MODELING ALKALI-SILICA-REACTION IN REINFORCED CONCRETE STRUCTURES COMBINING KINETICS AND FRACTURE MECHANICS

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Abstract. Alkali-silica reaction (ASR) is a reaction in concrete between alkali hydroxides and reactive siliceous aggregates. The paper presents a chemo-mechanical weakly coupled model for ASR. The chemical model predicts kinetics and volume expansion of macroscopically-unrestrained specimens. The volumetric strain depends on aggregate composition, characteristic and latency time, moisture ambient conditions and temperature. The mechanical material model is formulated on a macro scale, taking unrestrained volumetric strain as the main input. The volumetric strain governs deterioration of material characteristics (tensile strength, compressive strength, fracture energy) and contributes as an eigenstrain to material behaviour. The growths of ASR gel follows stress state where high compression inhibits further expansion and prevents further deterioration. A fracture-plastic material model for concrete delivers strain decomposition, stress, damage and plastic behaviour.

Validation focuses on macroscopically stress-free specimens where correct expansion is obtained. An example of reinforced concrete beam shows excellent performance for internally restrained concrete. The model has been implemented in ATENA software and extends its capability to examine lifetime of the structure.

1 INTRODUCTION

The present project aims to develop a module that can be used for improved predictions of durability and safety of civil engineering and transport structures. The module should cover all phases of their life cycle, starting from their design and construction, followed by their long-time service up to their removal. It builds up on previous research and software development that allows for assessment of carbonation and chloride penetration into concrete structure [1] and corrosion of its reinforcement[2]. This paper describes its extension that supports also analysis of alkali-aggregate reaction in concrete and related deterioration of the structure. The new module is implemented and tested in Atena software [3].

2   GENERAL FORMULATION

In the majority of concretes, aggregates are more or less chemically inert. However, some aggregates react with the alkali hydroxides in concrete, causing expansion and cracking over a period of many years. This alkali-aggregate reaction has two basic forms: alkali-silica reaction (ASR) and alkali-carbonate reaction (ACR).

Alkali–silica reaction (ASR), one of those common deleterious mechanisms, consists in a chemical reaction between "unstable" silica mineral forms within the aggregate materials and the alkali hydroxides (Na, K–OH) dissolved in the concrete pore solution. It generates a secondary alkali–silica gel that induces expansive pressures within the reacting aggregate material(s) and the adjacent cement paste upon moisture uptake from its surrounding environment, thus causing micro cracking, loss of material's integrity (mechanical/durability) and, in some cases, functionality in the affected structure.

Several aggregate types in common use, particularly those with a siliceous composition, may be attacked by the alkaline pore fluid in concrete. This attack, essentially a dissolution reaction, requires a certain level of moisture and alkalis (leading to high pH) within the concrete to take place. During the reaction, a hygroscopic gel is produced. When imbibing water is present, the gel will swell and thus cause expansion, cracking, and in the worst case spalling of the concrete [4].

Thus, the degree of reaction of an aggregate is a function of the alkalinity of the pore solution. For a given aggregate, a critical lower pH-value exists below which the aggregate will not react. Consequently, ASR will be prevented by lowering pH of the pore solution beneath this critical level where the dissolution of alkali-reactive constituents (silica) in the aggregates will be strongly reduced or even prevented, as discussed in[5]. No "absolute" limit is defined, because the critical alkali content largely depends on the aggregate reactivity [3], but from many experimental test we can estimate threshold value [4],[6].

Many studies carried out over the past few decades have shown that ASR can affect the mechanical properties of concrete as a "material". Usually, ASR generates a significant reduction in tensile strength and modulus of elasticity of concrete. These two properties are much more affected than compressive strength, which begins to decrease significantly only at high levels of expansion.

Several ASR models were developed over the years to predict expansion and damage on both ASR affected materials (microscopic models) [7], [8], [9] and ASR affected structures/structural elements (macroscopic models) [10], [11],[12]. The first group has a goal of modelling both the chemical reactions and the mechanical distresses caused by ASR or even the coupling of the two phenomena. The second group aims at understanding the overall distress of structures/structural concrete elements in a real context, simulating their likely in situ behaviour [13] seem to have finally bridged the gap between scientific rigor and practical applicability to real structures.

In terms of mechanical effects, it is known that ASR expansions occur over long time periods. During this process, ASR affected concretes are subjected to a progressive stress built up that is very likely to cause creep on the distressed materials.

ASR depends on the availability of three factors: alkalis liberated from cement during hydration, siliceous minerals present in certain kinds of aggregates and water. Several

microscopic and random factors are involved in ASR expansion, such as concrete porosity, amount and location of reactive regions in the material and permeability[13]. These parameters, added to concrete's intrinsic heterogeneity, turn simulating ASR expansion into a rather complex task.

Even though ASR process has not been well explained so far, the commonly accepted theory for describing it is that two distinct phases need to be considered: gel formation and water absorption by the gel, causing expansion. According to this mechanism, reaction does not always lead to expansion. As long as there is enough void space to be filled by the gel, i.e. pores and cracks, concrete volume remains unchanged.

Due to the lack of a model which is able to incorporate effects of relative humidity, alkali/silica content in the mixture, ambient temperature, authors suggest to combine ASR kinetics proposed by [10] with influence of moisture, published by [14] and influence of alkali/silica content proposed by [15].

Implementation of modelling expansion due to ASR consists of modelling engeinstrains in time-steps t on entire structure. Function for volumetric eigenstrain reads

$$\varepsilon_{ASR}(t) = \varepsilon_{cal}^{\infty}\xi(t)F_M \tag{1}$$

where $\varepsilon_{cal}^{\infty}$ is volumetric strain of ASR swelling at infinity time, $\xi(t) \in \langle 0,1 \rangle$ is the chemical extent of ASR and F_M is the coefficient reflecting moisture influence. It is described later in the text. In the case of varying the relative humidity, Equation (1) changes to incremental form, for time t_i

$$\varepsilon_{ASR}(t_i) = \varepsilon_{ASR}(t_{i-1}) + \varepsilon_{cal}^{\infty}\left(\xi(t_i) - \xi(t_{i-1})\right)F_M\left(\frac{t_i + t_{i-1}}{2}\right) \tag{2}$$

2.1 Influence of moisture FM

Approximately 75% relative humidity (RH) within concrete is necessary to initiate non-negligible expansion and it is assumed to vary F_M linearly between 75% RH and 100% RH as shown in Figure 1.
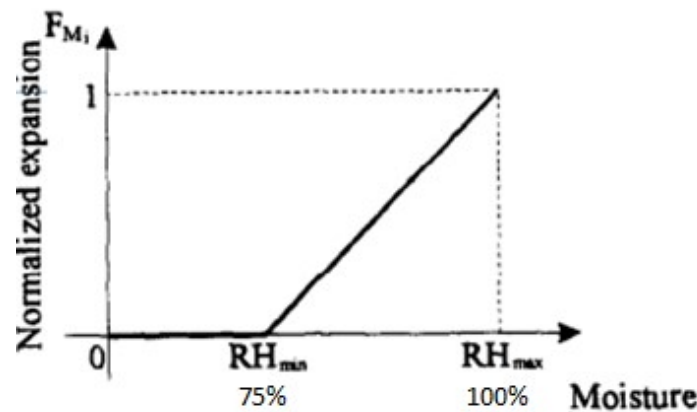

Figure 1: Parameter Factor of RH influencing ASR concrete expansion, reproduced from [16].

The coefficient F_M reflects influence of moisture h. The function for FM is approximated as

$$F_M(h) = \frac{1}{1-h_{min}}(h - h_{min}) \qquad (3)$$

where h_{min} is relative humidity threshold where ASR begins to appear, 0.75 by default. Other variables will be explained in the following text.

2.2   Model for ASR kinetics

For the complete 3D constitutive model we consider first-order reaction

$$1 - \xi = t_c(\theta, \xi)\dot{\xi} \qquad (4)$$

where $t_c(\theta, \xi)$ is the characteristic time. It has been found that t_c depends on temperature $\theta[K]$ and the ASR extent ξ. Referring to the implementation of the chemo elastic material law a suitable integration scheme is given in [10].

Consider an isothermal stress-free ASR expansion test carried out at constant temperature $\theta = \theta_0$. In this test, the volumetric strain ε_{ASR} is recorded as a function of time and ASR extent is calculated as

$$\xi(t) = \frac{\varepsilon_{ASR}(t)}{\varepsilon_{ASR}(\infty)} \qquad (5)$$

For macroscopically stress-free sample, it yields

$$\varepsilon_{ASR}(\infty)(1-\xi) = \varepsilon_{ASR}(\infty)t_c(\theta, \xi)\frac{\dot{\varepsilon}_{ASR}(t)}{\varepsilon_{ASR}(\infty)}$$

$$\varepsilon_{ASR}(\infty) - \xi\varepsilon_{ASR}(\infty) = t_c(\theta, \xi)\dot{\varepsilon}_{ASR}(t) \qquad (6)$$

$$\varepsilon_{ASR}(\infty) - \varepsilon_{ASR}(t) = t_c(\theta, \xi)\dot{\varepsilon}_{ASR}(t)$$

with $\varepsilon_{ASR}(t)$ and $\dot{\varepsilon}_{ASR}(t)$ being measurable functions of time. The characteristic time t_c can be determined from a stress-free expansion test. In a recent extensive series of stress-free expansion tests carried out at different constant temperatures[17], t_c has been found to depend on both temperature $\theta[K]$ and reaction extent $\xi[-]$ in the form

$$t_c = \tau_c(\theta)\lambda(\xi, \theta) \qquad (7)$$

$$\lambda(\xi, \theta) = \frac{1 + \exp[-\tau_L(\theta)/\tau_C(\theta)]}{\xi + \exp[-\tau_L(\theta)/\tau_C(\theta)]} \qquad (8)$$

In this experimentally determined kinetics function, $\tau_c(\theta)$ is a characteristic time [day] and $\tau_L(\theta)$ is a latency time [day]. The use of (7) and (8) , in (6) yields after integration

$$\xi(t) = \frac{1 - \exp(-t/\tau_C)}{1 + \exp(-t/\tau_C + \tau_L/\tau_C)} \qquad (9)$$

For variable temperature and cracking it is difficult to solve for $\xi(t)$ analytically and a numerical integration is needed. Suitable solution scheme is derived in [10] which is implemented in our model. Furthermore, proceeding as in physical chemistry [18], we explore the temperature dependence of the time constants τ_c and τ_L from stress-free expansion tests carried out at different constant temperatures. It is remarkable that the experimental values align (almost) perfectly along a straight line, matching the Arrhenius concept.

$$\tau_C(\theta) = \tau_C(\theta_0) \exp\left[U_c \left(\frac{1}{\theta} - \frac{1}{\theta_0} \right) \right] \tag{10}$$

$$\tau_L(\theta) = \tau_L(\theta_0) \exp\left[U_L \left(\frac{1}{\theta} - \frac{1}{\theta_0} \right) \right] \tag{11}$$

where $U_C = 5400 \pm 500\,K$; $U_L = 9400 \pm 500\,K$.

2.3 Prediction of free ASR swelling ε_{cal}^∞

ε_{cal}^∞ [-] is the predicted volumetric expansion at infinity time obtained by model proposed previously [15] under no external restraint. It is calculated based on reactive aggregates, amount of reactive silica in the aggregates and value of measured stress-free expansion test done in Poyet's study [6] and [4] on samples containing reactive particles only. ε_{cal}^∞ is defined as follows

$$\varepsilon_{cal}^\infty(t) = s \cdot p \cdot AC \cdot \varepsilon_F \frac{A_C}{A_R} \tag{12}$$

where ε_F [-] is measured ASR strain expansion on samples containing reactive particles only with enough sufficiency of alkali. See [6] for more details. A_C [kg/m^3 Na$_2$O$_{eq}$] and A_R [kg/m^3 Na$_2$O$_{eq}$] are amounts of consumed and required alkali respectively. AC is total aggregate content in [kg/m^3]. One of the main assumptions of the model is that the maximum expansion of mortar is achieved, if there is enough alkali to react with all the reactive silica of the mixture. This amount of required alkali content A_R [kg/m^3 Na$_2$O$_{eq}$] is defined as

$$A_R = r \cdot s \cdot p \cdot AC \tag{13}$$

where s is the proportion of quantity of soluble silica [-], p is the proportion of reactive aggregate [-], r states for the amount of required alkali per kg of reactive silica and it is a constant value r = 15.4 %. Value A_C is defined as min(A_R, A_A). A_A is the available amount of alkali for ASR reaction. A_A is defined as difference between initial amount of available alkali A_T [kg/m^3 Na$_2$O$_{eq}$] and alkali content threshold A_0 [kg/m^3 Na$_2$O$_{eq}$] when ASR reaction starts

$$A_A = A_T - A_0 \tag{14}$$

It should be noted that this model does not consider any alkali flow through boundaries inside the structure during the service life. By default, A_0 is equal to 3.7 kg/m³ Na₂O$_{eq[6]}$, but other values in range of $3 - 5$ kg/m³ Na₂O$_{eq}$ can be found in the literature [4]

Table 1: Mixtures and ASR expansions of mortars studied by [6] and[15]. F1-F3 are size fractions 80 μm-3.15 mm.

Non-reactive sand (%)			Reactive sand (%)			Measured ASR expansion
F1	F2	F3	F1	F2	F3	(%)
0	50	25	25	0	0	0.003
25	25	25	0	25	0	0.06
25	50	0	0	0	25	0.06
0	25	25	25	25	0	0.045
25	25	0	0	25	25	0.08

Value of p depends on the mix ratio of reactive aggregate, typically $p = 11,1\%$ [15] or 9,4% and 12,4%[7]. Value s depends on amount of reactive silica in aggregates.

2.4 Extension to ASR for 3D conditions

Expansion of externally unrestrained concrete specimens due to ASR has been summarized in[19]. The expansion model takes into account reaction kinetics, alkali content, reactive amount of aggregates, relative humidity and temperature. The model has been validated on 4 examples found in literature. Degradation of material due to ASR reaction is suggested in[20] Eqs.18,19 as follows:

$$E(t,\theta) = E_0 \left[1 - (1 - \beta_E) \xi(t,\theta) \right]$$
$$f_t(t,\theta) = f_{t,0} \left[1 - (1 - \beta_f) \xi(t,\theta) \right] \tag{15}$$
$$G_f(t,\theta) = G_{f,0} \left[1 - (1 - \beta_G) \xi(t,\theta) \right]$$

where $\beta_{E,f,G}$ are residual values of E/E₀, f/f₀, G$_f$/G$_{f0}$. Default values are $\beta_E = 0.1$, $\beta_f = 0.6$ [21] and $\beta_G = 0.6$. The general equation for the incremental volumetric AAR strain is given by [20]-Eq. 5

$$\dot{\varepsilon}_V(t) = \dot{\varepsilon}_I(t) + \dot{\varepsilon}_{II}(t) + \dot{\varepsilon}_{III}(t) =$$
$$\underbrace{\Gamma_t \Gamma_c(\overline{\sigma}, f_c') F_M(h) \dot{\xi}(t) \varepsilon_{cal}^{\infty}}_{\text{Only considered in implementation}} + \Gamma_t \dot{\Gamma}_c(\overline{\sigma}, f_c') F_M(h) \xi(t) \varepsilon_{cal}^{\infty} + \dots \dot{\Gamma}_t, \dot{\overline{\sigma}}, \dot{f}_c', \dot{F}_M, \dots \tag{16}$$

where Γ_c reflects effect of compressive stresses by [20]-Eq. 10, Γ_t accounts for the influence of tensile cracking, (assumed here as 1), F_M is the effect of relative humidity, see (3). Note that our model considers only the most relevant first term (16), which yields

$$\Delta\varepsilon_V\left(t_i\right) = \Gamma_t \cdot \Gamma_c\left(\overline{\sigma}_{i-1}, f'_{c_{i-1}}\right) \cdot F_M\left(h_{\overline{i}}\right) \cdot \varepsilon^{\infty}_{cal} \cdot \left(\xi\left(t_i\right) - \xi\left(t_{i-1}\right)\right)$$

$$\overline{i} = \left(i + (i-1)\right)/2 \tag{17}$$

Reduction Γ_c due to compressive stress is considered as follows

$$\Gamma_c = \begin{cases} 1 & if\ \overline{\sigma} \geq 0 & Tension \\ 1 + \dfrac{e^{\beta}\overline{\sigma}}{1 + \left(1 - e^{\beta}\right)\overline{\sigma}} & if\ \overline{\sigma} < 0 & Compresion \end{cases} \tag{18}$$

$$\overline{\sigma} = \frac{\sigma_I + \sigma_{II} + \sigma_{III}}{3\left|f'_c\right|}$$

where the shape factor β is -2 by default by [20]-Tab.2 and f'_c is compressive strength.

Under constrained conditions, ASR expansion depends on the stress state. It is known that compressive stress beyond approximately -10 MPa stops ASR expansions. It needs to be reflected within strain redistribution into principal direction[22]: Similarly to [20]-Fig. 5, weight factors are assigned to three directions. Let us assume that directions of principal stresses σ_I, σ_{II}, σ_{III} are known. Expansion is then assigned to each principal stress direction according to a weight factors W_1', W_2', W_3'. Starting from compressive stress -0.3 MPa the weight factor decreases until maximum stress -10 MPa is reached.

For compressive stress σ_i under -0.3 MPa, the following decay function is used, according to [14] where $\sigma_L \approx$ -0.3 MPa and $\sigma_u \approx$ -10 MPa.

$$W_i'\left(\sigma_i\right) = \begin{cases} \left[1 - \dfrac{1}{\log\left(\dfrac{\sigma_u}{\sigma_L}\right)}\log\left(\sigma_i / \sigma_L\right)\right] & for\ \sigma_i < -0.3 MPa \\ 1 & for\ \sigma_i \geq -0.3 MPa \end{cases} \tag{19}$$

Weight factors need to be normalized as

$$W_i = \frac{W_i'}{\sum_{i=1}^{3} W_i'} \tag{20}$$

Three principal strains from ASR are assigned as

$$\Delta\varepsilon_{ASR,i} = W_i \cdot \Delta\varepsilon_V\left(t_i\right) \tag{21}$$

This new approach simplifies the procedure outlined by [20]-Fig. 5 where several stress state cases were treated individually.

3   VALIDATION OF THE MODEL

This section brings a few analyses to validate the presented model.

3.1 Validation on free expansion

The Figure 2 validates experimental data for free expansion. The material parameters in the test are summarized in Table 2

Table 2: Summarized parameters for validation

| Variable	Symbol	Value	Source
REQUIRED ALKALI PER REAC. SILICA	r	15.4 %	[15]
PROPORTION REACTIVE SILICA	s	21.8 %	[15]
PROP. REACTIVE PARTICLES IN SAND	p	30 %	[15]
SAND MASS	AC	833 kg/m^3	[23]
ASR MEASSURED ASR STRAIN	ε_F	0.0525 %/kg	[6]
AMOUNT OF REQUIRED ALKALI	A_R	8.39 kg/m^3	[6]
TOTAL ALKALI IN MORTAR for Ca-5.4 (for Ca-9.0)	A_T	5.4 (9) kg/m^3	[23]
THRESHOLD ALKALI IN CONCRETE	A_0	3.7 kg/m^3	[6]
CHARACTERISTIC TIME	τ_C	20 day	
LATENCY TIME for Ca-5.4 (for Ca-9.0)	τ_L	55 (45) day	
ELASTIC MODULUS	E	27 GPa	[23]
COMPRESSIVE STRENGTH	Fc	26 MPa	[23]
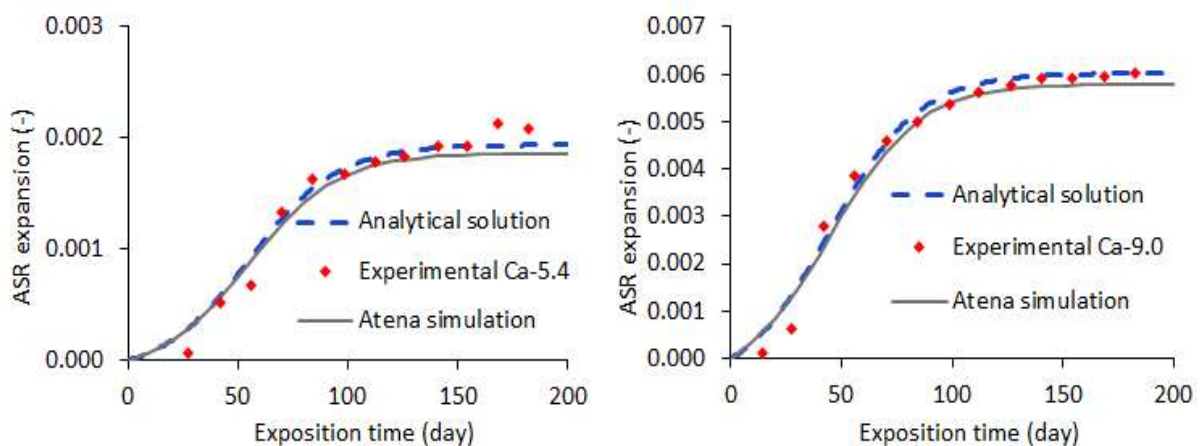
Figure 2: Validation of free expansion, [23]

3.2   Validation on free expansion, material degradation

This test compares computed material degradation against experiment. The parameters from Table 3 has been used in the analysis.

Table 3: Summarized parameters for validation.

Variable	Symbol	Value	Remarks [21]
ELASTIC MODULUS	E_0	21130 N/mm^2	at 28 day
TENSILE STRENGTH	ft_0	1.44 N/mm^2	at 28 day
COMPRESSIVE STRENGTH	Fc_0	41.0 N/mm^2	at 28 day
FRACTURE ENERGY	G_{f0}	0.142 N/mm	$G_{f0}=0.073f_{cm}^{0.18}$
Residual value of E/E$_0$	β_E	0.1	
Residual values of f/f$_0$, G$_F$/G$_{f0}$	$\beta_{f,G}$	0.6	

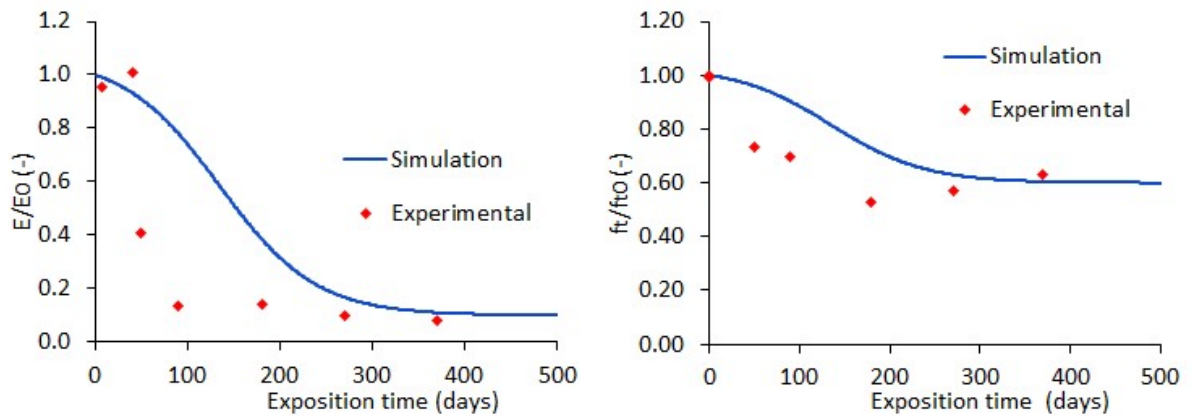The results are depicted in Figure 3.

Figure 3: Validation of stiffness and tensile strength degradation in ASR-affected concrete in free expansion, [21]

3.3   Validation on expansive pressure

This example demonstrates ASR in combination with compressive stress. It is based on experimental data from[23]. Expansive pressure of concrete prism is measured by apparatus,

where steel rods provide a certain stiffness during experiment. The results are presented in Figure 4. A_s/A_c ratio equal to 30.4, where A_s is transversal sectional area of two steel rods and A_c is transversal sectional area of concrete prism. (Assumed stiffness of apparatus is 1702.99 MN/m).
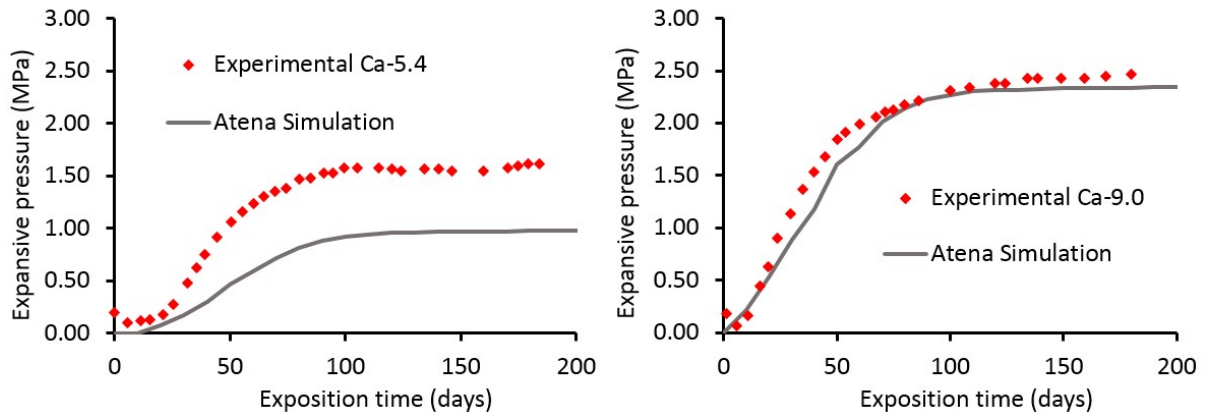

Figure 4: Evolution of compressive stress due to ASR reaction, [23]

12 CONCLUSIONS

The project develops a module for improved predictions of durability and safety analysis of structures due to ASR. It yields results with reasonable accuracy and is usable for typical analyses from engineering practice. It has been implemented into ATENA FEM software. The new module helps in development and maintenance of bridges, tunnels and other transport constructions affected by ASR.

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