# Macroscopic and mesoscopic approach to modelling the alkali-silica reaction in concrete

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## Abstract

Model of the alkali-silica reaction, predicted for both mesoscopic and macroscopic analyses, has been presented. It takes into account coupling between thermal, hygral, mechanical and chemical phenomena in concrete. In the macroscopic model, alkali silica reaction is modelled with the first-order kinetic law. In the mesoscopic approach, diffusion of alkalis from the cement paste to the aggregate and influence of alkali content on the reaction development is considered.

Keywords: alkali-silica reaction, cement-based materials, concrete damage

### 1. Introduction

Alkali-silica reaction (ASR) occurs between the hydroxyl ions, which are provided to the cement-based materials mainly during cement hydration, and reactive forms of silica, such as chert, quartzite, opal or strained quartz crystals. In high relative humidity, alkalis and hydroxyl ions diffuse from the cement paste to the reactive spots of aggregates. After dissolution of silica, the alkali-silica gel is formed. Product of the reaction imbibes water and increases its volume, what may results in failure of concrete.

Numerous numerical models of the alkali-silica reaction have been formulated in the past. First ones were designed for phenomenological analyses at the macroscopic scale, in which entire structures were considered [5]. Afterwards, several chemo-mechanical models were presented [9, 4, 10]. Recently, researchers began to investigate mechanisms of the reaction development also at the mesoscopic scale, in which single aggregates are considered [1]. Such an approach may allow to take into account influence of diffusion of alkalis between the cement paste and aggregate on the reaction extent. In the presented research, both approaches have been presented.

# 2. Mathematical model

Mathematical formulation presented in this article is based on the mathematical model of the hygro-thermo-chemo-mechanical phenomena in partially saturated porous media [2]. Macroscopic model of the ASR has been previously presented [3, 6]. It takes into account action of hygro-thermal, chemical and mechanical loads to describe chemical degradation of the cement-based materials. Four governing equations are considered in the model: mass balance equation of dry air, liquid water and water vapour, enthalpy balance equation and linear momentum balance equation. The ASR reaction extent rate is modelled with the first-order kinetic law:

$$\dot{\Gamma}_{ASR} = \frac{1 - \Gamma_{ASR}}{t_r},\tag{1}$$

where  $\Gamma_{ASR}$  is the ASR reaction extent and  $t_r$  it the characteristic time of the ASR reaction, given by equation proposed by Ulm *et al.* as [9]:

$$t_{r} = \tau_{r}(T, S_{w}) \cdot \frac{1 + \exp[-\tau_{L}(T, S_{w}) / \tau_{r}(T, S_{w})]}{\Gamma_{ASR} + \exp[-\tau_{L}(T, S_{w}) / \tau_{r}(T, S_{w})]},$$

$$(2)$$

where  $\tau_L(T, S_w)$  and  $\tau_r(T, S_w)$  are the latency and the reaction times, given by equations proposed by Ulm et al. [9] and Steffens et al. [8]. In Figure 1 comparison of the numerical results, obtained using the mathematical model, with experimental data of the ASR expansion obtained by Poyet et al. [7] for samples stored in variable relative humidity is presented. One can notice that the numerical results are in good accordance with the experimental results. However, influence of neither the aggregate size nor the diffusion of alkalis is taken into account. Therefore, such approach does not provide information how would this aggregate behave in other conditions and for a different grading curve.



Figure 1: ASR expansion obtained by means of mathematical model compared against experimental data by Poyet *et al.* [7].

In the recently formulated mesoscopic model additional balance equation was introduced as:

$$\frac{D}{Dt} \rho_{alk} + \rho_{alk} \operatorname{div} \mathbf{v}^{alk} = -\dot{m}_{alk,gel}, \qquad (3)$$

where  $\rho_{alk}$  is the phase averaged alkali density, t is the time,

 $\mathbf{V}^{alk}$  is velocity of the alkalis and  $\dot{m}_{alk,gel}$  is alkali source related to binding of alkalis by the ASR gel. Alkalis, present in the cement paste after the hydration, diffuse towards the aggregate grains. After reaching the alkali concentration threshold,  $c_{lim}$ , the ASR extent rate is modelled with equation:

$$\dot{\Gamma}_{ASR} = \begin{cases} 0, & c < c_{\lim}, \\ \frac{1 - \Gamma_{ASR}}{t_r}, & c \ge c_{\lim}. \end{cases}$$
(4)

Using eq. (4) we account for the initial alkali content, reactivity and the aggregate size. We validate the model using the experiment which considers the ASR progress in aggregates stored in various conditions: 1M NaOH water solution or liquid water. For the samples stored in water, no ASR expansion was observed. Comparison of experimental data with the numerical code is presented in Figure 2.

### References

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Figure 2: ASR expansion obtained by means of mathematical model compared against experimental data for the samples stored in water (A) and in 1M NaOH water solution (B).

## 3. Conclusions

Macroscopic and mesoscopic models of the ASR have been presented. For both models good accordance with experimental data has been obtained. However, using the macroscopic approach, it would not be possible to model the ASR progress in the samples stored in different conditions using the same set of parameters. The mesoscopic model allows to consider effect of material structure: aggregate grading, porosity, diffusivity, etc. It is also possible to take into account the alkali sources.

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