



An inverse analysis approach for the identification of the hygro-thermo-chemical model parameters of concrete

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ABSTRACT

Hygro-thermo-chemical models provide useful representations of the mechanisms of moisture transport and temperature variations that take place in concrete structures and that can influence their durability and service behaviour. Several material parameters need to be specified when performing a hygro-thermo-chemical simulation. While some of these parameters can be evaluated based on the concrete mix specifications or from data reported in the literature, some other parameters are not readily available from the literature, partly because of their large variability and partly because they do not possess a precise physical meaning. In this context, this paper presents a robust inverse analysis procedure for the identification of this latter set of material parameters. The inverse analysis problem is formulated by using temperature and relative humidity profiles taking place within a concrete component as input. The proposed approach is applied to evaluate the minimum number of temperature and relative humidity measurements that are necessary to be performed for a successful identification of the sought material parameters. Representative results of an extensive sensitivity analysis are presented to gain insight into the most effective locations within the concrete component for the measurements and instants in time when these measurements should be collected. The inverse analysis procedure is then presented and validated against a set of pseudo-experimental results affected by different levels of noise, highlighting the robustness of the proposed methodology when applied with the arrangements suggested in terms of discrete relative humidity and temperature measurements and monitoring periods.

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1. Introduction

Durability and serviceability limit states represent important requirements associated with the design of concrete structures. Excessive deformations, displacements and cracks may drastically affect the service behaviour of a structure and lead to increased maintenance costs. These effects are influenced by the time-dependent properties of the concrete and, in particular, by the physical and chemical mechanisms that take place in the concrete, especially in its early age. Moisture transport during hardening, occurring for release of water through the external surfaces and for internal water consumption due to chemical reactions such as cement hydration, causes volume changes that give rise to drying and autogenous shrinkage strains, respectively. The heat released during the cement hydration reaction may also cause volume changes inside the concrete. Different numerical and experimental studies on the early concrete behaviour exist in the literature and deal with the self-heating and self-drying phenomena. Bažant and Najjar [1] proposed a well-known material model for nonlinear moisture transport suitable for concrete

and similar materials. This model was extended in subsequent years, for example, by including the direct modelling of the cement hydration occurring in concrete at early age by means of a thermodynamics based approach (e.g. [2]); by considering the aging effect on strength development through a coupled thermo-chemo-mechanical model (e.g. [3]) or, more recently, by taking into account the permeability increase once a macro crack is formed (e.g. [4]). Kim and Lee [5] and Oh and Cha [6] proposed a model for moisture and temperature calculation at concrete early age, where a sink term was added to the diffusive moisture equation to account for internal water consumption. A multi-phase coupled thermo-chemo-mechanical model was proposed by Gawin [7] and more recently by Du [8] and it accounted for the porous nature of the concrete by considering a micro-scale description of the material. The effects of the 3D meso-structure, modelled with different aggregate particles shapes and porous cement paste matrix, and of microcracks distribution on diffusivity and permeability of concrete materials has been studied in [9,10]. A new cement hydration model has been proposed in [11], considering the effects of C-S-H layers forming around anhydrous cement grains to control the very long hydration process which may occur in thick concrete components. Di Luzio et al. [12,13] proposed a hygro-thermo-chemical model by considering the effect of

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cement hydration on both moisture and temperature calculations in terms of internal water consumption and self-heating generation.

While the use of such hygro-thermo-chemical models provides great insight into the material behaviour, it requires the knowledge and input of several material parameters. The latter can be subdivided into two major sets: (i) one set of parameters that can be evaluated based on the concrete mix specifications or from data reported in the literature; and (ii) a second set of parameters that are characterised by a large variability (based on data available in the literature) and, among these, many parameters do not possess a precise physical meaning and, for this reason, are not amenable to a direct measurement. The inability of the latter set of parameters to be easily identified provides a limitation on the wider use of the hygro-thermo-chemical model.

In this context, this paper aims to provide a robust procedure for the identification of the set of material parameters for the hygro-thermo-chemical modelling defined at point (ii), i.e. parameters characterised by a large variability, some of which not amenable to a direct measurement because not reflecting a precise physical property. The proposed approach relies on the use of an inverse analysis procedure (see [14–16]) that adopts temperature and relative humidity distributions as input data. The particularity of the proposed methodology is to give indication on the minimum number of temperature and relative humidity measurements that are required for a successful identification of the material parameters. This minimum requirement is established after evaluating through an extensive sensitivity analysis (of which representative results are presented in the following) the most effective locations and instants from concrete casting for the temperature and relative humidity measurements to take place through the thickness of a typical concrete component. The identification of the optimal locations and instants in time for the temperature and humidity measurements has significant practical implications, because supporting the effective planning of monitoring and measurement setups for laboratory or in-situ investigations. This becomes particularly significant considering the fact that recent technological advancements have led to a growing use and acceptance of temperature and relative humidity sensors embedded in concrete [17], for example, for its real-time strength monitoring. The outcomes of the proposed study will enable to optimise the number, locations and durations of the measurements while maximising the information collected.

In the first part of the paper, the hygro-thermo-chemical model is presented. In this section, a clear distinction is provided between the sets of parameters required by this model that can be determined from either the concrete mix specifications or from data available in the literature, and those that are characterised by a large variability and that are the focus of the present study. In view of using recorded temperature and relative humidity information as input in the inverse analysis process, the influence and responsiveness of the different material parameters on these two fields is discussed and representative trends are reported. The inverse analysis procedure is then introduced and its robustness is tested considering different scenarios constructed using pseudo-experimental data subjected to different degrees of noise. Representative results are provided to highlight the robustness of the proposed methodology when applied with the arrangements suggested for the discrete relative humidity and temperature measurements and with the recommended monitoring periods.

2. Hygro-thermo-chemical model

This section presents the hygro-thermo-chemical model capable to describe, over a spatial domain Ω , how the variations of the relative humidity h and temperature T take place over time t in a concrete component while accounting for different environmental conditions.

The model here adopted has been proposed in [12] and here applied, without any loss of generality, to a concrete mix without the presence of silica fume. The water transport mechanisms taking place in the concrete

are described by the combination of the Fick's law, expressing the flux of water mass $\mathbf{j}$ as proportional to the gradient of the relative humidity h (i.e. $\mathbf{j} = -D_h \nabla h$) and the water mass balance equation, e.g. [1–12]:

$$\frac{\partial w}{\partial t} = \nabla \cdot [D_h \nabla h] \quad \text{in } \Omega \quad (1)$$

where the total water content w depicts the sum of the evaporable water w_e and the non-evaporable water w_n , i.e. the water chemically bonded, for example, by cement hydration. The moisture diffusion parameter D_h depends on the relative humidity h and temperature T as highlighted by the following expression [12]:

$$D_h(h, T) = \psi(T) D_1 \left[1 + \left(\frac{D_1}{D_0} - 1 \right) (1 - h)^n \right]^{-1} \quad (2)$$

in which $\psi(T) = e^{(E_{ad}/RT_0 - E_{ad}/RT)}$, with T_0 being the reference room temperature (taken as 296°K in the simulations presented in the following), considers the influence of the temperature on the moisture diffusion (see [18]), while it is usually assumed that $E_{ad}/R = 4700\text{K}$ (see e.g. [1]), and parameters D_0 , D_1 and n depend on the specific concrete mix. In the literature, it is recognized that moisture diffusion depends on different transport mechanisms, which can be modelled individually to achieve a more physical description of the process. However, such an approach requires a series of information, such as concrete pore structure, pore radii and connectivity, that is usually not readily available or easily measurable from experimental tests. As this paper is focused at the identification of optimal or acceptable sets for practical experimental measurements, it is felt that the use of this single phenomenological law for the modelling of the different underlying physical mechanisms is acceptable, as also adopted by others in the literature [1,12].

Under the assumption that the non-evaporable water can be expressed as $w_n(\alpha_c) = k_c \alpha_c c$, with c being the cement ratio content and k_c a material parameter that, according to [12] and references herein, can be assumed equal to 0.253, and assuming the evaporable water to be expressed as a function of the relative humidity and of the degree of cement hydration α_c , i.e. $w_e = w_e(h, \alpha_c)$, Eq. (1) can be rewritten as follows:

$$\frac{\partial w_e}{\partial h} \frac{\partial h}{\partial t} = \nabla \cdot [D_h \nabla h] - \left(\frac{\partial w_e}{\partial \alpha_c} + k_c c \right) \dot{\alpha}_c \quad \text{in } \Omega \quad (3)$$

where the dot operator represents partial differentiation with respect to time t and α_c is calculated as the ratio between the level of hydration X_c and its theoretical asymptotic value $X_c^{\infty, th}$ exhibited in ideal hygro-thermal conditions. The maximum level of hydration at time infinity X_c^∞ is usually assumed to remain below $X_c^{\infty, th}$ and, therefore, the maximum value of the reaction degree $\alpha_c^\infty = X_c^\infty / X_c^{\infty, th}$ is usually smaller than one, i.e. $\alpha_c^\infty < 1$. According to [19], we may assume $\alpha_c^\infty = (1.032w/c)/(0.194 + w/c)$, with w/c being the water-to-cement ratio.

Eq. (3) highlights how the local variation of humidity depends on the divergence of the moisture flux and on two additional terms describing the microstructure variation (gel formation) and the internal consumption of water due to cement hydration.

The variation of α_c over time increases with relative humidity content and reduces while approaching its asymptotic value α_c^∞ as described by:

$$\dot{\alpha}_c = A_{c1} \left(\frac{A_{c2}}{\alpha_c^\infty} + \alpha_c \right) \cdot (\alpha_c^\infty - \alpha_c) \cdot e^{\left(-\frac{\eta_c \alpha_c}{\alpha_c^\infty} \right)} \cdot \frac{1}{[1 + (a - ah)^b]} \cdot e^{\left(-\frac{\gamma_c}{T} \right)} \quad (4)$$

where $\gamma_c = E_{ac}/R$ with E_{ac} being the hydration activation energy and R the universal gas constant. Parameters A_{c1} , A_{c2} and η_c have no precise physical meaning and govern the so-called normalized chemical affinity. Constants a and b enter into the empirical function $b_h(h) = [1 + (a - ah)^b]^{-1}$, which takes into account the slowing of the hydration process when relative humidity decreases below a certain

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