Construction and Building Materials 162 (2018) 202–214

Contents lists available at ScienceDirect

Construction and Building Materials

journal homepage: www.elsevier.com/locate/conbuildmat

Identification of the hygro-thermo-chemical-mechanical model parameters of concrete through inverse analysis

Massimiliano Bocciarelli [a,*], Gianluca Ranzi [b]

[a] Architecture, Built Environment and Construction Engineering Department, Politecnico di Milano (Technical University), Italy
[b] School of Civil Engineering, The University of Sydney, Australia

HIGHLIGHTS

- Inverse analysis procedure for a hygro-thermo-chemical-mechanical model.
- Temperature, humidity and deformation data used in input for the inverse analysis.
- Minimum experimental data required for the model parameter characterization.

ARTICLE INFO

Article history:
Received 5 July 2017
Received in revised form 27 November 2017
Accepted 30 November 2017

Keywords:
Concrete
Inverse analysis
Long-term behaviour
Moisture diffusion
Sensitivity analysis
Shrinkage

ABSTRACT

A wide range of parameters is required in input when applying hygro-thermo-chemical-mechanical models to concrete components with the aim of determining the variations over time of temperature, relative humidity and shrinkage induced deformations. While a sub-set of these material parameters can be evaluated on the basis of the concrete mix specifications or from literature data, this paper presents a robust inverse analysis procedure for the identification of the remaining sub-set of parameters that are characterised by a large variability and, in some cases, do not have a precise physical meaning and are not amenable to a direct measurement. The particularity of this paper is to propose different strategies for the characterisation of these material parameters that account for the presence of different exposure conditions, as these affect the outcomes and requirements of the parameter identification procedure. After introducing the adopted hygro-thermo-chemical-mechanical model, representative results of an extensive sensitivity analysis are presented in the first part of the paper to give insight into most effective number, location and duration of measurements to be used in input of the inverse analysis. The inverse analysis procedure is then presented and applied to a number of selected scenarios to highlight its robustness considering different boundary conditions in terms of external temperature and relative humidity surrounding the concrete. The ability to characterise these parameters will support a wider use of these hygro-thermo-chemical-mechanical models, especially for those applications in which humidity and temperature profiles significantly influence the structural response, for example when predicting curling in industrial pavements and non-uniform shrinkage profiles in composite steel-concrete slabs.

1. Introduction

Concrete structures are significantly influenced by the time-dependent behaviour of the concrete that affects their serviceability and durability. An inaccurate evaluation of this service response can lead to undesired excessive deformations and occurrence of cracking. Concrete time effects are significantly dependent on the moisture transport and heat transfer mechanisms that take place in the concrete and that control, for example, the hardening process, water release, cement hydration, and volume changes. Different numerical and experimental studies are available in the literature that deal with the concrete behaviour, especially considering its early age. Bažant and Najjar [1] presented a material model capable of describing the nonlinear moisture transport that takes place in concrete. Several researchers extended this approach in following years, for example, by incorporating a thermodynamics based approach for the cement hydration [2] or by establishing a thermo-chemo-mechanical model to account for the aging effect on strength development and the micro-scale description of the

* Corresponding author.
E-mail address: massimiliano.bocciarelli@polimi.it (M. Bocciarelli).

https://doi.org/10.1016/j.conbuildmat.2017.11.167

material [3–5]. Other recent contributions considered the influence of cracking on the permeability [6] or included a sink term into the diffusive moisture equation to capture the internal water consumption occurring during cement hydration [7,8]. The use of an enhanced cement hydration model was presented in [9] while the influence of the meso-structure was investigated in [10–12]. A hygro-thermo-chemical model that accounted for the effect of cement hydration on both moisture and temperature calculations was considered in [13,14]. In these models the mechanical coupling is usually based on a linear relationship between the variations over time of the relative humidity and the consequent free shrinkage deformations (see, e.g. [13,14,15,16]).

The use of these models is particularly relevant in applications where the effect of shrinkage induced deformations are important, such as curling in industrial pavements [17,18] and shrinkage gradients in composite floor systems [19–22] (where the presence of different exposure conditions, due to the presence of subgrade/waterproofing membrane and profiled steel sheeting, respectively, influence the mechanical response). In the latter case, the occurrence of the non-uniform shrinkage profiles has been only recently identified [19] and the ability to couple the hygro-thermo-chemical behaviour to the mechanical response will enable more accurate structural predictions associated to the serviceability limit state requirements of building floors. For these applications, the wider use of hygro-thermo-chemical-mechanical models for service design and modelling needs to be supported by techniques capable of adequately identifying the required material parameters. Not all material parameters to be specified in input in these hygro-thermo-chemical-mechanical models can be easily determined and, to better highlight this aspect, the model material parameters are subdivided into the following two 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 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.

In this context, the main contribution of this paper relies on the development of a robust inverse analysis procedure for the identification of the second set of material parameters (i.e. listed at point (ii) above) that are required in input for the use of the hygro-thermo-chemical-mechanical models. This paper contributes to this effort by proposing different strategies for the characterisation of the material parameters considering different exposure conditions.

In this work, the robustness of the proposed inverse analysis procedure is determined based on the use of pseudo-experimental results as input data (e.g. [23–25]) that includes measurements of temperature, relative humidity and total deformations. This data has been generated considering the same exposure conditions of commonly available reinforced or prestressed concrete slabs, i.e. exposed on both its surfaces, and of slabs exposed only from one side because sealed on its opposite side (e.g. composite slabs and industrial pavements). The proposed methodology is developed with the idea of minimising the number and the duration of the measurements to be carried out and of investigating how these are influenced by different exposure conditions. After introducing the key features of the hygro-thermo-chemical-mechanical model considered in this study, the main outcomes and representative results obtained from an extensive sensitivity analysis are presented because providing insight into the most effective number, location and duration of the measurements to be used as input of the inverse analysis procedure. The basis of the inverse analysis procedure is then presented and its robustness is tested against selected scenarios constructed using pseudo-experimental data subjected to different degrees of noise and for different external temperatures and relative humidities surrounding the concrete. Representative results are reported in the paper to give insight into the use and effectiveness of the proposed methodology. These results are also expected to support the effective planning of the instrumentation setup to be used in experimental tests on service conditions performed in controlled laboratory environments and for the arrangement of in-situ monitoring and investigations, for example during construction or during day-to-day service operations, associated to applications whose service response is influenced by shrinkage.

2. Hygro-thermo-chemical-mechanical model

The hygro-thermo-chemical-mechanical model considered in this paper is able to predict the variations of the relative humidity h, temperature T and deformation ε that take place over time within the spatial domain Ω of a concrete component taking into account its environmental conditions. The model here presented has been proposed in [13] and applied to a concrete mix without the presence of silica fume. The main features of the model and its numerical implementation are described in the following.

The principal chemical reaction occurring during hardening of a concrete mix is cement hydration, whose extent is here expressed through a scalar variable α_c, computed as the ratio between the actual level of hydration X_c and its theoretical asymptotic value $X_c^{\infty,th}$ achievable under ideal hygro-thermal conditions. The maximum level 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 [26], we may assume $\alpha_c^\infty = (1.032w/c)/(0.194 + w/c)$, in which w/c depicts the water-to-cement ratio. The variation over time $\dot{\alpha}_c$ increases with relative humidity content and reduces while approaching its asymptotic value α_c^∞ as expressed by the following Arrhenius type equation:

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

where $\gamma_c = E_{ac}/R$, E_{ac} is the hydration activation energy and R represents 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. The function $b_h(h) = \left[1 + (a - ah)^b\right]^{-1}$ takes into account the slowing of the hydration process when relative humidity decreases below a certain value (around 80%). Parameters a and b are usually taken equal to 7.5 and 4.0, respectively, (see [1]).

The total water content w, present in the concrete mix, is expressed as the sum of the evaporable water w_e and the non-evaporable water w_n, the latter being the water chemically bonded by cement hydration and 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 [13] and references herein, can be assumed equal to 0.253. The evaporable water is expressed as a function of the relative humidity (sorption isotherm curve) and of the degree of cement hydration α_c as follows:

$$\begin{aligned} w_e(h, \alpha_c) = {} & \kappa_{vg}^c \alpha_c c(1 - 1/\bar{e}_2) \\ & + \left[w_0 - 0.188\alpha_c c - \kappa_{vg}^c \alpha_c c(1 - 1/\bar{e}_1)\right] \cdot \frac{\bar{e}_2 - 1}{\bar{e}_1 - 1} \end{aligned} \tag{2}$$

in which $w_0(=(w/c)c)$ is the initial water content and it is assumed that $\bar{e}_2 = e^{10\left(g_1\alpha_c^\infty - \alpha_c\right)h}$ and $\bar{e}_1 = e^{10\left(g_1\alpha_c^\infty - \alpha_c\right)}$. Eq. (2) also depends on material parameters κ_{vg}^c and g_1 that govern the amount of water contained in the cement gel pores and the shape of the sorption curve, respectively.

Starting from the consideration that $w = w_e(h, \alpha_c) + w_n(\alpha_c)$, the variation of the humidity field over time and space is described