Numerical modelling of concrete degradation due to alkali-silica reaction in variable hygro-thermal conditions

Dariusz Gawin[1], **Francesco Pesavento**[2], **Witold Grymin**[1], **Mateusz Wyrzykowski**[1], **Luciano Simoni**[2]

[1]*Department of Building Physics and Building Materials, Technical University of Łódź, al. Politechniki 6, Łódź 90-924, Poland*
e-mail: dariusz.gawin@p.lodz.pl, witold.grymin@p.lodz.pl, mateusz.wyrzykowski@p.lodz.pl

[2]*Department of Structural and Transportation Engineering, University of Padova, via Marzolo 9, 35131 Padova, Italy*
e-mail: pesa@dic.unipd.it, simoni@dic.unipd.it

Abstract

A new numerical model for the simulation of ASR in cement-based materials considering both the effect of temperature and moisture content is presented. A mechanistic approach, based on the mechanics of porous media, was used to obtain the governing equations by means of a hybrid mixture theory. The model equations, mass (water species and dry air), energy and momentum balances are written in terms of the chosen primary variables: gas pressure, capillary pressure, temperature and displacement vector, while the ASR evolution is described by the reaction extent being the internal variable. The model takes into account full coupling between hygral, thermal and chemical phenomena, as well as changes of concrete properties caused by chemical reaction, i.e. porosity, density, permeability. Phase changes and chemical processes, as well as the related heat and mass sources are considered. Material chemical and mechanical degradation is considered with the isotropic damage theory. The model equations are numerically solved using finite element method for discretization in space and finite differences for time integration. The model results are validated by comparison with some published experimental data concerning ASR expansion in constant and variable hygro-thermal conditions.

Keywords: concrete, damage, porous media, coupled fields, finite elements method

1. Introduction

Durability of cement-based materials in normal and chemically aggressive environment has been an important subject of research in recent two decades. Several mathematical models have been developed for predicting the service life of concrete structures. Different chemical degradation processes are considered, including also those due to the alkali-silica reaction (ASR). Most of the models describing the latter process are based on a phenomenological approach. Here a mechanistic-type mathematical model of chemical degradation of concrete, based on mechanics of multiphase porous media, due to combined action of hygro-thermal, chemical and mechanical loads, is presented.

2. Mathematical model

The proposed mathematical model is an extension of the one that describes the heat and moisture transport in concrete at early ages and beyond [1], considering additionally the ASR reaction evolution and its influence on the heat and moisture transport properties. A porous material consists of a solid skeleton, voids of which are partly filled with liquid water, and partly with a mixture of dry air and water vapour. It is assumed that the moist air is perfect gas. The moisture content is described by the water saturation degree, S_w.

Concrete strains are described as a function of the effective stresses, while the material degradation due to simultaneous action of chemical processes and mechanical loads is modelled with the isotropic damage theory, similarly as done by the authors for concrete exposed to calcium leaching, [2].

The mathematical model consists of four governing equations: water mass conservation, dry air mass conservation, energy conservation and linear momentum conservation as well as evolution equation describing the ASR reaction kinetics. The chosen primary variables of the model are: gas pressure $p^g(\mathbf{x}, t)$, capillary pressure $p^c(\mathbf{x}, t)$, temperature $T(\mathbf{x}, t)$, and displacement vector $\mathbf{u}(\mathbf{x}, t)$, and the ASR reaction extent $\Gamma_{ASR}(\mathbf{x}, t)$ is internal variable of the model.

The ASR is modelled as a two stage process, involving chemical reactions causing first silica dissolution and then gel formation, [3, 4]. The effect of moisture content on the kinetics of the first process is considered similarly to Steffens et al. [4] and effect of temperature following approach proposed by Ulm et al. [5]. Here the two effects are considered jointly, resulting in the following ASR evolution equation,

$$\frac{\partial \Gamma_{ASR}}{\partial t} = \frac{1-\Gamma_{ASR}}{\tau_r(T,S_w)\cdot\lambda(T,S_w,\Gamma_{ASR})} \tag{1}$$

where $\tau_r(T,S_w)$ is the characteristic time of ASR reaction at temperature T and moisture content S_w, while $\lambda(T,S_w,\Gamma_{ASR})$ is an experimentally determined material function [5].

It is assumed that the gel formation process causes expansion of the material skeleton and the maximal chemical strain is dependent on the moisture content, Fig. 1a, and to a much lesser extent on the temperature value, Fig. 1b. The gel is assumed to be in equilibrium with moisture in its pores, hence any variation of relative humidity causes an immediate change of chemical strains, also during the decrease of water content.

3. Numerical solution

The model equations are discretized in space using finite element method, and integrated in time with the fully implicit scheme of finite difference method, resulting in the following equation set, [2],

$$\mathbf{C}_{ij}\left(\bar{\mathbf{X}}_j^{n+1}\right)\frac{\bar{\mathbf{X}}_j^{n+1}-\bar{\mathbf{X}}_j^{n}}{\Delta t}+\mathbf{K}_{ij}\left(\bar{\mathbf{X}}_j^{n+1}\right)\bar{\mathbf{X}}_j^{n+1}=\mathbf{f}_i\left(\bar{\mathbf{X}}_j^{n+1}\right) \tag{2}$$

where

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\mathbf{K}_{ij} = \begin{bmatrix} \mathbf{K}_{gg} & \mathbf{K}_{gc} & \mathbf{K}_{gt} & \mathbf{0} \\ \mathbf{K}_{cg} & \mathbf{K}_{cc} & \mathbf{K}_{ct} & \mathbf{0} \\ \mathbf{K}_{tg} & \mathbf{K}_{tc} & \mathbf{K}_{tt} & \mathbf{0} \\ \mathbf{K}_{ug} & \mathbf{K}_{uc} & \mathbf{K}_{ut} & \mathbf{K}_{uu} \end{bmatrix}, \quad \bar{\mathbf{X}}_j = \begin{Bmatrix} \bar{\mathbf{p}}^g \\ \bar{\mathbf{p}}^c \\ \bar{\mathbf{T}} \\ \bar{\mathbf{u}} \end{Bmatrix}, \tag{3}
$$

$$
\mathbf{C}_{ij} = \begin{bmatrix} \mathbf{C}_{gg} & \mathbf{C}_{gc} & \mathbf{C}_{gt} & \mathbf{C}_{gu} \\ \mathbf{0} & \mathbf{C}_{cc} & \mathbf{C}_{ct} & \mathbf{C}_{cu} \\ \mathbf{0} & \mathbf{C}_{tc} & \mathbf{C}_{tt} & \mathbf{C}_{tu} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}, \quad \mathbf{f}_i = \begin{Bmatrix} \mathbf{f}_g \\ \mathbf{f}_c \\ \mathbf{f}_t \\ \mathbf{f}_u \end{Bmatrix}, \tag{4}
$$

The non-linear equation set (2) - (4) is first linearized using the Newton-Raphson method, and then solved with a monolithic approach [2].

The first numerical example is based on the experimental tests performed by Larive [5] and it deals with a cement mortar specimens exposed to various, but constant in time, hygral and thermal conditions. The material contained reactive aggregates hence considerable swelling strains due to the ASR reaction were observed. The simulations are performed for four different values of ambient relative humidity, 100% (in water), 98%RH, 92% and 86% at the same temperature of 38°C, and then three different values of ambient temperature, 23°C, 38°C and 60°C, at the same relative humidity of 92%. The comparison of the simulation results with the experimental ones [5] is presented in Fig. 1, showing their good agreement.

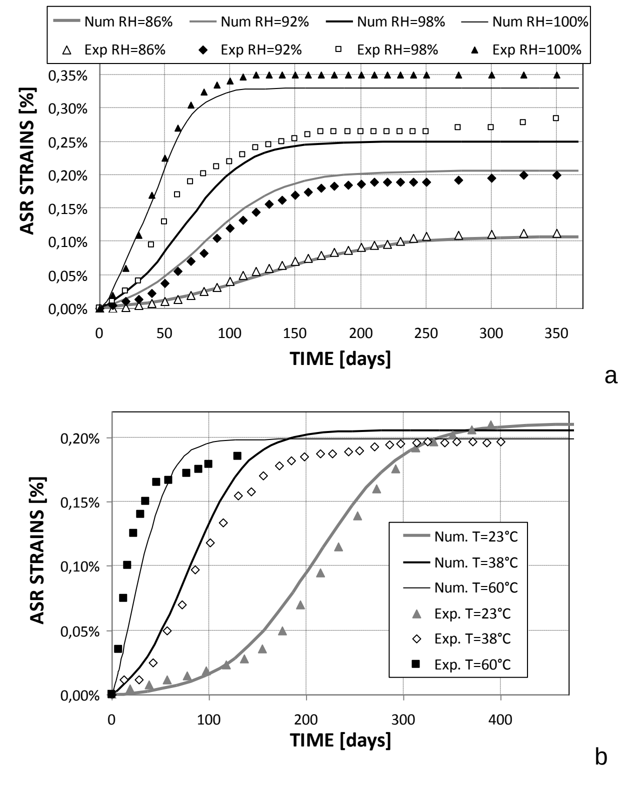

Figure 1. Comparison of the ASR strains obtained from simulations with the experimental data [5]: a) for different values of RH at T=38°C, b) for different values of temperature at RH=92%.

The second numerical example is based on the experimental tests performed by Poyet [6] and it deals with a cement mortar specimens exposed to variable in time hygral conditions. The specimens were placed alternately in two chambers, one with the RH of 96% and the second one with the RH of 59%, for the time periods of 14 days (short cycle) and 28 days (long cycle). The comparison of the simulation results with the experimental ones [6] is presented in Fig. 2, showing their good agreement.

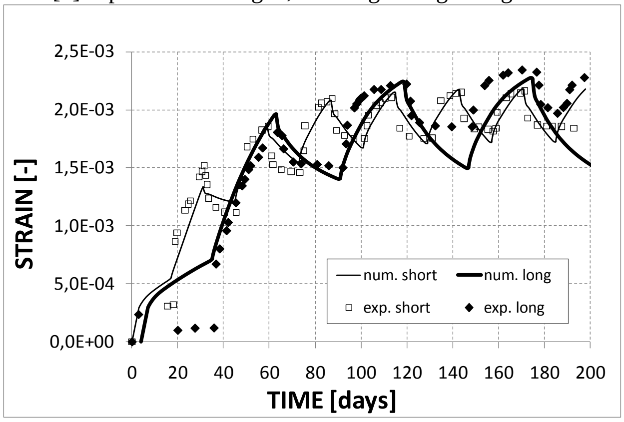

Figure 2. Comparison of the ASR strains obtained from simulations with the experimental data [6].

4. Conclusions

A mechanistic-type mathematical model for chemo-thermo-hygro-mechanical behaviour of cement-based materials exposed to the alkali-silica reaction, considering their multiphase nature, has been presented. The model is thermodynamically consistent and it has been developed within framework of mechanics of multi-phase porous media. The presented simulation results are in a good agreement with experimental data, both for the constant and variable in time hygral conditions. The model can be useful for prediction of the service life of concrete structures exposed to the ASR degradation.

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