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Micromechanics-based multifield framework for early-age concrete

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ABSTRACT

In the process of hydration of concrete, there are considerable interacting physical and chemical changes inside the material, affecting both composition and morphology of concrete at early ages. These changes are properly considered within multiscale models comprising several scales of observation and giving access to the effective properties via upscaling. In this paper, a multiscale model for early-age concrete is implemented into a multifield (thermo–hygro–chemo–mechanical) framework, which accounts for all major processes among the solid, liquid, and gas phases of concrete by means of mass, energy, and momentum equilibrium. The proposed modeling approach is employed for the investigation of the effect of formwork removal (stripping) of early-age concrete, exposing the concrete surface to the outside environment which may cause early-age cracking of concrete structures. Based on the multiscale approach, the authors evaluate the cracking risk of concrete members with respect to the underlying mix-design, size of the concrete member, and stripping time, providing first insight into the influence of these parameters on the cracking risk of early-age concrete.

1. Introduction

Early-age concrete experiences severe physical and chemical changes during its hydration process, causing deformation and, thus, inducing stress inside concrete. Realistic prediction of these stresses shall assist to optimize the curing conditions and setting of concrete members and, thus, to minimize the risk of early-age cracking. For determination of these stresses, multifield models were proposed in the literature, focusing on the thermo-chemical field (energy field) [1–3] and the moisture-gas field (mass-transport field) [4–6]. When the thermo-chemical field and moisture-gas field are determined, the total strain theory [4] and effective stress theory [7,8] are used to solve the underlying mechanical field problem. In application, the weak-coupled multifield models solve the energy field, mass-transport field (or ignore mass-transport field), and mechanical field by turns, which ignores mass-transport process or ignores the impact of mass-transport on the energy field [9]. More recently, fully-coupled (thermo–hygro–chemo–mechanical) analysis tools were developed [10]. Both weak-coupled and fully-coupled approaches have been validated and proved effective for different types of concrete (OPC as well as HPC) [11,10], while the former has advantages on efficiency, the latter may be applied to open systems. Such systems are encountered in case of removal of formwork, representing the first direct contact of concrete with the outside environment. Hereby, vaporization and convection at the concrete surface are induced, resulting in a rapid drop of temperature on the concrete surface, referred to as thermal shock. Several codes (such as [12]) emphasis the importance of proper removal of formwork, which was investigated numerically in [11] by means of thermo-chemical analysis.

In order to capture the heterogeneous nature of concrete, multiscale models were developed to predict the elastic properties of early-age concrete [13,14], autogenous-shrinkage [15], and creep [16]. Multiscale models provide a routine for homogenization of the behavior of concrete, giving access to effective material properties as basis for further analysis.

In this paper, a multiscale model for early-age concrete is combined with a fully-coupled multifield framework. Hereby, both the elastic properties of concrete as well as Biot's coefficient appearing in the constitutive law of the mechanical field problem are related to finer-scale properties of concrete. In Section 2, the multiscale model for early-age concrete and the multifield framework are discussed, in the meanwhile, the boundary conditions related to formwork removal are described. In Section 3, numerical studies are conducted, focusing on the difference between weak-coupled analysis and fully-coupled analysis as well as possible remedies to minimize the error introduced by the weak-coupled analysis. Moreover, concrete members with different size and stripping time are studies with respect to the maximum stress and, hence, cracking risk as a function of material and processes specifications (mix design, stripping time).

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Nomenclature

List of symbols

$\widetilde{A}$	chemical affinity of hydration reaction (s^{-1})
b^{hom}	Biot's coefficient (–)
a, b, c	parameters defining $\widetilde{A}$ (s^{-1}), (–), (–)
c_p	heat capacity of concrete (J kg^{-1} K^{-1})
c_p^g, c_p^w, c_p^s	heat capacity of gas, water, solid part of concrete (J kg^{-1} K^{-1})
$\mathbb{C}^{hom}$	homogenized elastic stiffness tensor
D^{eff}	effective diffusivity of concrete (m^2 s^{-1})
E_a	activation energy of hydration process (J mol^{-1})
E	Young's modulus of concrete (MPa)
f_x	volume fraction of component x
f_t, f_c	tensile and compressive strength of concrete (MPa)
$f_{t,\infty}$, $f_{c,\infty}$	tensile and compressive strength of mature concrete (MPa)
h	specific enthalpy of vaporization (J kg^{-1})
$\mathbf{1}$	second-order unity tensor
$\mathbf{k}$	intrinsic-permeability tensor of concrete (m^2)
K^{hom}, K^s	homogenized bulk modulus and bulk modulus of solid part (MPa)
k^{rg}, k^{rw}	relative permeability of gas and liquid phase (–)
$\mathcal{L}$	the structural dimension of heat diffusion (m)
l_ξ	hydration heat per unit mass of hydration products (J kg^{-1})
$\dot{m}_{hydr}$	rate of mass of hydration products per unit volume concrete (kg m^{-3} s^{-1})
$\dot{m}_{vap}$	change of vapor mass per unit volume concrete (kg m^{-3} s^{-1})
M_a, M_w, M_g	molar mass of dry air, water, gas mixture (kg mol^{-1})
n	porosity of concrete (–)
p^g, p^w, p^c	gas, water, capillary pressure of concrete (Pa)
p^{ga}, p^{gw}	air partial pressure and vapor partial pressure in gas (Pa)
p	
$_{satb}$, $p_{sat\infty}$	saturation vapor pressure at the boundary of concrete and in the environment (Pa)
R	universal constant for ideal gases (J mol^{-1} K^{-1})
Rh_b, Rh_∞	relative humidity at the boundary of concrete and in the environment (–)
S_w	saturation degree of pores in concrete (–)
S	moisture boundary coefficient considering surface cover (–)
T	absolute temperature in concrete (K)
T_b, T_∞	temperature at the boundary of concrete and in the environment (K)
v	wind speed (m s^{-1})
α_T	convection coefficient (J s^{-1} m^{-2} K^{-1})
α_V	equivalent convection coefficient caused by vaporization (J s^{-1} m^{-2} K^{-1})
β_s	thermal expansion coefficient of solid part of concrete (K^{-1})
λ, λ^{eff}	thermal conductivity and effective thermal conductivity coefficient of concrete (J s^{-1} m^{-1} K^{-1})
η^g, η^w	viscosity of gas, water phase (Pa s)
ρ^g, ρ^w, ρ^s	density of gas, water, solid part of concrete (kg m^{-3})
ρ^{ga}, ρ^{gw}	density of dry air and water vapor (kg m^{-3})
ξ	hydration degree (–)
ξ_0	percolation threshold (–)
$\boldsymbol{\Sigma}$	microscopic and macroscopic stress tensor (MPa)
$\mathbf{E}$	macroscopic strain tensor (–)
$\mathbf{E}^T$	thermal strain tensor (–)

2. Model

2.1. Multiscale model

The degree of hydration $\xi(t)$ of early-age concrete is defined by the volume fraction of cement in the material system, $f_{cem}(t)$, related to the respective initial volume fraction, $f_{cem}^{initial} = f_{cem}(t=0)$, $\xi(t) = 1 - f_{cem}(t)/f_{cem}^{initial}$. The evolution of ξ is determined by an Arrhenius-type law [17,3]:

$$\dot{\xi} = \widetilde{A} \exp\left(-\frac{E_a}{RT}\right), \tag{1}$$

where E_a/R is set to 4000 K. A mathematical relation for the chemical affinity $\widetilde{A}$ is given by $\widetilde{A} = a\xi^b(1-\xi)^c$, where a, b, c can be acquired from adiabatic tests [18]. Eq. (1) accounts for the thermo-chemical coupling, giving an increased hydration rate with increasing temperature, or vice versa. In this paper, changes in pore water saturation due to drying/wetting is assumed to not affect the hydration kinetics. On the other hand, the hydration reaction cannot continue when free water is exhausted. Within this paper, the hydration process is assumed to stop when the saturation degree S_w drops below a certain threshold value $\overline{S_w}$, where $\overline{S_w}$ is set to 58.6%.[1]

As an engineering approximation, the hydration of cement is represented by the hydration stoichiometry of tricalcium silicate (C_3S[2]), i.e., the main clinker phase in all Portland cement-based material systems [19]:

$$C_3S + 5.3H \rightarrow 0.5C_{3.4}S_2H_8 + 1.3CH \tag{2}$$

Using the intrinsic material properties summarized in Table 1, Eq. (2) can be written as mass balance:

$$\begin{aligned} &228 + 5.3 \times 18 \rightarrow 0.5 \times 454 + 1.3 \times 74 \quad \text{in(g)} \\ &323 \rightarrow 323 \quad \text{in(g)} \end{aligned} \tag{3}$$

or volumetric balance:

$$\begin{aligned} &\frac{228}{3.15} + 5.3\frac{18}{0.998} \rightarrow 0.5\frac{454}{1.99} + 1.3\frac{74}{2.24} \quad \text{in } (cm^3) \\ &167.97 \rightarrow 157.02 \quad \text{in } (cm^3) \end{aligned} \tag{4}$$

Hence, the water-to-cement mass ratio (w/c) needed for completion of full hydration, $\overline{w/c}$, can be determined from Eq. (3) as

$$\overline{w/c} = \frac{5.3 \times 18}{228} = 0.418 \tag{5}$$

On the other hand, the chemical shrinkage associated with the stoichiometric relation given in Eq. (2) is determined from Eq. (4) as

$$1 - \frac{157.02}{167.97} = 6.52\% \tag{6}$$

[1] According to [4], the hydration stops completely when the relatively humidity drops below 80%, with the corresponding saturation degree being about 58.6% at 20 °C (see Eq. (15)). However, this threshold value does not concern the results of the numerical simulation in this paper. Because stripping is conducted after 24 h and the maximum stress will emerge 3 h after stripping (the conclusions will be given later), the increase of the hydration degree within these 3 h is negligible.

[2] Standard cement chemistry abbreviations are used throughout this paper: C = CaO, S = SiO_2, H = H_2O.