frac{x'}{2b}) \quad (19)$$

(c) Mapped infinite elements

The two types of mapped infinite elements presented here are based on the bilinear rectangular element described in the preceding and illustrated in Fig. 5(a) in the natural coordinate system (ξ, η). These are [15]:

- (1) *bilinear singly infinite element*, which extends to infinity in the ξ direction only, as shown in Fig. 5(b). This may be derived from the bilinear rectangular element, if the two nodes corresponding to $\xi=+1$ are positioned at infinity.
- (2) *bilinear doubly infinite element*, which extends to infinity in both the ξ and η directions, as shown in Fig. 5(c). This is derived from the bilinear rectangular element by positioning at infinity the nodes corresponding to both $\xi=\eta=+1$. This element is employed as a *corner* element in a mesh where transition is needed between regions extending to infinity along two different directions [14].

The geometry of both elements is interpolated according to $x(\xi, \eta) = [M]\{X\}$ and $y(\xi, \eta) = [M]\{Y\}$, where $[M]$ is a row vector of geometric mapping functions and $\{X\}$ and $\{Y\}$ are the vectors containing the global x and y coordinates of the finite nodes, respectively. Mapping functions for the bilinear singly and doubly infinite elements are listed below [14].

$$\left(\begin{array}{l} M_i = \frac{-\xi(1-\eta)}{1-\xi} \\ M_j = \frac{(1+\xi)(1-\eta)}{2(1-\xi)} \\ M_k = \frac{(1+\xi)(1+\eta)}{2(1-\xi)} \\ M_l = \frac{-\xi(1+\eta)}{1-\xi} \end{array} \right); \quad \left(\begin{array}{l} N_i = \frac{1}{4}(1-\xi)(1-\eta) \\ N_l = \frac{1}{4}(1-\xi)(1+\eta) \end{array} \right); \quad \left(\begin{array}{l} M_i = \frac{4\xi\eta}{(1-\xi)(1-\eta)} \\ M_j = \frac{-2\eta(1+\xi)}{(1-\xi)(1-\eta)} \\ M_k = \frac{(1+\xi)(1+\eta)}{(1-\xi)(1-\eta)} \\ M_l = \frac{-2\xi(1+\eta)}{(1-\xi)(1-\eta)} \end{array} \right); \quad N_i = \frac{1}{4}(1-\xi)(1-\eta) \quad (20)$$

Bilinearsingly infinite element

Bilineardoubly infinite element

For the geometrical mapping to be independent of the selection of the coordinate system, it is required that the sum of infinite element mapping functions be equal to 1 [12]. When forming a singly infinite element from the bilinear rectangular element, it is difficult to enforce simultaneously the singularity at $\xi = +1$ and the invariance requirement under change of coordinate origin [14]. To solve the problem, Marques and Owen [14] suggest that two extra

nodes be included for the geometric mapping only (represented by the white nodes in Fig. 5(b)). Similarly, three additional nodes are required to define the geometric mapping of the doubly infinite element (Fig. 5(c)).

The field variable ϕ is interpolated within the mapped infinite elements using the standard shape functions of the parent finite element (the bilinear rectangular element in this case) according to $\phi^{(e)} = [N]\{\Phi^{(e)}\}$. If the value of ϕ can be manipulated so that it approaches zero at infinity, the effect of the interpolation functions $[N]$ associated with those nodes located at infinity ($\xi = +1$ for the singly infinite and $\xi = \eta = +1$ for the doubly infinite) can be removed from the mathematical formulation, since, by doing so, the zero boundary condition is automatically satisfied [14, 15]. This reduces the size of the elements as well as the associated matrices and vectors and increases the efficiency of the computational analysis. The bilinear singly infinite element can thus employ only two nodes for the field variable description (nodes i and l in Fig. 5(b)), whereas the bilinear doubly infinite element can employ only one (node i in Fig. 5(c)), i.e.,

$$\phi^{(e)} = \begin{cases} N_i\phi_i + N_l\phi_l & \text{when } \phi(\xi = +1) = 0 & \text{for the singly infinite} \\ N_i\phi_i & \text{when } \phi(\xi = +1) = \phi(\eta = +1) = 0 & \text{for the doubly infinite} \end{cases} \quad (21)$$

Note that the nodes used for interpolation of the field variable ϕ (black nodes in Fig. 5(b, c)) are not the same set of nodes used for geometrical mapping (black and white nodes in Fig. 5(b, c)). Since the standard shape functions $[N]$ are of lower degree than the mapping functions $[M]$, the mapped infinite elements illustrated in Fig. 5(b, c) are superparametric. The geometry and field variable expansions involved in the mapped infinite elements are both referred to a set of poles, i.e., singular points about which the field quantity, ϕ , decays [14]. The poles must be located outside the infinite element, but their positioning is arbitrary and depends on the geometric and physical characteristics of the problem (Fig. 5(b, c)). The external nodes of the infinite elements are located halfway between the poles and the first set of internal nodes [12, 14, 15].

(d) Boundary conditions at infinity

The use of mapped infinite elements is restricted to problems where the field variable, ϕ , tends monotonically to a limiting value at infinity. It has been previously mentioned that when ϕ approaches zero at infinity, the boundary condition is automatically satisfied by removing the influence of nodes located at infinity in the finite element formulation (Eqn. (21)). However, for the type of problems being solved here, the field variable at infinity does not always tend to zero but to a constant initial value. For the latter case, the zero-boundary condition approach can still be preserved if the initial value is subtracted from the field variable ϕ [12, 15]. The problem is

then expressed in terms of a new field variable, ψ , which is defined as, $\psi(x,y,t) = \phi(x,y,t) - \phi(x,y,0)$ for $t > 0$, where $\phi(x,y,0)$ is the specified initial condition of the problem. In light of this definition, Eqn (16) simplifies to:

$$[C]\{\dot{\Psi}\} + [K]\{\Psi\} - \{F\} = 0 \quad (22)$$

which is solved for ψ with initial condition $\psi(x,y,0)=0$, whereas the transient and spatial distribution of ϕ is calculated from the above definition of ψ . Note that external boundary conditions in the transformed problem also have to be decreased by $\phi(x,y,0)$.

Fluxes along any edge extending to infinity are incompatible with the assumption of ϕ vanishing at infinity [14]. Thus fluxes in infinite elements can only be specified along the edge common to the finite elements to which they are connected, and they can be assigned to the finite element instead of the infinite element for the sake of simplicity. Therefore, Eqn. 14 that results from specifying fluxes along the boundary of an element does not need to be evaluated for the mapped infinite elements described above.

(c) Evaluation of element matrices

The capacitance and property matrices and the inter-element vector were evaluated in closed form for the element types described in the preceding ([4], Appendix I). Particularly for calculating the integrals for the mapped infinite elements, the domain of integration dA was written in terms of the natural coordinates (ξ, η) :

$$dA = dx \cdot dy = \det[J] d\xi \cdot d\eta; \quad [J] = \begin{bmatrix} \frac{\partial[M]}{\partial\xi} \\ \frac{\partial[M]}{\partial\eta} \end{bmatrix} \begin{bmatrix} X & Y \end{bmatrix} \quad (23)$$

where $[M]$ is the row vector containing the mapping functions given in Eqn. (20), and X and Y are the vectors containing the global x and y coordinates of the nodes defining the element geometry, respectively (black and white nodes in Fig. 5(b, c)). The geometric mapping functions $[M]$ are therefore used to relate the coordinates in the global system x - y to the natural system ξ - η through the computation of the Jacobian matrix $[J]$. Matrix $[B]$ in Eqn. (12), which contains the derivatives of the shape functions $[N]$ with respect to the global coordinates x and y , is evaluated for mapped infinite elements according to:

$$[B]^T = \begin{bmatrix} \frac{\partial[N]^T}{\partial x} & \frac{\partial[N]^T}{\partial y} \end{bmatrix} = [J]^{-1} \begin{bmatrix} \frac{\partial[N]^T}{\partial\xi} & \frac{\partial[N]^T}{\partial\eta} \end{bmatrix} \quad (24)$$

SOLUTION PROCEDURE

The implementation of Eqn. (17) to each of the transport problems considered in this formulation results in a system of nonlinear equations for moisture, chloride and oxygen transport in concrete. Assuming λ , c_q and ρ_c constant, the solution of the equation governing heat transfer in concrete yields a system of linear equations. The nonlinearity of the moisture and chloride problems arises from the dependence of coefficients D_h and D_c on the unknowns h and C_{fc} , respectively. The dependence of D_c on the free chloride concentration C_{fc} is only manifested when nonlinear binding (Fig. 2) is considered. The nonlinearity of the oxygen transport problem is due to the dependence of the imposed boundary conditions at the steel/concrete interface on the concentration of dissolved oxygen C_o available at the reinforcing steel surface.

Equation (17) was solved by means of a frontal solver [16], which takes advantage of the symmetry of the capacitance and most of the property matrices by only storing their upper triangle in a one-dimensional array. In the problem describing chloride ingress into concrete, the property matrices resulting from integration of the sorptive term are nonsymmetric (Appendix I), and thus the frontal solver was modified for this particular case by storing the element matrices in their entirety [4].

(a) Numerical parameters

Solutions to Eqn. (17) were obtained using $\theta \geq 0.5$ (unconditional stability for a constant time step Δt). Sudden changes in the imposed boundary conditions such as for example step-wise increase in the supply of chlorides at the boundary (simulating exposure to de-icing salts in winter) caused oscillations in the solution of the chloride transport equation. Oscillations were numerically dampened by increasing θ to $2/3$ and by approximating the step increase/decrease in the value of C_{en} with a very steep linear function.

The time step was selected based on considerations of accuracy and efficiency. Initially, the nonlinear solution of Eqn. (17) was iterated at each time step by evaluating coefficients from the values of ϕ obtained at a previous iteration. To increase the rate of convergence in a given time step, successive underrelaxation was employed. Iterations were terminated when a predefined convergence criterion ε was reached at the given time step:

$$\left| \frac{\phi^{i+1} - \phi^i}{\phi^i} \right| \leq \varepsilon; \quad \phi^{i+1} = \omega \phi^{i+1} + (1 - \omega) \phi^i \quad \text{with} \quad 0 < \omega < 1 \quad (25)$$

where ω is the relaxation parameter.

To determine the optimum time step, moisture profiles along the diagonal 1-104 of the two-dimensional mesh shown in Fig. 6(a), which represents the corner of a reinforced concrete member section, were calculated and are plotted in Figure 6. With reference to Fig. 3(b), which represents the moisture boundary conditions at the free surface of the member, h_{max} and h_{min} were taken as 90% and 65%, respectively. Results were obtained using $\Delta t = 1, 2$ and 5 days, and a duration of exposure of either 120 or 365 days. The largest difference between solutions was observed in the early stages of exposure and tended to decrease with time. After 5 years of exposure the profiles were practically identical regardless of the selected time step. However, the number of iterations required to achieve convergence increased significantly with Δt (using $\varepsilon = 10^{-4}$). For this reason, Δt was taken as 1 day in the subsequent analyses.

The optimum value of ω , for which convergence was faster, was found to be 0.1, which means that more weight is put on the solution of variable ϕ obtained at a previous iteration. However, it was noticed that the problem of chloride transport with nonlinear binding posed convergence problems, especially at the points where de-icing salts are no longer applied ($C_{en} = 0$ in the step function, Fig. 3(a)). In these cases the problem was treated as a linear one evaluating D_h and D_c from humidity and chloride concentration values obtained at a previous time level without any iterations. To minimize the error, the time step Δt was then reduced to 12 hours.

(b) Solution algorithm

After input of the general geometry of the finite element mesh, material properties, chloride threshold concentration, and initial and boundary conditions, the solution proceeds as follows:

b.1. Initiation stage:

- b.1.1 Evaluate temperature distribution $T(x,y)$ throughout the mesh.
- b.1.2 Evaluate moisture profile $h(x,y)$ throughout the mesh. Coefficient D_h is evaluated as a function of T .
- b.1.3 Determine amount of evaporable water, $\omega_e(x,y)$, from sorption isotherms.
- b.1.4 Evaluate free chloride profile $C_{fc}(x,y)$ throughout the mesh. Coefficient D_c is evaluated as a function of T and h .
- b.1.5 Determine concentration of total chlorides in concrete, $C_{tc}(x,y)$, from chloride binding relationships.
- b.1.6 If total chloride concentration at the reinforcing bar surface has reached the threshold value, corrosion is assumed to have initiated => **go to step b.2.** Otherwise, increment time and **go to step b.1.1.**

b.2. Propagation stage:

- b.2.1 Estimate the anodic current density, i_a .
- b.2.2 Evaluate the dissolved oxygen profiles, $C_o(x,y)$, throughout the mesh. Coefficient D_o is evaluated as a function of ω_e .
- b.2.3 Calculate amount of hydrated red rust and displacement of volume of concrete. *From here proceed with the solution of the associated mechanics/fracture problem to solve for the state of stress in the cover (optional).*
- b.2.4 If end of service life has been reached (according to some predefined criterion), end computations. Otherwise, increment time and **go to step b.1.1**.

EXAMPLE APPLICATION

The numerical performance of the finite element model was evaluated by considering two distinct cases: one simulating one-dimensional flow, as in the case of concrete slabs of highway structures or parking garages exposed to de-icing salts, and the other representing two-dimensional flow, found in concrete pillars in marine structures or concrete columns in bridges. For the first case, the numerical simulations were based on a linear strip of reinforced concrete with a cover to the reinforcement of 50 mm, as illustrated in Fig. 7(a). The finite element mesh was only subject to flux boundary conditions along the left side. This problem represents the “semi-infinite medium” for which an analytical solution for the case of constant diffusivity and constant surface concentration exists (for initial condition $C(x>0, t=0)=0$ and boundary condition $C(x=0, t>0)=C_s$, where C_s is the surface concentration in kg/m^3 [17]):

$$C(x,t) = C_s \left[1 - \text{erf} \left(\frac{x}{2\sqrt{D \cdot t}} \right) \right] \quad (\text{kg/m}^3) \quad (26)$$

In Eqn. (26), x denotes the depth (m), D is the diffusivity (m^2/s), and t is the time of exposure (s).

To determine the influence of the element size on the results for the one-dimensional flow example, the concrete cover was discretized using fifty 1×1 mm, twenty 2.5×2.5 mm, and ten 5×5 mm rectangular elements, respectively. The “far field” (i.e., $x > 50$ mm) was approximated by one singly infinite element in the three cases. Figure 8(a) shows the resulting free chloride profiles for a concrete with $D_c = 1.0 \times 10^{-12} \text{ m}^2/\text{s}$ (assumed to be constant over time, i.e., the effect of temperature, time of exposure and chloride binding has been ignored) and immersed in a 0.5M chloride solution after an exposure period of one year, five years, and 10 years, respectively. Also shown in the graphs are the corresponding profiles obtained from the closed-form solution given by Eqn. (26), which assumes both the chloride surface concentration and diffusion coefficient to be constant over time [17]. The numerical solutions obtained for the different one-dimensional meshes are identical regardless of the element size used. The 5×5 mm mesh yielded the same results as the other two more refined meshes, and the computation time was greatly decreased as

fewer elements were needed in the analysis. Note that the numerical approximation to the diffusion problem with bilinear rectangular elements (a linear approximation of the concentration of chlorides within the element) compares very well with the analytical solution given by Eqn. (26). However, as the period of exposure increases, the singly infinite element used to approximate the “far field” boundary condition tends to underestimate the buildup of chlorides at the reinforcement level as compared with the analytical solution. This can already be observed after 10 years of exposure, although the discrepancy is more significant at 25 years as is illustrated in Fig. 8(b). This trend was further studied by plotting the free chloride history at $x=50$ mm over a 100 years given by the 5×5 mm finite element mesh solution and by Eqn. (26). Comparison between the analytical and numerical solutions confirms the lower buildup of chlorides at the reinforcing steel resulting from the latter (Fig. 8(c)); however, the rate at which both solutions increase with time seems to be similar. According to Damjanic and Owen [15] bilinear infinite elements do not give sufficient accuracy in areas near the finite edge of the infinite domain, and the authors suggest the use of higher order elements instead to get better approximations.

Comparison between one-dimensional and two-dimensional flows can be seen in Fig. 9, where the chloride profiles corresponding to the mesh shown in Fig. 7(b) are plotted along diagonal A-B. The amount of chloride buildup along the concrete cover is significantly greater if the two-dimensional problem is considered, even after 1 year of chloride exposure. Note the flattening of the chloride penetration curve near the exposed surface due to the “corner” effect. These results highlight the need for properly modeling the boundary conditions at hand.

CONCLUSIONS

Transport of chlorides, moisture, oxygen and heat convection through concrete is a coupled boundary-initial value mathematical problem that underlies the mechanics of corrosion of embedded reinforcement in concrete. In this paper, all these processes were described by modified versions of Fick’s 2nd law of diffusion, and thus the resulting PDE’s had all the same order and mathematical structure. To solve the space aspect of the problem, a 2-D finite element formulation was proposed through which concentrations of the various species assisting the mechanism of corrosion in concrete could be resolved at any point in space. For this purpose, four element types were developed. These were: (a) *linear triangular* and *bilinear rectangular* elements, to be used in discretizing the near-field conditions (such as in the cover concrete adjacent to the reinforcing bar surface); and (b) *singly* and *doubly infinite* elements, to be used in

representing the far-field boundary conditions of the member (i.e., the area of the cross section that is distant from the rebars). A time step integration procedure (based on Finite Differences) was also incorporated in the formulation in order to determine the variation in time of the species concentrations in response to seasonal variations in exposure conditions of the concrete member surface throughout the year. The model correlated successfully with closed form solutions of the diffusion equation (such solutions exist only for few cases of simplified boundary conditions). The sensitivity of the solution to mesh density and time evolution increment were evaluated from parametric studies.

APPENDIX I

Calculated values for capacitance and property matrices as well as the corresponding force vector for the three element types considered are given below:

Linear triangular element:

$$[C^{(e)}] = \frac{\kappa A}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}; \quad [k_1^{(e)}] = \frac{D}{4A} \begin{bmatrix} b_i^2 + c_i^2 & b_i b_j + c_i c_j & b_i b_k + c_i c_k \\ b_i b_j + c_i c_j & b_j^2 + c_j^2 & b_j b_k + c_j c_k \\ b_i b_k + c_i c_k & b_j b_k + c_j c_k & b_k^2 + c_k^2 \end{bmatrix}; \quad [k_2^{(e)}] = \frac{D_h}{12A} \begin{bmatrix} m_1 & m_2 & m_3 \\ m_1 & m_2 & m_3 \\ m_1 & m_2 & m_3 \end{bmatrix}$$

$$\begin{aligned} m_1 &= (b_i^2 + c_i^2)h_i + (b_i b_j + c_i c_j)h_j + (b_i b_k + c_i c_k)h_k \\ m_2 &= (b_i b_j + c_i c_j)h_i + (b_j^2 + c_j^2)h_j + (b_j b_k + c_j c_k)h_k; \quad \{f^{(e)}\} = \frac{M}{2} \left[l_{ij} \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix} + l_{jk} \begin{Bmatrix} 0 \\ 1 \\ 1 \end{Bmatrix} + l_{ik} \begin{Bmatrix} 1 \\ 0 \\ 1 \end{Bmatrix} \right] \\ m_3 &= (b_i b_k + c_i c_k)h_i + (b_j b_k + c_j c_k)h_j + (b_k^2 + c_k^2)h_k \end{aligned}$$

$$[k_3^{(e)}] = \frac{\partial \omega_e}{\partial h} \frac{A}{60} \begin{bmatrix} 6\dot{h}_i + 2\dot{h}_j + 2\dot{h}_k & 2\dot{h}_i + 2\dot{h}_j + \dot{h}_k & 2\dot{h}_i + \dot{h}_j + 2\dot{h}_k \\ 2\dot{h}_i + 2\dot{h}_j + \dot{h}_k & 2\dot{h}_i + 6\dot{h}_j + 2\dot{h}_k & \dot{h}_i + 2\dot{h}_j + 2\dot{h}_k \\ 2\dot{h}_i + \dot{h}_j + 2\dot{h}_k & \dot{h}_i + 2\dot{h}_j + 2\dot{h}_k & 2\dot{h}_i + 2\dot{h}_j + 6\dot{h}_k \end{bmatrix} \quad \begin{aligned} &\text{where } h_i \text{ is the nodal value of } h \\ &\text{and } \dot{h}_i \text{ is the time derivative of } h_i \end{aligned}$$

$$[k_4^{(e)}] = \frac{L}{6} \left\{ l_{ij} \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix} + l_{jk} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} + l_{ik} \begin{bmatrix} 2 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 2 \end{bmatrix} \right\} \quad \text{where } l_{ij} \text{ is the length of side } ij, \text{ etc.}$$

Bilinear rectangular element:

$$[c^{(e)}] = \frac{\kappa ab}{9} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}; \quad [k_1^{(e)}] = \frac{D}{6ab} \begin{bmatrix} 2(a^2+b^2) & -(2a^2-b^2) & -(a^2+b^2) & (a^2-2b^2) \\ -(2a^2-b^2) & 2(a^2+b^2) & (a^2-2b^2) & -(a^2+b^2) \\ -(a^2+b^2) & (a^2-2b^2) & 2(a^2+b^2) & -(2a^2-b^2) \\ (a^2-2b^2) & -(a^2+b^2) & -(2a^2-b^2) & 2(a^2+b^2) \end{bmatrix}$$

$$[k_2^{(e)}] = \frac{D_h}{24ab} \begin{bmatrix} k_2^{11} & k_2^{12} & k_2^{13} & k_2^{14} \\ k_2^{21} & k_2^{22} & k_2^{23} & k_2^{24} \\ k_2^{31} & k_2^{32} & k_2^{33} & k_2^{34} \\ k_2^{41} & k_2^{42} & k_2^{43} & k_2^{44} \end{bmatrix}; \quad [k_3^{(e)}] = \frac{\partial \omega_e}{\partial h} \frac{ab}{36} \begin{bmatrix} k_3^{11} & k_3^{12} & k_3^{13} & k_3^{14} \\ k_3^{21} & k_3^{22} & k_3^{23} & k_3^{24} \\ k_3^{31} & k_3^{32} & k_3^{33} & k_3^{34} \\ k_3^{41} & k_3^{42} & k_3^{43} & k_3^{44} \end{bmatrix}$$

$$[k_4^{(e)}] = \frac{Lb}{3} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \frac{La}{3} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 \\ 0 & 1 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \frac{Lb}{3} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{bmatrix} + \frac{La}{3} \begin{bmatrix} 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 \end{bmatrix}$$

$$\begin{aligned} k_2^{ii} &= (3a^2 + 3b^2)h_i - (3a^2 - b^2)h_j - (a^2 + b^2)h_k + (a^2 - 3b^2)h_l; & k_3^{ii} &= 9\dot{h}_i + 3\dot{h}_j + \dot{h}_k + 3\dot{h}_l \\ k_2^{ij} &= -(3a^2 - b^2)h_i + (3a^2 + b^2)h_j + (a^2 - b^2)h_k - (a^2 + b^2)h_l; & k_3^{ij} &= k_3^{ji} = 3\dot{h}_i + 3\dot{h}_j + \dot{h}_k + \dot{h}_l \\ k_2^{ik} &= -(a^2 + b^2)h_i + (a^2 - b^2)h_j + (a^2 + b^2)h_k - (a^2 - b^2)h_l; & k_3^{ik} &= k_3^{ki} = \dot{h}_i + \dot{h}_j + \dot{h}_k + \dot{h}_l \\ k_2^{il} &= (a^2 - 3b^2)h_i - (a^2 + b^2)h_j - (a^2 - b^2)h_k + (a^2 + 3b^2)h_l; & k_3^{il} &= k_3^{li} = 3\dot{h}_i + \dot{h}_j + \dot{h}_k + 3\dot{h}_l \end{aligned}$$

$$\{f^{(e)}\} = Mb \begin{Bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{Bmatrix} + Ma \begin{Bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{Bmatrix} + Mb \begin{Bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{Bmatrix} + Ma \begin{Bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{Bmatrix}$$

Mapped elements:

$$[c^{(e)}] = \begin{cases} \kappa x_p \delta \begin{bmatrix} 1/3 & 1/6 \\ 1/6 & 1/3 \end{bmatrix}; & [k_1^{(e)}] = \begin{bmatrix} \frac{D}{18x_p \delta} \begin{bmatrix} 2\delta^2 + 18x_p^2 & \delta^2 - 18x_p^2 \\ \delta^2 - 18x_p^2 & 2\delta^2 + 18x_p^2 \end{bmatrix}, & \text{for singly infinite} \\ \frac{D}{3} \begin{pmatrix} x_p^2 + y_p^2 \\ x_p y_p \end{pmatrix} & \text{for doubly infinite} \end{cases}$$

$$[k_2^{(e)}] = \begin{cases} \frac{D_h}{48x_p\delta} \begin{bmatrix} (3\delta^2 + 12x_p^2)h_i + (\delta^2 - 12x_p^2)h_l & (\delta^2 - 12x_p^2)h_i + (\delta^2 + 12x_p^2)h_l \\ (\delta^2 + 12x_p^2)h_i + (\delta^2 - 12x_p^2)h_l & (\delta^2 - 12x_p^2)h_i + (3\delta^2 + 12x_p^2)h_l \end{bmatrix} & \text{for singly infinite} \\ \frac{D_h}{8} h_i \left(\frac{x_p^2 + y_p^2}{x_p y_p} \right) & \text{for doubly infinite} \end{cases}$$

$$[k_3^{(e)}] = \begin{cases} \frac{\partial \omega_e}{\partial h} \frac{x_p \delta}{24} \begin{bmatrix} 3\dot{h}_i + \dot{h}_l & \dot{h}_i + \dot{h}_l \\ \dot{h}_i + \dot{h}_l & \dot{h}_i + 3\dot{h}_l \end{bmatrix} & \text{for singly infinite} \\ \frac{\partial \omega_e}{\partial h} \frac{1}{4} x_p y_p \dot{h}_i & \text{for doubly infinite} \end{cases} ; \quad [k_4^{(e)}] = 0$$

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FIGURE CAPTIONS

Figure 1: Idealizing the initiation and propagation stages as two distinct phases [1].

Figure 2: Models for binding isotherms.

Figure 3: Yearly distribution of environmental values for chlorides, moisture and temperature.

Figure 4: Linear triangular and bilinear rectangular elements.

Figure 5: Mapped infinite elements: **(a)** Reference bilinear rectangular element in natural coordinates; **(b)** Bilinear singly infinite element; **(c)** Bilinear doubly infinite element [15].

Figure 6: **(a)** Mesh for a corner of a reinforced concrete member; Influence of time step Δt on calculated pore relative humidity profile at **(b)** 120 days and **(c)** 1 year of exposure.

Figure 7: Finite element meshes simulating **(a)** a linear semi-infinite concrete strip and **(b)** a corner of a concrete section.

Figure 8: **(a)** Calculated free chloride profiles after 1 year, 5 years, and 10 years of exposure, for meshes with 1×1, 2.5×2.5, and 5×5 mm rectangular elements; **(b)** Free chloride profiles after 25 years of exposure; **(c)** Free chloride build-up at $x=50\text{mm}$ over an exposure period of 100 years.

Figure 9: Calculated free chloride profiles after 1 year and 5 years of exposure for one and two dimensional flows.

Table 1: Correspondence between Eqn. 1 and transport differential equations.

Physical Problem	ϕ	κ	J_x	J_y	J_x'	J_y'
Chloride ingress	C_{fc}	1	$-D_c^* \cdot \partial C_{fc} / \partial x$	$-D_c^* \cdot \partial C_{fc} / \partial y$	$C_{fc} \cdot J_{mx}$	$C_{fc} \cdot J_{my}$
Moisture diffusion	h	$\partial \omega_e / \partial h$	$-D_h \cdot \partial h / \partial x$	$-D_h \cdot \partial h / \partial y$	0	0
Heat transfer	T	$\rho_c c_q$	$-\lambda \cdot \partial T / \partial x$	$-\lambda \cdot \partial T / \partial y$	0	0
Oxygen transport	C_o	1	$-D_o \cdot \partial C_o / \partial x$	$-D_o \cdot \partial C_o / \partial y$	$C_o \cdot J_{mx}$	$C_o \cdot J_{my}$

J_{mx} and J_{my} refer to moisture fluxes.

Table 2: Correspondence of L and M values with the imposed boundary conditions.

Physical Problem	Diffusive Term			Sorptive Term		
	ϕ_b	L	M	ϕ_b	L	M
Chloride ingress	C_{fc}	B_c	$B_c \cdot C_{en}$	h	$B_h \cdot C_{en}$	$B_h \cdot h_{en} \cdot C_{en}$
Moisture diffusion	h	B_h	$B_h \cdot h_{en}$	-	-	-
Heat transfer	T	B_T	$B_T \cdot T_{en}$	-	-	-
Oxygen transport (to steel surface)	0	0	$-k i_a^*$	-	-	-

* $k=8.291 \times 10^{-8} A_a/A_c + 4.144 \times 10^{-8}$, i_a is the anodic current, and A_a/A_c is the ratio of anodic to cathodic areas.

(a)

(b)

(c)

mapped elements in
natural coordinates

infinite elements in
global coordinates