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Multiscale hydro-thermo-mechanical model for early-age and mature concrete structures

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ABSTRACT

Temperature and early-age mechanical properties in hydrating concrete structures present a significant risk for cracking, having a major impact on concrete durability. In order to tackle these phenomena, a multiscale analysis is formulated. It accounts for a high variety of cement properties, concrete composition, structure geometry and boundary conditions.

The analysis consists of two steps. The first step focuses on the evolution of moisture and temperature fields. An affinity hydration model accompanied with non-stationary heat and moisture balance equations are employed.

The second step contains quasi-static creep, plasticity and damage models. It imports the previously calculated moisture and temperature fields into the mechanical problem in the form of a staggered solution. The whole model has been implemented in the ATENA software, including also the effect of early-age creep, autogenous and drying shrinkage.

Validation on selected structures shows a good prediction of temperature fields during concrete hardening and a reasonable performance of the mechanical part.

1. Introduction

Thermal expansion, shrinkage and external restraints present a serious threat to concrete durability due to early-age cracking [1]. These problems may be investigated by means of virtual material and structure testing. Based on an accurate mathematical formulation of the underlying phenomena these models can assist in the prediction of structural deterioration. Sensitivity analysis and optimization present further extension of these multiscale models.

Extensive experimental research carried out in this area has already resulted in a number of precautions and recommendations incorporated in civil engineering guidelines and codes [2]. The formulation of numerical hydro-thermo-mechanical models followed historical evolution. The simplest models were formulated for the temperature evolution in hardening concrete under adiabatic curing conditions [3,4]. Recognizing a heterogeneous temperature distribution on the structural scale led to the development of multiscale models for temperature prediction [5,6] to cite a few. The most sophisticated models are based on chemo-mechanical coupling, adding optionally concrete creep, tensile failure with damage, plasticity or moisture transport [6–13]. These models are quite accurate and versatile, although they may suffer from a considerable number of input parameters being sometimes difficult to calibrate. Consequently, they are seldom used for routine engineering analyses.

This paper aims at developing a new simulation tool that can handle hydrating concrete in its complexity and heterogeneity. Emphasis is put on versatility, accuracy and rational simplicity, opening ways for wider engineering practice. A coupled multiscale approach was selected since it provides a robust modelling framework accommodating both material and structural scales. Now it is possible to account directly for cement properties, concrete composition, creep and shrinkage behaviour, structural topology, reinforcement and various boundary conditions.

The validation and verification present indispensable processes of any model. The international benchmark for crack control of reinforced concrete structures, known as ConCrack, see www.concrack.org, was chosen to illustrate the performance of the newly formulated multiscale model. It is worthy to review the results from 18 participating teams competed in the modelling of two reinforced beams using various software tools. A blind stage revealed that the maximum concrete core temperature in a RG8 experiment was predicted between 48 and 65 °C against the measured 55 °C. None of the competing teams reproduced correctly a dormant period and hydration kinetics strongly deviated. The results from the RG8 restrained shrinkage test revealed that only one model gave reasonable predictions for displacements. After

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the calibration stage, the majority of models were able to correct their predictions.

2. Formulation of hydro-thermo-mechanical model

Fig. 1 provides a flowchart of the developed multiscale hydro-thermo-mechanical model employing a staggered solution strategy. Firstly, moisture and heat transport analysis is carried out using a five-component model for concrete. Secondly, thermal and moisture fields are passed to the mechanical analysis of the structure. A weak coupling between hydro-thermal and mechanical parts is assumed, meaning that structural conditions in the mechanical model have no influence on the calculated hydro-thermal fields. The presented model has been implemented in the ATENA software [14].

2.1. Heat and moisture transport analysis

Heat and moisture analysis predicts the evolution of moisture and temperature fields. Both are used in the subsequent mechanical analysis for:

- Determination of the maximum temperature and its gradients.
- Calculation for thermal expansion and contraction strain.
- Accuracy enhancement of creep prediction models, e.g. the calculation of drying creep, drying shrinkage, the temperature effect on creep scaling.

2.1.1. Heat transport

The heat balance equation for non-stationary heat transport requires

$$\frac{\partial}{\partial t}(Q) = -\mathrm{div}(\bar{q}_T) \tag{1}$$

where Q is the total amount of heat accumulated in a unit volume of concrete in J/m^3 and $\bar{q}_T$ is a heat flux in J s^{-1} m^{-2}. A change of thermal energy occurs due to a temperature change and released hydration heat

$$\frac{\partial Q}{\partial t} = \frac{\partial Q_c}{\partial T}\frac{\partial T}{\partial t} + \frac{Q_h}{\partial t} = C_T\frac{\partial T}{\partial t} + \frac{\partial Q_h}{\partial t} \tag{2}$$

where Q_c is a heat gain or loss due to conduction in J/m^3, C_T is the heat capacity in J K^{-1} m^{-3}, Q_h is the total hydration heat released at the time t in J/m^3. The heat flux $\bar{q}_T$ is calculated via Fourier's law

$$\bar{q}_T = -\lambda\nabla(T) \tag{3}$$

where λ represents thermal conductivity in J s^{-1} m^{-1} K^{-1} for isotropic material. Substituting Eqs. (2) and (3) into Eq. (1) provides differential equation from which the unknown temperature field can be obtained.

2.1.1.1. Hydration heat. The affinity hydration model provides the framework for accommodating all stages of cement hydration and presents the core of the multiscale hydro-thermal formulation. It is accompanied by the calculation of released heat and consumed water during hydration stages. The degree of hydration $\alpha \in \langle 0,1\rangle$ can be approximated experimentally by the amount of liberated heat scaled to the potential hydration heat of cement, $Q_{h,pot}$, in J kg^{-1}

$$\frac{Q_h}{Q_{h,pot}} = \alpha \tag{4}$$

In the modelling, the degree of hydration is approximated by integrating the chemical affinity $\tilde{A}_{25}$. Expressing affinity at 25 °C has an advantage of easy scaling hydration kinetics with temperature while the other parameters inside the affinity model remain constants. The evolution of the degree of hydration under an arbitrary temperature T reads

$$\frac{\partial\alpha}{\partial t} = \tilde{A}_{25}\exp\left[\frac{E_a}{R}\left(\frac{1}{T_{25}} - \frac{1}{T}\right)\right] \tag{5}$$

where R is a gas constant 8.31441 J mol^{-1} K^{-1}, T is the current temperature in K, T_{25} is a reference temperature in K, and the activation energy E_a is approximately 40 kJ/mol, see [15].

Cervera et al. [16] developed an analytical form of the normalized affinity which was refined in [12]. A slightly modified formulation is proposed here

$$\tilde{A}_{25} = B_1\left(\frac{B_2}{\alpha_\infty} + \alpha\right)(\alpha_\infty - \alpha)\exp\left(-\eta\frac{\alpha}{\alpha_\infty}\right) \tag{6}$$

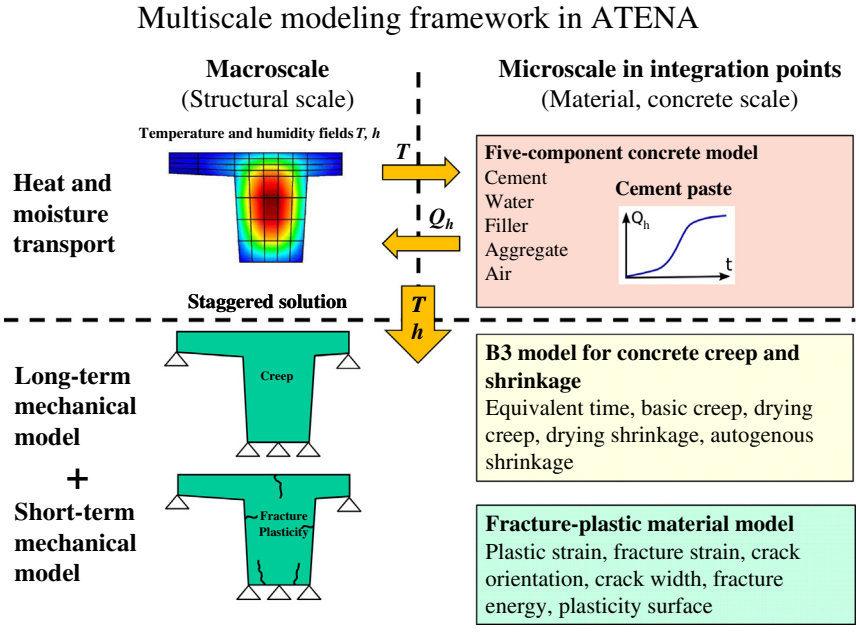

Fig. 1. Flowchart of the multiscale hydro-thermo-mechanical model.