Wetting and Drying of Concrete: Modelling and Finite Element Formulation for Stable Convergence

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Abstract

The simulation of moisture movement in concrete is vital for estimating its durability performance under the given conditions of service. A robust analysis of the nonlinear phenomenon relies on the implementation of an efficient numerical algorithm. This entails a comprehension of the underlying mathematical models, the numerical analysis scheme and the related issues of stability and convergence. This paper describes a computational scheme to facilitate the estimation of moisture distribution in concrete subjected to wetting–drying exposure due to intermittent rains, an exposure type which severely impairs the durability performance of structural concrete under tropical climatic conditions. Beginning with a brief review of the conventional moisture transport models for concrete, this paper proposes a modified model using dimensionless parameters, which enhances the computational efficiency of the delineated scheme. This paper also describes the formulation of a one-dimensional, nonlinear finite element scheme for the modified model and discusses the issue of numerical oscillations concomitant to the numerical analysis of the problem. The suitability of the first-order element in providing stable convergence when implemented in conjunction with a lumped-mass scheme has been mathematically interpreted. The validity of the delineated proposition has been illustrated using a test problem.

Keywords: wetting–drying exposure; moisture transport models; FE analysis; numerical oscillation; concrete; wetting–drying exposure.

Introduction

Structural concrete during service constantly remains exposed to the action of temperature and humidity cycles operating at diurnal and seasonal scales. Under tropical climatic conditions, it is also subjected to intermittent spells of rainfall. These conditions induce flow of moisture in liquid and vapour phases through the porous matrix of concrete, often rendering it unsaturated.1–5 The subsequent interaction of concrete with gases and other invading species carried by the imbibed liquid phase alters its physical and chemical constitution resulting in gradual degradation and consequent disruption of durability. The degradation mechanisms being critically moisture dependent necessitate the study of moisture movement in concrete to enable a reliable prediction of its performance while under service. The pertinence is especially critical for exposure conditions that strongly influence the state of moisture in concrete and hence expedite the impending degradation.

In this context, the effect of alternating wet and dry conditions is known to be very severe in causing corrosion of steel reinforcement embedded in structural concrete. In a tropical climate, the exposure is predominantly due to the occurrence of intermittent rainfall events. While exposure to rain causes a conspicuous ingress of moisture in concrete, subsequent drying renders the medium unsaturated and the embedded reinforcement susceptible to corrosion owing to the presence of both air and moisture in the pores. Estimating the possible extent of ensuing degradation requires appropriate modelling of moisture transport and implementation of an efficient numerical scheme to address the highly nonlinear character of the problem. The modelling of moisture movement in hydrated cement systems has been conventionally carried out using two distinct approaches. The more rigorous of the two starts with the formulation of mass and energy balance equations at a microlevel followed by volume averaging to obtain the macroscopic description. The method is particularly suitable for modelling the hygrothermal behaviour of concrete at early ages6 and the deformations occurring due to the effect of shrinkage and creep.7 This approach however relies on the experimental estimation of several material properties and is thus less viable for durability studies. The alternative approach is phenomenological and starts directly from the macroscopic level, with the effect of various influencing factors lumped into a few model parameters to be determined experimentally. This approach culminates into a diffusion model, and which, because of its relative simplicity, has been used extensively to describe the transfer of moisture and heat in porous building materials.6–10 Most of these studies have implemented numerical methods to handle the mathematical nonlinearity of diffusion model but have not elaborated adequately the associated issues of numerical stability and oscillation-free convergence. In contrast, several studies pertaining to the domain of water-infiltration modelling in unsaturated soil medium have evaluated the efficiency of numerical schemes and tested their stability in relation to element order, mass type and time-step size11–13; the delineated conclusions, however, remain to be testified and adapted for the analysis of moisture movement in cement-based materials.

This paper provides an exhaustive description of the outlined problem, reviews the associated aspects of moisture transport modelling and elaborates the constitution of a robust finite element (FE) scheme for efficient analysis of the problem. At the outset, the paper briefly describes the formulation of conventional equations governing the phenomena of moisture transport in unsaturated concrete. The
model is subsequently restated using a set of nondimensional terms to minimize the range of orders involved in the underlying calculations. This aids in reducing the numerical errors concomitant to computer arithmetic and in easily adapting the simulated results to predict the behaviour of hydraulically similar materials. Further, using the modified model, this paper elucidates the formulation of a one-dimensional, nonlinear FE scheme to determine the evolution of moisture distribution in concrete subjected to wetting–drying exposure due to intermittent rains. The paper also discusses the issue of numerical oscillations typically related to the FE-based analysis of nonlinear diffusion models. A prudent evaluation of the system of nonlinear algebraic equations generated in the FE analysis has been carried out to ascertain the suitability of the mass type to be implemented with a linear element for obtaining an oscillation-free convergence. The study leads to a set of criteria governing the maximum permissible value of time-step size for stable convergence. The validity of the derived criteria has been tested for a typical concrete subjected to rainfall exposure.

The thrust of the present work is therefore on establishing the conditions that enable a robust one-dimensional, transient, nonlinear FE analysis of moisture flow in concrete described using a phenomenological model. The developed scheme can be implemented to examine the impact of various influencing parameters on the state of moisture distribution in concrete without resorting to extensive experimental programmes. The present work thus bears a special significance in the context of model-based service life analysis of concrete structures; in particular, for tropics where the occurrence of rainfall in intermittent spells is a characteristic climatic phenomenon.

Brief Review of Phenomenological Moisture Transport Models

Moisture Ingress

When a concrete surface is exposed to rain flux, the concomitant ingress of moisture is caused due to the action of capillary forces, and the resulting distribution of moisture is governed by the gradient of capillary pressure. It is thus rational to represent the ensuing movement of water using convection models that consider the gradient of pressure as the primary driving force.19 Darcy’s law, the first convection model, was proposed in the form of an empirical equation to describe the flow of water through saturated porous media.20 Mathematically, Darcy’s law is stated as

\[ Q = -k_s A \Delta p/L \]  

i.e. \( u = -k_s \Delta p/L \)  

In a local sense Eq. (1b) can be expressed as

\[ u = -k_s \nabla p \]  

where \( Q \) is the volume rate of flow \((m^3 s^{-1})\), \( k_s \) is the Darcean permeability \((kg^{-1} m^2 s)\), \( A \) is the cross-sectional area of specimen \((m^2)\), \( p \) is the hydrostatic head \((kg m^{-1} s^{-2})\), \( L \) is the thickness of the medium \((m)\) and \( u \) is the average velocity of flow \((m^3 s^{-1})\).

By expressing the hydrostatic pressure in terms of pressure potential, the equation further reduces to

\[ u = -K_s \nabla \psi \]  

where \( K_s = k_s \rho_w g \) is the permeability of the saturated medium \((m^3 s^{-1})\), \( P = \rho w g \) is the pressure potential \((m)\), \( \rho_w \) is the density of water \((kg m^{-3})\) and \( g \) is the acceleration due to gravity \((m^3 m^{-1} s^{-2})\). When applied to the analysis of unsaturated flow, the permeability term in Darcy’s relation is replaced by a generalized transport property called the capillary conductivity \( K(\theta)\) \((m^3 m^{-1} s^{-1})\), which is a strong function of the liquid water content, and the pressure potential is replaced by the capillary potential \( \psi(\theta)\). Thus, Eq. (1d) gets modified to

\[ u = -K(\theta) \nabla \psi \]  

The above relation can be applied directly to describe the steady-state unsaturated flow. However, to incorporate the effect of unsteady conditions, Eq. (1e) for apparent velocity has to be combined with the mass balance equation,

\[ \Delta \rho \nabla \psi \]  

where \( \rho \) is the partial moisture density \((kg m^{-3})\), \( t \) is the time variable \((s)\) and \( j_l \) is the liquid flux \((m^2 s^{-1})\). Equation (2a) can be restated in terms of volumetric liquid water content \( \theta \) \((m^3 m^{-3})\) as

\[ \partial(\rho_w \theta)/\partial t + \nabla (\rho_w u) = 0 \]  

The combination of Eqs (1c) and (2b) results in

\[ \frac{\partial \theta}{\partial t} = -D(\theta) \nabla \theta \]  

Equation (2c) can be expressed in terms of \( \theta \) rather than \( \psi \) as

\[ \frac{\partial \theta}{\partial t} = \frac{D(\theta)}{K(\theta)} \nabla \theta \]  

with \( D(\theta) = K(\theta) \nabla \psi / (\partial \theta/\partial \psi) = K(\theta) / (\partial \theta/\partial \psi) = K(\theta) / (\partial \theta/\partial \psi) \), where \( c(\theta) \) is specific water capacity \((m^3 kg^{-1})\).

The extended Darcy’s law represented by Eq. (2d) governs the flow of water in unsaturated porous medium and is also referred to as Richard’s equation. Mathematically, it is analogous to Fick’s law of diffusion.

Moisture Egress

The evaporative drying of moisture imbibed in concrete starts soon after the end of a rainfall event and involves flow in both liquid and vapour phases. This multiphase movement of water can be described using the diffusion models that assume concentration gradient to be the primary driving force. Krischer’s model, in particular, considers the transport of water and water vapour as caused separately due to the respective gradients of liquid moisture content and partial pressure of vapour in air. Thus, the liquid and vapour fluxes are expressed as

\[ j_l = -\rho_w D(\theta) \nabla \theta \]  

\[ j_v = -\frac{D_v}{\mu} \nabla p_v \]  

The corresponding mass balance equations are given by

\[ \rho_w \frac{\partial \theta}{\partial t} = \rho_w \frac{D(\theta)}{K(\theta)} \nabla \theta \]  

\[ \frac{1}{RT} \frac{\partial p_v}{\partial t} = \frac{1}{RT} \nabla \left( \frac{D_v}{\mu} \nabla p_v \right) \]  

Here, \( D_v(\theta) \) is the diffusivity of liquid water \((m^2 s^{-1})\), \( R \) is the gas constant of water vapour \((1 k g^{-1} K^{-1})\), \( T \) is the temperature \((K)\), \( p_v \) is the partial vapour pressure \((Nm^{-2})\), \( D_v \) is the diffusion coefficient of water vapour in air \((m^2 s^{-1})\) and \( \mu \) is the resistance factor of the porous medium to vapour diffusion.

The total mass balance of moisture after accounting for the effects of the Stefan diffusion and the concentration of water in the pores can be obtained from Eqs (4a) and (4b) as

\[ \rho_w \frac{\partial \theta}{\partial t} + \frac{1}{RT} \frac{\partial p_v}{\partial t} = \rho_w \frac{D(\theta)}{K(\theta)} \nabla \theta \]  

\[ + \frac{1}{RT} \nabla \left( \frac{D_v}{\mu} (\theta - \theta_R - \frac{p_v}{p_v - p_r} \nabla p_v) \right) \]  

where $\phi$ is the open porosity ($m^3/m^3$) and $p_r$ is the pressure of vapour–air mixture ($N/m^2$).

Equation (4c) represents Krischer’s model for combined liquid and vapour transport. The expression can be further simplified by considering the aspects of capillary pressure and relative humidity that prevail within the porous matrix.

For a given moisture content the capillary pressure within the porous matrix is constant and the relative humidity of the associated vapour phase is

$$ h = p_r/p_s $$

where $p_s$ is the saturated vapour pressure ($N/m^2$). Now, using Kelvin’s equation $p_r$ can be stated as

$$ p_r = h p_s = p_s \exp \left( \frac{p_s}{\rho_v R_T} \right) $$

where $p_s$ is the capillary pressure ($N/m^2$).

From the above expression, it becomes evident that under isothermal conditions the partial vapour pressure depends only on capillary pressure and hence varies as a function of the moisture content. Thus, from Eq. (5b),

$$ \nabla p_v = p_s (\partial h/\partial \theta)_T \nabla \theta $$

The vapour flux in Eq. (3b) can now be expressed as

$$ j_v = -\frac{p_s}{R_T} \left( \frac{\partial h}{\partial \theta} \right)_T \frac{D_v}{\mu} \nabla \theta $$

Thus, as in Eq. (4c), the total mass balance of moisture can now be expressed as

$$ \rho_v \frac{\partial \theta}{\partial t} + \rho_s \frac{\partial h}{\partial t} = \rho_s \nabla \left[ D_v \nabla \theta \right] $$

$$ + \nabla \left[ \frac{p_s}{R_T} \left( \frac{\partial h}{\partial \theta} \right)_T \frac{D_v}{\mu} \left( \theta - \theta_v \right) \right] $$

that is,

$$ \frac{\partial \theta}{\partial t} = \nabla (D_v \nabla \theta) $$

which is of the form

$$ \frac{\partial \theta}{\partial t} = \nabla (D(\theta) \nabla \theta) $$

Here, $\theta_v$ is the volumetric water vapour content ($m^3/m^3$), $D_v(\theta)$ is the diffusivity of water vapour in porous medium ($m^2/s$), $\theta = \theta_v + \theta_i$ is the total volumetric moisture content and $D(\theta) = D_s(\theta) + D_w(\theta)$ is the isothermal moisture diffusivity ($m^2/s$). The derived equation governing the combined flow of liquid and vapour phases of water takes up the form of Fick’s law of diffusion.

**Models for Diffusivity Function**

Diffusivity of a porous material is a measure of its tendency to transmit fluid through its interconnected pore space while in a state of unsaturation. When the fluid being transmitted is water, it is referred to as the hydraulic diffusivity. The hydraulic diffusivity is a continuum level property that takes into account the combined effect of pore structure geometry, state of saturation of pore space and the transport mechanisms driving the moisture movement phenomenon. In a phenomenological model, the hydraulic diffusivity is the only decisive parameter that governs the evolution of moisture distribution in a medium. Considering the pore structure to remain stable, the strong dependence of hydraulic diffusivity on moisture content is generally represented using monotonically increasing functions. The trend follows from the underlying mechanisms of moisture transport, which enhance the rate of mass transfer with increasing levels of pore saturation; initiating with the slow gaseous diffusion of vapour in a near-dry state, the rate compounds through the movement of water in adsorbed and condensed layers to the phase of bulk flow in pore space under the rising levels of saturation.

Furthermore, the empiric modelling of hydraulic diffusivity leads to typical functional forms for wetting and drying conditions characterizing the associated moisture transport mechanisms. For liquid water ingress, which owes to the effect of capillarity, the hydraulic diffusivity has been successfully represented by an exponential function of the form $e^{21-28}$

$$ D_r(\theta) = D_{w,dry} \exp \left( n \theta \right) $$

where $D_{w,dry}$ is the drying diffusivity of concrete in completely wet state ($m^2/s$), $n$ is the ratio of minimum to maximum diffusivity, and the parameters $n$ and $\theta$ characterize, respectively, the spread and the location of drop of the curve.

The empirical diffusivity models broadly describe the hygroscopic behaviour of concrete under wetting and drying conditions. The application of these models for a given concrete is, however, dependent on the experimental estimation of the function parameters. Comprehensive studies to establish the dependence of these parameters on temperature, initial saturation level and parameters governing the pore structure properties of concrete would enable a direct implementation of these models for durability studies.

**FE Formulation**

**Governing Equation**

As has been described in the Brief Review of Phenomenological Moisture Transport Models section, the phenomenon of one-dimensional isothermal moisture transport in a porous medium can be represented using the equation

$$ \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left( D(\theta) \frac{\partial \theta}{\partial x} \right) $$

Eq. (8a) is a nonlinear parabolic partial differential equation. The nonlinearity is caused by the term $D(\theta)$, a strong function of moisture content that follows distinct characteristic trends for wetting and for drying conditions, respectively. Owing to its highly nonlinear nature, Eq. (8a) is not amenable to analytical solution and requires the implementation of numerical procedures. The equation being first order in time and second order in space, the
solution of the problem relies on the specification of an initial condition and two boundary conditions. The boundary conditions may either be provided as the value of moisture content \( \theta \) (Dirichlet/essential boundary condition) or as the value of moisture flux stated as \( D(\theta)\partial \theta/\partial x = -V_r \) (Neumann/natural boundary condition), where \( V_r \) is the orthogonal rain flux incident on the exposed surface (\( \text{ms}^{-1} \)). The initial moisture content across the physical domain of analysis is generally described by an initial moisture profile \( \theta(x,t = 0) = \theta_i(x) \).

Since the parameters constituting the given problem range over several orders of magnitude, restating Eq. (8a) using the following dimensionless terms,

- Reduced moisture: \( \theta_r = (\theta - \theta_o)/\theta_i \) (8b)
- Reduced distance: \( x_r = (V_r/D_{d,wet})x \) (8c)
- Reduced time: \( t_r = (V_r/D_{d,wet})t \) (8d)

Aids in minimizing the computing errors.

Restating Eq. (8a) in terms of non-dimensional parameters gives:

\[
\frac{\partial \theta_r}{\partial t_r} = \frac{1}{D_{d,wet}} \frac{\partial D(\theta_r)}{\partial t} \left( \frac{\partial \theta_r}{\partial x_r} \right)^2 + \frac{D_r(\theta_r)}{D_{d,wet}} \frac{\partial^2 \theta_r}{\partial x_r^2} \tag{8e}
\]

A scrutiny of these terms reveals their appropriateness in reducing the range of orders involved in computation; the most prominent aspect in the modified model represented by Eq. (8e) is the normalization of the diffusivity function \( D_r(\theta) \) with the term \( D_{d,wet} \). Moreover, expressing the model in terms of these parameters enables adaptation of results to determine the behaviour of all hydraulically similar materials. The idea will be clarified further in the following section.

Considering the following simplified representations for the hydraulic diffusivity function,

- for wetting: \( D_r(\theta) = D_{d,wet} f_w(\theta_r) \) (8f)
- for drying: \( D_r(\theta) = D_{d,wet} f_d(\theta_r) \) (8g)

where \( f_w(\theta_r) \) and \( f_d(\theta_r) \) are functions of reduced moisture content in wetting and drying diffusivity functions, respectively, and subsequently equating the boundary flux term

\[
V_r(\theta_r - \theta_o) \frac{D_r(\theta_r)}{D_{d,wet}} \frac{\partial \theta_r}{\partial x_r} \tag{8h}
\]

to wetting and drying fluxes yields, respectively, the following conditions, for wetting: \( f_w(\theta_r) \frac{\partial \theta_r}{\partial x_r} = -1/(\theta_r - \theta_o) \) (8h)

and for drying: \( (D_r(\theta_r)/D_{d,wet}) f_d(\theta_r) \frac{\partial \theta_r}{\partial x_r} = J_r/V_r(\theta_r - \theta_o) \) (8i)

where \( J_r \) is drying boundary flux acting in the direction of outward normal to the surface (\( \text{ms}^{-1} \)).

It is worth mentioning that the adaptation of Eq. (8a) most widely used in previous studies implements only the reduced moisture content as in Eq. (8b) and has the form,

\[
\frac{\partial \theta_r}{\partial t_r} = \left( D_r(\theta_r) \frac{\partial \theta_r}{\partial x_r} \right) \tag{8j}
\]

**Formulation of Element-Level Governing Equation**

Using the governing differential equation stated in Eq. (8e), the FE formulation can be carried out using Galerkin’s weighted residual technique. For the given problem, the weighted residual statement is given as

\[
\int_0^l w_k \left[ \frac{\partial \theta_r}{\partial t_r} - \frac{1}{D_{d,wet}} \frac{\partial D(\theta_r)}{\partial t_r} \left( \frac{\partial \theta_r}{\partial x_r} \right)^2 \right] dx_r = 0 \tag{9a}
\]

where \( w_k \) is the weight function (\( k = 1 \) to number of nodes in an element) and \( l \) is the reduced size of element constituting the FE mesh.

Integration of Eq. (9a) by parts leads to

\[
\int_0^l \left[ \frac{\partial \theta_r}{\partial x_r} \right] dx_r + \int_0^l \frac{D_r(\theta_r)}{D_{d,wet}} \frac{\partial \theta_r}{\partial x_r} \frac{\partial \theta_r}{\partial x_r} dx_r = w_k \frac{D_r(\theta_r)}{D_{d,wet}} \frac{\partial \theta_r}{\partial x_r} \bigg|_{x_r=0}^{x_r=l} \tag{9b}
\]

where \( w_k \) is the weight function (\( k = 1 \) to number of nodes in an element) and \( l \) is the reduced size of element constituting the FE mesh.

Now, for a linear element with two nodes, it is known that

\[
\theta_r = \left[ 1 - \frac{x_r}{l} \right] \theta_{r,0} + \left[ \frac{x_r}{l} \right] \theta_{r,l} \tag{9c}
\]

Thus,

\[
\frac{\partial \theta_r}{\partial x_r} = \left[ -\frac{1}{l} \right] \theta_{r,0} + \left[ \frac{1}{l} \right] \theta_{r,l} = [H] \{ d' \} \tag{9d}
\]

where \([H]\) is the interpolation matrix, \([B]\) is the gradient matrix and \([d']\) is the vector of elemental degrees of freedom.

Following Galerkin’s method, the weights in Eq. (9b) are taken equal to the interpolation functions.

Thus, for \( w_1 = 1 - (x/l) \), Eq. (9b) yields,

\[
\int_0^l \left[ \frac{1}{l} \frac{\partial}{\partial t_r} \frac{\partial (d')}{\partial x_r} \right] dx_r + \frac{D_r(\theta_r)}{D_{d,wet}} \left[ \frac{\partial \theta_r}{\partial t_r} \right] \bigg|_{x_r=0}^{x_r=l} = \frac{D_r(\theta_r)}{D_{d,wet}} \frac{\partial \theta_r}{\partial x_r} \bigg|_{x_r=0}^{x_r=l} \tag{9e}
\]

And for \( w_2 = (x/l) \),

\[
\int_0^l \left[ \frac{1}{l} \frac{\partial}{\partial t_r} \frac{\partial (d')}{\partial x_r} \right] dx_r + \frac{D_r(\theta_r)}{D_{d,wet}} \left[ \frac{\partial \theta_r}{\partial t_r} \right] \bigg|_{x_r=0}^{x_r=l} = \frac{D_r(\theta_r)}{D_{d,wet}} \frac{\partial \theta_r}{\partial x_r} \bigg|_{x_r=0}^{x_r=l} \tag{9f}
\]

Combining Eqs (9e) and (9f), the general element-level governing equation can be obtained as

\[
\int_0^l \left[ \frac{1}{l} \frac{\partial}{\partial t_r} \frac{\partial (d')}{\partial x_r} \right] dx_r + \frac{D_r(\theta_r)}{D_{d,wet}} \left[ \frac{\partial \theta_r}{\partial t_r} \right] \bigg|_{x_r=0}^{x_r=l} = 0 \tag{9g}
\]

Substituting Eqs (8f) and (8g) in Eq. (9g) and using Eqs (8h) and (8i) in tandem, the governing equation for the boundary element respective to the cases of wetting and drying can be obtained as

\[
\int_0^l \left[ \frac{1}{l} \frac{\partial}{\partial t_r} \frac{\partial (d')}{\partial x_r} \right] dx_r + \frac{D_r(\theta_r)}{D_{d,wet}} \left[ \frac{\partial \theta_r}{\partial t_r} \right] \bigg|_{x_r=0}^{x_r=l} = 0 \tag{9h}
\]

and

\[
\int_0^l \left[ \frac{1}{l} \frac{\partial}{\partial t_r} \frac{\partial (d')}{\partial x_r} \right] dx_r + \frac{D_r(\theta_r)}{D_{d,wet}} \left[ \frac{\partial \theta_r}{\partial t_r} \right] \bigg|_{x_r=0}^{x_r=l} = 0 \tag{9i}
\]
An inspection of Eqs (9h) and (9i) reveals their dependence on the functions \( f_s(\theta) \) and \( f_d(\theta) \), which are known to follow characteristic exponential and S-shaped forms for the respective cases of wetting and drying of concrete. Also, as the terms \( D_{w, \text{dry}} \) and \( D_{f, \text{wet}} \) are relative in nature, the derived expressions can be considered to represent the behaviour of all hydraulically similar materials.

Equations (9h) and (9i) are semi-discrete and can be represented in matrix form as

\[
[m][d'] + [k][d'] = [q]
\]  

(9j)

where \([m]\) and \([k]\) are the element-level mass and the diffusivity matrices, respectively, \([d']\) is the vector of time derivatives of elemental degrees of freedom and \([q]\) is the vector of elemental nodal fluxes.

In order to obtain a fully discretized system of equations, the time derivatives of the field variable in these equations are to be further approximated using the method of finite difference. Adopting the Crank–Nicolson scheme, a completely discrete system of equations is obtained as

\[
([m] + 0.5\Delta t[K]^m)[d']^{n+1} + ([m] – 0.5\Delta t[K]^m)[d']^n = 0.5\Delta t[Q]^m + [q]^n
\]  

(9k)

where the superscripts \( n \) and \((n+1)\) denote the previous and present time levels, respectively, in the course of transient analysis.

**Numerical Stability of the FE Scheme**

The highly nonlinear nature of the problem necessitates the implementation of an extremely refined mesh and a small time-step size to facilitate the stable convergence of simulated results. However, earlier studies based on FE analysis of parabolic partial differential equations reported that the minimization of the time-step size beyond a certain threshold value induces numerical oscillations in the simulated results. The issue was addressed in the context of heat diffusion problems by determining the minimum time-step sizes for some typical one- and two-dimensional elements. These criteria that had actually been developed for strictly constant material properties were tested for unsaturated seepage problems involving mildly nonlinear material properties and were found to be equally useful. In another study, it was demonstrated that the use of lumped-mass scheme with linear elements offers stable convergence and consistent results for FE-based solution of Richard’s equation. The observation was, however, empirical and was not deduced mathematically.

In the following section, an attempt has been made to mathematically interpret the issue of numerical oscillations and to ascertain the suitability of a lumped-mass type implemented with linear elements in providing a stable convergence. In addition, a set of criteria has been developed for the modified model to regulate the variation of time-step size as a function of element length and hydraulic diffusivity for stable convergence of the FE scheme.

**General Conditions for Stability**

To determine the nodal values of the field variable at a particular time-step, all the element-level equations are assembled to obtain a set of nonlinear algebraic equations in the form, \([A][X] = [b]\) with

\[
[A] = [M] + 0.5\Delta t[K]^m
\]  

(10a)

\[
[b] = ([M] – 0.5\Delta t[K]^m)[X]^n + \Delta t([Q]^m + [Q]^n)
\]  

(10b)

where \([M]\) and \([K]\) are, respectively, the global consistent mass and diffusivity matrices, and \([X]\) and \([Q]\) are the global vectors for degrees of freedom and nodal fluxes, respectively.

It is evident that spatial oscillations in the simulated results are caused by the numerical characteristics of matrix \([A]\) and vector \([b]\). From basic reasoning it can be perceived that the occurrence of numerical oscillations can be eliminated if:

1. \([A]\) is strictly diagonally dominant with positive terms in the principal diagonal and negative terms elsewhere with magnitudes lesser than the smallest element of the principal diagonal.
2. All the elements of \([b]\) are positive, which necessarily depends on the diagonal elements of \([M] – 0.5\Delta t[K]^m\) to remain positive.

Depending on the method to be implemented for solving the system, \([A][X] = [b]\) the implications of the stated conditions would be as follows:

(a) The constitution of \([A]\) would be such that its manipulation using any of the elimination methods will not produce negative elements on its principal diagonal; will not require row subtractions during the elimination phase; thus, the elements in \([b]\) shall always remain positive provided condition (2) is already met.

(b) If \([A]\) is to be inverted for \([X] = [A]^{-1}[b]\), then none of the elements in the inverted matrix would be negative; it would otherwise fetch negative values in the resulting vector.

(c) The diagonal dominance of \([A]\) is a sufficient condition for the iterative methods to converge for any initial solution vector. The specified conditions restrict the generation of negative values at nodes which generally manifest in an alternating pattern when a wetting front invades a dry medium. They also arrest the oscillations causing a saw-tooth pattern in simulated moisture profile. Fulfilling the proposed conditions thus eliminates both forms of oscillations that are reported to influence the quality of results simulated under a FE scheme. Furthermore, it is to be recognized that the numerical oscillations are primarily caused due to the composition of matrix \([A]\); that is, in relation to the violation of condition (1). The perturbations caused due to the multiplication of the negative diagonal elements of \([M] – 0.5\Delta t[K]^m\) with the elements of vector \([X]^n\) are largely counterbalanced by the contribution of the off-diagonal elements in the respective rows, which are always positive and have the same order of magnitude.

The mathematical criteria to be adopted to enforce the proposed conditions depend on the type of element being implemented in the FE model. This study considers only the instance of linear element in the following section.

**Stability Criteria**

For the FE formulation presented in the Formulation of Element Level Governing Equation section, the global characteristic matrices for the phase of wetting will be tri-diagonal and are defined as

\[
M = \frac{1}{6} \begin{cases} 
2, & i = j = 1, m \\
4, & i = j = 2 \text{ to } (m-1) \\
1, & \text{for } i = 2 \text{ to } m, j = (i-1) \\
0, & \text{for } i = 1 \text{ to } (m-1), j = (i+1) \\
0, & \text{for all other elements}
\end{cases}
\]

(11a)
where $M_{ij}$ is an element of the $i$th row and $j$th column of lumped-mass matrix.

The revised criteria for satisfying conditions (1) and (2) would now be

$$0,5\Delta t \left[ \frac{0,5}{l} - 2f_u(q_{\text{max}}^r) \right] < \frac{3l}{6} + 0,5\Delta t, 0,5 \left[ -2f_u(q_{\text{min}}^r) \right] > 0$$

which reduces to

$$\Delta t < p/3f_u(q_{\text{max}}^r)$$

Equations (12b) and (12c) establish that adopting the lumped-mass scheme in conjunction with a two-noded linear element allows the minimization of time-step size to achieve convergence without the need of simultaneously refining the mesh density. It is important here to note that although the condition in Eq. (12c) imposes a more stringent limit on $\Delta t$, in comparison to Eq. (12b), the two conditions converge within a value of $\theta_{\text{max}} = 0.2$ for $f_u(\theta)$ = exp $(6\theta)$, $\theta_{\text{min}} = 0$ and $l = 0.5$ as depicted in Fig. 1. In fact, the convergence occurs at a steeper rate for finer meshes and remains within the stated threshold for the coarsest meshes practicable for the problem. The delineated criteria are thus particularly stringent for near-dry conditions and can be relaxed at higher levels of moisture content using average value of moisture content; that is, $\theta_{\text{avg}}$ in place of $\theta_{\text{max}}$.

Similarly, for the phase of drying, the governing criteria for time-step size corresponding to conditions (1) and (2) would be

$$\Delta t < D_{\text{water}}^r/f_{\theta_{\text{max}}}^r$$

Implementing the Time-Step Size Criteria

To illustrate an application of the delineated time-stepping criteria and the influence of mass type on numerical oscillations, we consider a one-dimensional moisture ingress problem involving an initially dry (i.e., $\theta = 0$ at $t_r = 0$) concrete medium of length $L = 0.10$ m subjected to a rainfall of intensity, $I_r = 10 \text{ mm/h}$ until the attainment of surface saturation (i.e., $\theta = 1$ at $x_r = 0$). The typical material parameters opted for the analysis are $\theta_{\text{max}} = 0$ m$^3$/m$^2$, $\theta_{\text{min}} = 0.1811$ m$^3$/m$^2$, $D_{\text{water}} = 9.45 \times 10^{-10}$ m$^2$/s and $n = 6$. The FE mesh has been constituted using linear elements of reduced size, $l = 0.5$, which equals $0.17$ mm for the adopted parameter values.

The FE analysis of the considered problem, governed by Eq. (8), has been carried out by four distinct approaches:

(i) using a consistent mass type and varying the time-step size in accordance to Eq. (11c);
(ii) with a lumped-mass type and varying the time-step size as per Eqs (12b) and (12c);
(iii) as in (i) but relaxing the time-stepping constraints in Eq. (11c) by replacing $\theta_{\text{max}}$ by $\theta_{\text{avg}}$;
(iv) as in (ii) but relaxing the time-stepping constraints in Eqs (12b) and (12c) by replacing $\theta_{\text{max}}$ by $\theta_{\text{avg}}$.

The time-stepping in FE analysis has been implemented using the following scheme:

1. At any instant $t_r$, calculate the present time-step size ($\Delta t_{\text{present}}$), if $t_r = 0$, take $\Delta t_{\text{present}} = 0.01I_p/\theta_{\text{max}}$ and for $t_r > 0$, take $\Delta t_{\text{present}} = \Delta t_{\text{next}}$, as determined in the previous instant of analysis.
2. Compute moisture distribution at the present instant $t_r$.
3. Calculate the limiting-time-step size ($\Delta t_{\text{limit}}$) using appropriate criteria.
4. Calculate time-step size for next instant to be simulated ($\Delta t_{\text{next}}$), if ($\Delta t_{\text{limit}} > 2 \Delta t_{\text{present}}$), then $\Delta t_{\text{next}} = 2 \Delta t_{\text{present}}$ else, $\Delta t_{\text{next}} = 0.95 \Delta t_{\text{limit}}$.
5. Increment time, $t_r = t_r + \Delta t_{\text{present}}$.

Figures 2–5 present the simulated results corresponding to each of the analysis approaches. These illustrations describe the evolution of reduced moisture content at nodes in successive time-steps and the distribution of moisture across the medium at the attainment of surface saturation. The observations clearly depict that the FE analysis based on consistent mass approach induces numerical oscillations in the simulated results. An inspection of Figs 2 and 4 further reveals that the oscillations strongly influence the initial stages of analysis and then gradually reduce to a relatively less intense level with a consistent effect on the nodes in a near-dry state at the toe of the wetting front. The analysis based on lumped-mass scheme, on the other hand, ensures a stable convergence of nodal values as is depicted in Figs 3 and 4 and also leads to convergence in relatively fewer time-steps, thereby economizing the computation time. Table 1 provides a summary of the time-steps computed and the simulated results. Relaxing the time-stepping constraints as in approaches (iii) and (iv) causes some perturbations in the initial evolution of nodal values as depicted in Figs 4 and 5. However, as summarized in Table 4, the analysis leads to satisfactory results with a significantly reduced computational time. These findings thus establish the advantage of implementing a lumped-mass scheme in conjunction with the relaxed time-stepping criteria delineated in the study for achieving computational efficiency and stability in the FE analysis of moisture transport in concrete.

The conventional model stated in Eq. (8j), which has been widely adopted in several previous studies, was also implemented to analyse the considered test problem. The observed trends of numerical stability were found to be similar to the ones obtained with the model proposed in this study. However, the computational expense for analysing the conventional model was found to be higher in relation to the proposed model. A comparison of the results has been summarized in Table 1.

![Fig. 2: Approach (i): (a) evolution of nodal values; (b) oscillating emergence of nodal values from initial dry state; (c) final moisture distribution across the medium](image1)

![Fig. 3: Approach (ii): (a) evolution of nodal values; (b) oscillation-free emergence of nodal values from initial dry state; (c) final moisture distribution across the medium](image2)

![Fig. 4: Approach (iii): (a) evolution of nodal values; (b) oscillating emergence of nodal values from initial dry state; (c) final moisture distribution across the medium](image3)
Discussion and Conclusions

A rational study of moisture movement in concrete rests on appropriate modelling of associated mass transport phenomena and on the efficacy of the numerical analysis of the constituted mathematical model. A sound comprehension of these facets is essential for a plausible treatment of the problem. The present work has addressed these aspects in the context of a rain-induced wetting–drying scenario, and in its discourse has emphasized the following ideas:

(a) The parabolic partial differential equation provides a phenomenological description of the flow of moisture in concrete under wetting and drying conditions albeit with distinct diffusivity functions.

(b) The presently available empirical models for hydraulic diffusivity incorporate parameters which are known to depend on temperature and the pore structure properties of concrete. This dependence, however, remains to be established mathematically in terms of the generic concrete properties. Future studies towards the refinement of hydraulic diffusivity models would enable a direct application of the delineated phenomenological approach in analysing the moisture transport in structural concrete.

(c) The restatement of the governing equation using the set of dimensionless terms, \( \theta_i = (\theta - \theta_0)/(\theta_f - \theta_0); x_i = (V_i/D_{d,wet})x \) and \( t_i = (V_i/D_{d,wet})t \) reduces the range of orders involved and hence minimizes the errors inherent in numerical computations; (ii) provides a representation characteristic of all hydraulically similar materials and (iii) economizes the computation time.

(d) Galerkin’s method can be effectively implemented to formulate a FE scheme for numerical analysis of the moisture transport problem. Its application has been elaborated using the modified model to describe the constitution of the characteristic matrices in detail.

(e) The occurrence of numerical oscillations inherent to the FE analysis of diffusion models relates to the nature of the matrices involved in the analysis and can be effectively controlled by imposing the conditions outlined in the study.

(f) The efficiency of lumped-mass scheme implemented in conjunction with a linear element for one-dimensional analysis has been mathematically interpreted. A concomitant time-stepping criterion for stable convergence has been derived, and its viability has been demonstrated through a test problem.

The deliberations presented in this paper provide an insight into the mathematical framework underlying the study of moisture transport phenomena in concrete and facilitate a robust FE analysis of moisture distribution in concrete subjected to wetting–drying exposure.

References


[34] Reddy JN. *An Introduction to the Finite Element Method*, 3rd edn, TMH; New Delhi, 2005.

