



A coupled thermo-hygro-chemical model for characterising autogenous healing in ordinary cementitious materials



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ABSTRACT

Experimental work has demonstrated that cracks can be healed in ordinary cementitious materials in the presence of water. The primary healing mechanisms are hydration of the unreacted nuclei of cement particles and the long-term formation of calcite. A mathematical model for simulating early-age autogenous healing of ordinary cement-based materials is proposed, which employs a coupled thermo-hygro-chemical (THC) framework and which uses a reactive water transport component to predict the movement of healing materials. A single concentration variable is employed for the healing component of the model that is derived directly from the quantity of unreacted cement and computed using a generalised cement hydration model component. The hydration component is directly linked to an expression for capillary porosity and for the porosity of the material within a healed crack. The results from a series of model simulations are in good general agreement with experimental data from tests on autogenous healing.

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Nomenclature

a	material parameter	K_X	order of reaction of mineral X
a_i	constant; $i \in [1,5]$	m	material parameter
A_k, A_f, A_p, A_w	material parameters	m_i	mass of i per unit volume [kg m^{-3}]
A_λ	material parameters	$\dot{m}_\pi^i$	type i mass rate of phase π [$\text{kg m}^{-3} \text{s}^{-1}$]
A_{crack}	area under the crack width curve [μm^2]	m_{c_i}	type i moisture content
b	material parameter	M_w	molar mass of the water [kg kmol^{-1}]
b_i	constant; $i \in [1,5]$	ne	number of finite elements
B_v	material coefficient	nn	number of nodes
c_1, c_2	empirical constants	$\bar{n}$	unit normal vector
c_{FA}	porosity coefficient due to FA	$\mathbf{N}$	vector of shape function
$c\eta$	material parameter	p_i	pressure type i [Pa]
$\hat{\mathbf{C}}$	global secant capacity matrix	q_π	imposed flux of phase π [$\text{kg m}^{-2} \text{s}^{-1}$; $\text{J m}^{-2} \text{s}^{-1}$]
C_{1S}^i	material coefficient of porosity type i	Q_h	rate of heat generation [$\text{J m}^{-3} \text{s}^{-1}$]
C_p^π	specific heat capacity of π [$\text{J K}^{-1} \text{kg}^{-1}$]	R	ideal gas constant [$\text{J K}^{-1} \text{kmol}^{-1}$]
d_{cz}	porosity material coefficient in crack zone	RH	relative humidity
D_π^i	type i diffusion coefficient of π [m^2/s]	R_{ck}	average radius of the clinker grain [m]

E	activation energy of the reaction [J kmol^{-1}]	S_π	saturation degree of phase π
f_i	weight ratio of i in terms of total cement content [%]	t	time [s]
f_s	structure coefficient	T	temperature [K]
$\mathbf{\bar{F}}$	global right-hand side vector	$\bar{v}^{ws}$	mass-averaged velocity of water phase with respect to solid phase [m s^{-1}]
$\bar{g}$	gravity vector [m s^{-2}]	V_i	volume of iper unit volume [$\text{m}^3 \text{m}^{-3}$]
H_i	total heat of hydration of material i [J m^{-3}]	w_{crack}	crack width [μm]
J_π^i	type i flux of phase π [$\text{kg m}^{-2} \text{s}^{-1}$]	w_{ref}	reference crack width [μm]
k_π^i	type i permeability coefficient of π [m^2]	w_π^{ult}	ultimate quantity of the gel water i [kg m^{-3}]
$\mathbf{\bar{K}}$	global secant hydraulic conductivity matrix	w/c	water-cement ratio

Greek symbols

α	empirical constant	$\delta\Phi$	increment of the vector of unknowns
α_g	longitudinal dispersivity	ΔH_v	specific heat of evaporation [J kg^{-1}]
α_p	precipitation parameter	Δt	time increment [s]
β	hydration shape parameter	η	porosity
β_{Tr}	transversal dispersivity	κ_X	rate constant of the mineral X
	coefficient [m]		

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β_p	precipitation parameter	λ_{dry}^{eff}	effective thermal conductivity of a dry material [$\text{W K}^{-1} \text{m}^{-1}$]
γ	filling fraction	μ_w	dynamic viscosity of liquid water [$\mu\text{Pa s}$]
γ_{norm}	normalized filling fraction	ρ_π	density of phase/material π [kg m^{-3}]
Γ	degree of hydration	$\bar{\rho}_\pi$	phase-averaged density of π [kg m^{-3}]
Γ_q	boundary of the domain	$\bar{\rho}C_p$	storage heat capacity [$\text{J m}^{-3} \text{K}^{-1}$]
δ_{ij}	Kronecker delta	τ	hydration time parameter
δ_T	heat transfer coefficient [$\text{W m}^{-2} \text{K}^{-1}$]	Φ	vector of unknowns
δ_{wv}	moisture transfer coefficient [m s^{-1}]	Ψ	residual vector
δ_ω	solute transfer coefficient [$\text{kg s}^{-1} \text{m}^{-2}$]	ω	mass of unreacted cement per mass of capillary solution [kg kg^{-1}]
		Ω	domain

Subscripts/superscripts

<i>agg</i>	aggregate	<i>eff</i>	effective value	<i>P</i>	precipitate
<i>atm</i>	atmospheric	<i>endST1</i>	end of stage 1	<i>ref</i>	reference value
<i>A</i>	advective	<i>env</i>	environmental value	<i>rel</i>	relative value
<i>AW</i>	adsorbed water	<i>FA</i>	fly ash	<i>res</i>	residual value
<i>cap</i>	capillary	<i>g</i>	gas	<i>s</i>	solid
<i>cem</i>	Portland cement	<i>GGBF</i>	ground-granulated blast-furnace slag cement	<i>sat</i>	saturated value
<i>clink</i>	clinker	<i>hyd</i>	hydration	<i>str</i>	strain
<i>cr</i>	critical value	<i>int</i>	intrinsic value	<i>SCM</i>	supplementary cementing materials
<i>cz</i>	crack zone	<i>int_{mat}</i>	intrinsic value of the matured paste	<i>SGW</i>	small gel water
<i>CBW</i>	chemically combined water	<i>I</i>	end of the induction period	<i>tot</i>	total
<i>CD</i>	conductive	<i>IGW</i>	intraglobular water	<i>T</i>	temperature
<i>CW</i>	capillary water	<i>ILW</i>	interlayer water	<i>ult</i>	ultimate value
<i>da</i>	dry air	<i>k</i>	iteration number	<i>UCP</i>	unreacted cement paste
<i>des</i>	desorption	<i>LGW</i>	large gel pore water	<i>v</i>	water vapour
<i>dry</i>	dry condition value	<i>mol</i>	molecular	<i>w</i>	liquid water
<i>D</i>	diffusive	<i>n</i>	step number	<i>wv</i>	moisture
<i>DD</i>	diffusive-dispersive	<i>NG</i>	end of the nucleation and growth controlled period	ω	solute
<i>e</i>	elemental value	<i>per</i>	percolation threshold of Γ	0	initial value
<i>ea</i>	entrapped air	<i>pm</i>	porous material		

Notations

• time derivative of X	$\frac{D^s}{Dt}$	material time derivative with respect to the solid phase	<i>div</i>	divergence operator (spatial description)
	$\frac{\partial}{\partial X}$	partial derivative with respect to X	<i>grad</i>	gradient operator (spatial description)

1. Introduction

Cementitious composites are quasi-brittle materials that develop their porous internal micro-structure during hydration. The complex pore structure within these materials, along with any micro-cracks present, largely governs the moisture and heat transfer properties of the composite material. Structures formed from these cementitious materials have frequently suffered from poor durability that has resulted in expensive repair and maintenance work. In recent years, researchers have investigated new cementitious materials that have the ability to self-repair, as a possible remedy to these durability problems.

Since Turner's first discussion on crack repair [1], the pace of experimental research on self-healing in cementitious materials has greatly accelerated [2–4]. Van Tittelboom and De Belie [2] provided an extensive state-of-the-art review of research on self-healing in cementitious materials in which the authors identified two main groups of self-healing techniques: (i) 'autonomic' healing, in which a single or multi-component healing agent is released from embedded capsules or vascular systems by damage and temperature activation [3] and (ii) 'intrinsic'/'autogenic' self-healing, based on the chemical reactions between the components of the cementitious matrix. In the latter case, the recovery of mechanical or durability properties is obtained either by autogenous healing or by healing in a polymer modified concrete [2]. Initially, autogenous healing was attributed solely to ongoing hydration of the remnant clinker and intercrystallisation of the fractured crystals [1]. More recent research suggests that continuous hydration is only predominant in the first weeks after casting, when the amount of unreacted cement is significant, but that calcite formation is the main mechanism thereafter [2,4–6]. Experimental tests showed a decrease of water permeability, a recovery of stiffness and a regain of compressive and flexural strengths [4–11]. The number of numerical studies on autogenous healing is still limited. Ter Heide [12] incorporated the bar and ribbon models developed by Lokhorst [13] and Koenders [14] and used bridging particles to fill the existing gaps between the clusters of hydrates formed as a result of the expansion of unhydrated cement. The distribution and further hydration of these particles were simulated considering diffusion and thermodynamic principles in the HYMOSTRUC [15] model. Huang and collaborators proposed an alternative modelling approach for autogenous healing in high performance concrete [16]. Again, the distribution and fraction of the unreacted cement particles were determined with the microstructural model HYMOSTRUC 3D. This time though, the dissociated ions from the clinker minerals were transported to the crack surface via a diffusion model, while the precipitation of the hydrates was represented in a thermodynamic model comprising mass and charge balance as well as chemical equilibrium. The mechanical recovery of the cracked cement paste was investigated using finite element models by Remmers and de Borst [17] and Hilloulin et al. [18]. Remmers and de Borst introduced momentum and mass balance equations for a fluid-saturated porous medium and modelled crack rebonding by adding a strength and stiffness increment of the interface to the constitutive relation that governs the crack opening. Hilloulin et al., on the other hand, solved a hydro-chemo-mechanical problem in which the chemical reactions were simulated in a hydration model based on the Arrhenius law.

In this paper a numerical study is presented on the simulation of autogenous healing of young cement-based materials. Dissolved clinker is modelled as a single solute that can be diffused and advected due to concentration and water pressure gradients, respectively. The thermohygral model formulated for transport phenomena in a porous medium [19,20] has been extended with a mass balance equation for the healing product. The kinetics of phase change, from dissolved clinker to precipitated material, is modelled using Freundlich equilibrium isotherm. The formation and variation of the porous network before and during crack recovery is assessed using the microstructural model STOICH_HC2 [21, 22]. The model is validated using data from recent tests undertaken at Cardiff University as well as from autogenous healing experiments reported in the literature. As discussed more fully in Section 3, the authors consider that the efficiency of this semi-phenomenological model would allow it to be coupled to a mechanical analysis and employed in the analysis of full-scale structures. The assumptions upon which the model is based means that is more applicable to early age self-healing than to long-term calcite formation.

2. Structure of the hydrated cement

The hydration of cement based materials leads, in the early stages of the reaction, to the appearance of an unstable chemical system with varying physical and chemical properties.

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