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Modelling of Expansion Induced by ASR — New Approaches

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Abstract

The mechanism of ASR expansion has been approached by thermodynamics and kinetics of the chemical reaction considering the diffusion law and by probabilistics of random gradients of alkalis and silica reactive sites and local formation of gel. Induced mechanical effects are elucidated through: (1) the capillary pressure relating the volume of expansive gels dissipated in connected porous zones to the initiation of cracks the linear fracture mechanics applied to the propagation and orientation of initiated cracks; and (2) a law of proportionality between confinement, temperature, relative humidity and reactivity describing the non-uniform anisotropic three-dimensional (3-D) distribution of the AAR expansion. Numerical results are very close to experimental data for the pessimun content of reactive silica, the evolution of linear expansions vs the consumed alkalis and the benefit of an isotropic confinement on expansion. © 1997 Elsevier Science Ltd. All rights reserved.

Keywords: ASR, computations, mechanics, probabilistics, thermodynamics modelling.

INTRODUCTION

Mechanisms and kinetics of the alkali–silica reaction were characterized by three steps:[1,2] (1) diffusion of Na^+, K^+, OH^- ions through the pore solution towards the aggregate; (2) dissolution of reactive silica due to the attack of OH^- ions; (3) precipitation of an expansive alkaline silicate gel.

The resulting expansion has been attributed either to an osmotic pressure by Dent-Glasser and Kataoka or to a physical sorption of water molecules by the gel by Diamond *et al.*[2] In fact, the measurement of the free linear expansion of concrete samples does not specifically separate the effects of the heterogeneity of the material and more particularly the random distribution of reactive sites.

New models using pluridisciplinary approaches such as thermodynamics, probabilistics and fracture mechanics have recently been published. They significantly improve our knowledge of structural effects induced by the alkali–silica reaction. They will be reviewed in this paper.

MECHANISM OF EXPANSION

New models predicting the expansion due to alkali–silica reaction, consider concrete as a heterogeneous porous material and reactive aggregates as spherical inclusions surrounded by a reaction layer which exerts an isotropic pressure on the matrix. In the chemical reactions, driving forces are the dissolution of silica and diffusion of Na^+ or $K^+$and OH^- ions through the pore solution. Theories used in these models are those relating to absorption of water by the gel.

Analytical model of heterogeneous materials [3]

In this model, a spherical particle of silica is surrounded by a porous zone which is progressively filled up by reaction products. The thickness of the reaction layer depends primarily on the apparent diffusion of OH^- ions into the aggregate (Fig. 1), but also on the type

global model

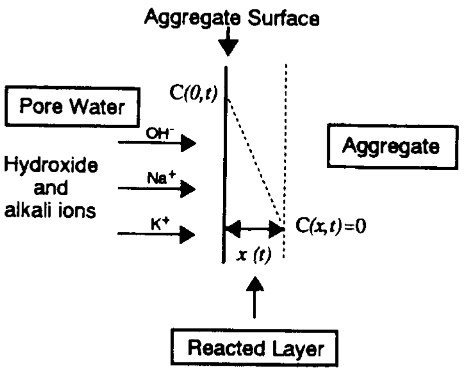


Fig. 1. Diffusion of alkali ions into reactive aggregates.[3]

of aggregate and temperature. The expansion is initiated when the volume of reaction products is larger than that of the porous zone as implied by eqn (1):

$$\varepsilon = f(Pt - Pabs) \qquad (1)$$

where Pt is the total amount of reaction product and Pa is the capacity of the porous zone. The model applied to the expansion of mortar bars confirms that the induction period is related to the porosity of the matrix (Fig. 2). The length of the induction period is a function of the apparent diffusion coefficient. However, the calculated expansion rapidly reaches a plateau at around 0.32% for the mixture studied which is characterized by this unique limiting value. This can be explained by the choice of a global model.

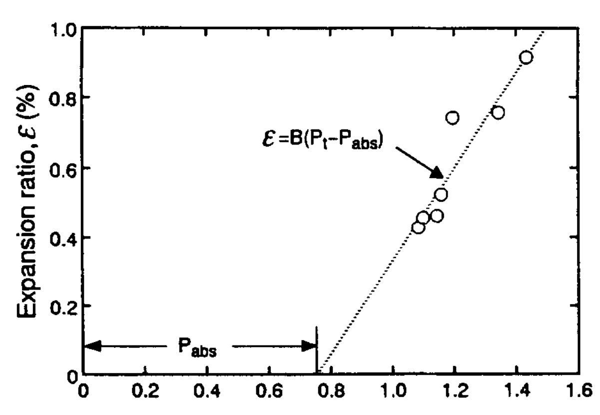


Fig. 2. Relationship between reaction products and expansion.[3]

Probabilistic model (4,5)

This probabilistic approach takes into account the localizaton, size and degree of reactivity of silica and also the probability of local and global presence of Na^+, K^+, OH^- ions. As in the previous model, an equivalent diffusion coefficient of alkaline ions is defined: at a given time, only a thin layer of silica can be attacked by Na^+, K^+, OH^- ions.

Local chemical reactions

The ionic diffusion follows Fick's law. Due to the random distribution of the reactive sites, the chemical reaction can occur in an elementary volume called ECRV, elementary chemical representative volume. The alkalis involved in the reaction are in an equivalent volume named EV. If the distribution of alkalis in ECRV is constant, the diffusion law can be integrated (Appendix 1). The local probabilities of gel formation and of remaining alkalis have been calculated. The chemical process is represented in Fig. 3. The global kinetics is driven first by the rate of alkalis diffusing into the reactive silica (OAB). Then the gel consumes alkalis (BC). At last, when the reactive silica is exhausted, alkalis are present again (from C).

Gel pressure

The gel absorbs water and is able to spread into the matrix through the porous system. The swelling occurs when the volume of gel exceeds the volume of the connected porosity. The gel is apparently able to absorb in volume 200–400% water of its weight in a saturated atmosphere.[6] In the model, the value has been taken equal to 300%.

The capillary pressure of this gel considered as a fluid follows Laplace's law:

$$P_c = \frac{2\sigma \cos \theta}{r_p} \qquad (2)$$

where P_c is capillary pressure; r_p is pore radius and $2\sigma\cos\theta$ is capillary characteristic of the gel (superficial tension). Let us suppose a random porous distribution, Fig. 4, similar to the Hg porosimeter curve. P_g, the gel pressure can be written as:

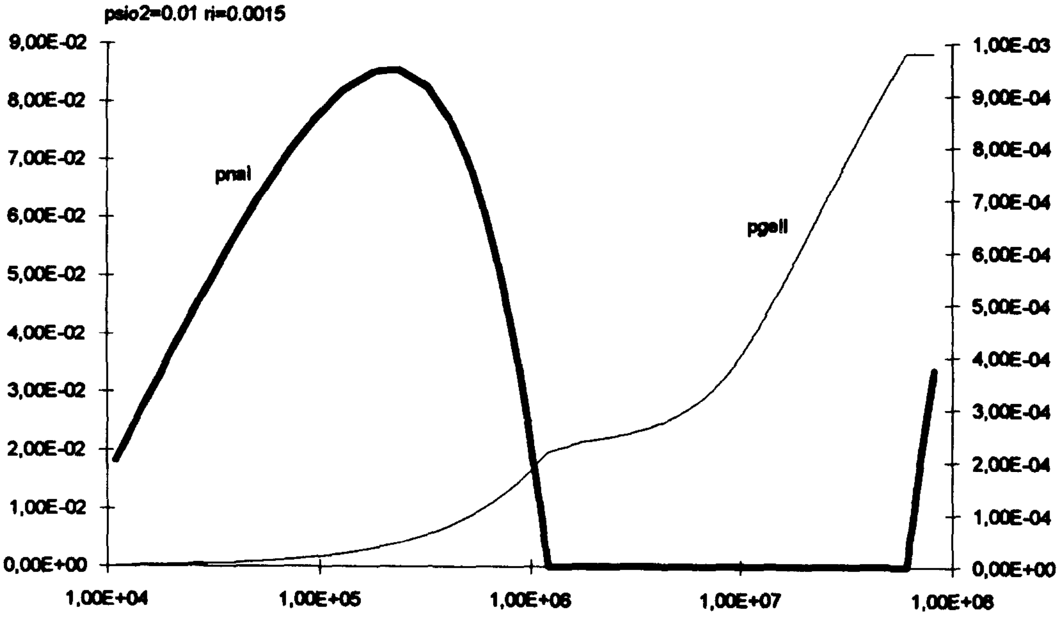


Fig. 3. Local probability of presence of gel Pgell and alkalies Pnal, around a reactive aggregate as a function of time.[5]

$$P_g = \frac{E_g}{3}\left[1 - \frac{V_{vo}}{V_{gel}}\,\phi\left(-\frac{ln(2\sigma cos(\theta)/P_c)}{\overline{\overline{lnr_p}}}\right.\right.$$

$$\left.\left.-\frac{\overline{lnr_p}}{\overline{\overline{lnr_p}}}\right)+ks.\gamma\right] \tag{3}$$

E_g is the Young's modulus of the gel; P_c is the capillary pressure; V_{vo} is the pore volume connected to the reactive site; V_{gel} is the gel volume at atmospheric pressure; and ϕ is the Gaussian distribution function.

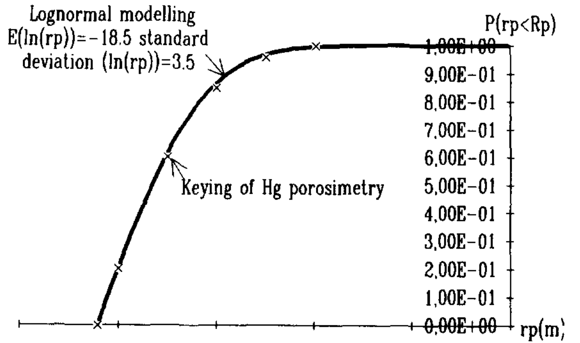


Fig. 4. Probability to find a pore Rp > rp, rp = pore radius.[7]

Cracking

Considering that swelling leads to cracking and that cracks progress in mode I, a rectilinear propagation as it is often observed on thin sections of concretes deteriorated by AAR (Fig. 5), the fracture mechanics is able to calculate the widening and, consequently, the volume of a crack (Appendix 1). The gel penetration in the crack is a function of the porous system of the matrix and of the opening of the crack under the gel pressure (Fig. 6). Connected pores are located from the reactive site at a distance lower than a critical distance l_c which represents the connectivity of pores.

Crack progression

There is no kinetic energy if the rate of energy restitution *G* is lower or equal to a critical value

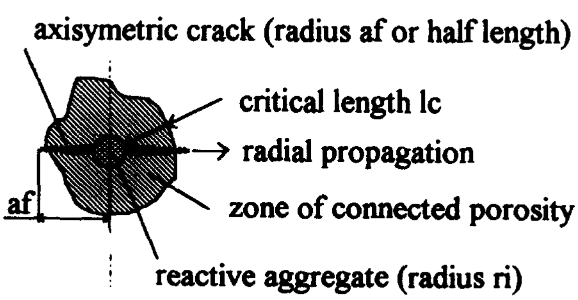


Fig. 5. Progression of a circular and plane crack in mode I from a reactive aggregate.[5]

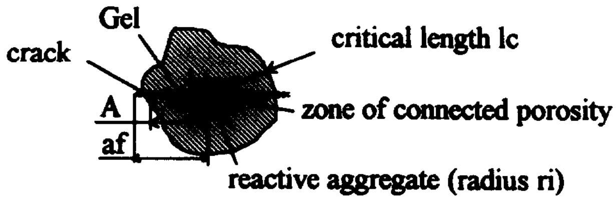


Fig. 6. Gel progression in the crack and in the connected porosity of the matrix.[7]

G_c. The swelling is due to the widening of cracks so ε can be related to V_f. A simulation of the gel pressure and propagation of cracks is given in Fig. 7. The gel pressure first increases with no cracking, then the crack appears. Its later propagation results in the decreasing of the gel pressure. The stress in the gel is relatively high (maximum 6.5×10^7 Pa). Sellier *et al.*[5,7] consider, later on, a random size of the crack, independent of the reactive site, instead of a crack size equal to the size of the reactive site.

The simulation of expansion by the model is in good agreement with experimental results. It confirms the induction period as already shown by Diamond *et al.*[2] and Chatterji & Christensen[8]. As an example, around 30% of alkalis produce a gel which is non-efficient regarding the swelling. Swelling and cracking are, in fact, due to the later consumption of alkalis between 25 and 45%. So only half of the gel formed is responsible for concrete deterioration in this case.

Pessimun

The pessimun content[9] of reactive silica obtained by simulation, confirms the experimental observations (Fig. 8). It is interpreted as the availability of alkalis. For low amounts of SiO_2, every reactive site is able to react with alkalis and to generate a pressure. If the amount of silica is high, some sites will be free of alkalis and will not produce the minimun amount of gel generating a high pressure responsible for cracking.

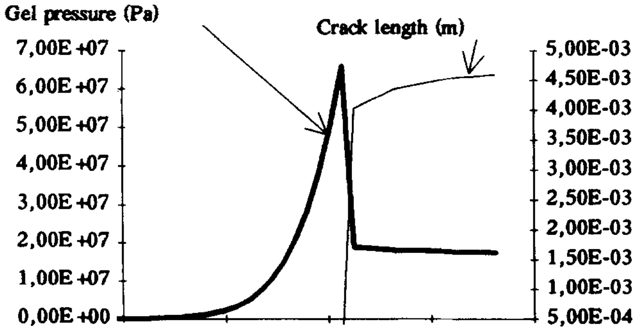


Fig. 7. Calculated evolution of the gel pressure and crack length in function of time.[5]

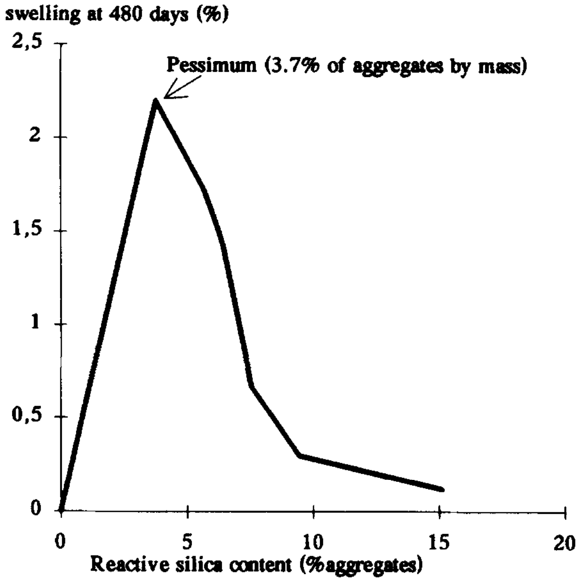


Fig. 8. Simulated pessimun content of silica.[7]

This probabilistic model which implies chemical, physical and mechanical characteristics of the alkali–silica reaction explains and simulates the behaviour of concrete at local and global levels. It is already promising and has been applied to the case of steam-cured concretes. Results are presented at this conference.[10] Some results can be discussed on the basis of the high value of the gel pressure, partly a consequence of the volume of water molecules absorbed by the gel. An improvement will also be brought out by the new data on the chemistry and composition of reaction products, including the presence of calcium ions in gels or precipitates as already shown by Way and Shayan,[11] Dron *et al.*[12] and Nieto *et al.*[13] and also the amount of water molecules in the gel.

Thermodynamical model of reactive porous materials[14]

The model describes the behaviour of concrete through the knowledge of chemical reactions at the level of a laboratory sample. Considering a closed reactive system, the chemical reaction between A and B is related to the mass variations of A and B.

$$\overset{\circ}{m}_{A\to B} = \overset{\circ}{m}_B = \overset{\circ}{m}_A = \overset{\circ}{\xi} \qquad (4)$$

m_A and m_B are the mass of phases A and B per unit of volume, ξ the reaction rate. $\mathring{m}_{A\to B}$ is the mass of phase A transformed into phase B, during the time interval d*t*.

The free energy, if the material is considered as elastic and isotropic in isothermal conditions, the state laws and kinetics of chemical reactions, following the Arrhenius' law (Appendix 2), have been coupled in the following equation for the free swelling ε.

$$\varepsilon = \varepsilon_\infty\left(1 - exp\left(-\frac{t}{\tau}\right)\right) \qquad (5)$$

ε_∞ and τ are constants expressed in relation to variables and intrinsic parameters K (tensor of elastic characteristics), α (coefficient of coupling between chemistry and mechanics), F_0 (initial chemical affinity of the reaction) L, η (constant of kinetics), E_a (activation energy). New developments are presented at this conference.[15] The variation of ε vs time is satisfactorily related to the curves of experimental linear expansion. A software called MINERALS, developed by Deloye,[16] evaluates the amount of silica that has reacted in the ASR and thus ξ. As the model describes the behaviour of a concrete presumably linear elastic, it is necessary to measure the mechanical characteristics of concrete samples. The storage of samples controls the stress, humidity and temperature.[17] New data are presented at this conference.[18]

Thermodynamics of damaged concretes [19,20]

The use of thermodynamics of irreversible processes, associated with the continuum damage theory[21] represents a non-linear calculation of cracking and is able to directly get zones deteriorated by ASR. The following variables are involved in the calculation of expansion due to ASR:

swelling due to AAR ε^{aar};
potential of reactivity A;
temperature T;
relative humidity H;
stress σ.

The free expansion due to AAR can be expressed by $\varepsilon^{aar} = \varepsilon^{aar}(A,T,H,\sigma)$.

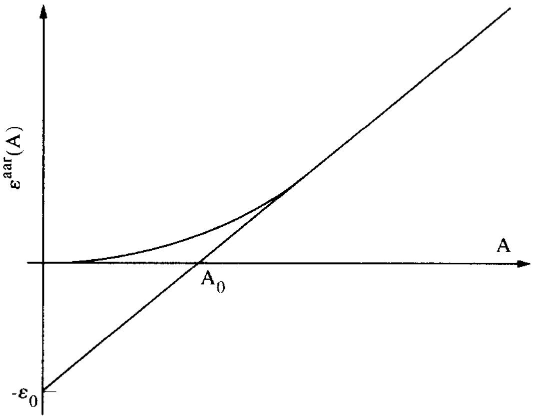


Fig. 9. Determination of ε_o and A_o.[23]

Expansion and chemical reaction

The free linear expansion is an average value of local expansions of the specimen. The amount of alkalis which has reacted, already emphasized by Diamond *et al.* is considered as a representative variable of the chemical reaction. There is expansion when the porosity around the reactive sites is filled by the gel. If the relation between ε^{aar} and A is assumed to be linear, as follows eqn (6), there is an induction period with no swelling (Fig. 9).

$$A < A_o : \varepsilon^{aar} = 0$$

and

$$A > A_o : \varepsilon^{aar} = \frac{\varepsilon_o}{A_o}(A - A_o) \qquad (6)$$

The kinetics of reaction is of a first-order and the law is described by:

$$\frac{dA}{dt} = k_0 e^{-\frac{E_a}{RT}} .(1 - A) \qquad (7)$$

The free expansion as a function of the chemical reactivity potential is for $A > A_o$:

$$\varepsilon^{aar}(t,T) = \frac{\varepsilon_o}{A_o}\left(1 - A_o - e^{-k_0 exp\left(\left(\frac{E_a}{RT}\right).t\right)}\right) \qquad (8)$$

This last formula simulates experimental results with good agreement. The same good agreement has been obtained regarding the influence of the relative humidity represented by a power function. Experimental results used in this comparison were published by Poole:[24]

$$\frac{\varepsilon^{aar}}{\varepsilon_0} = H^m, \text{ with } \varepsilon_o\text{: free expansion at } 100\% \text{ RH} \qquad (9)$$

where H is the relative humidity and m is a parameter of wedging.

Damage and cracking

In the theory of concrete damage[24] the level of observation is a material volume called REV, representative elementary volume, considered as homogeneous and small enough for a point. As the behaviour is local, the thermodynamics of irreversible processes can be applied to mechanics. Microcracks generated by mechanical strains modify the elastic characteristics and more particularly the Young modulus as follows:

$$E = E_o(1 - D) \qquad (10)$$

D represents the scalar damage variable varying between 0 and 1, E_o is the Young modulus of elasticity of the virgin material.

$$D = \alpha_c D_c + D_t \alpha_t \qquad (11)$$

where c is the compression, t is the tension and $\alpha_c + \alpha_t$. A probabilistic approach which assigned at each finite element its own evolution by a random sampling[20] was able to simulate the map cracking (Fig. 10) observed on concrete structures deteriorated by AAR and differential displacements noticed on testing bars, but the number of simulations is too high for a routine procedure.

Stress and expansion

Shayan and Quick,[25] showed that prestressed concrete railway sleepers deteriorated by AAR were cracked parallel to the prestress. So it appears that an applied stress can reduce, by a structural effect, the expansion in this direction, but is inefficient in the perpendicular direction. Moreover, it enhances cracking in the perpendicular direction by producing extra tensile stresses. This case was treated by the fracture mechanics.[22] Cracks were considered to open in mode I (linear expansion) and the volume of gel, V_g, was proportional to the free expansion when structural expansions have started.

$$g(t) = \alpha_1 \varepsilon_o^{aar}(t) \qquad (12)$$

α_1 is the coefficient of proportionality.

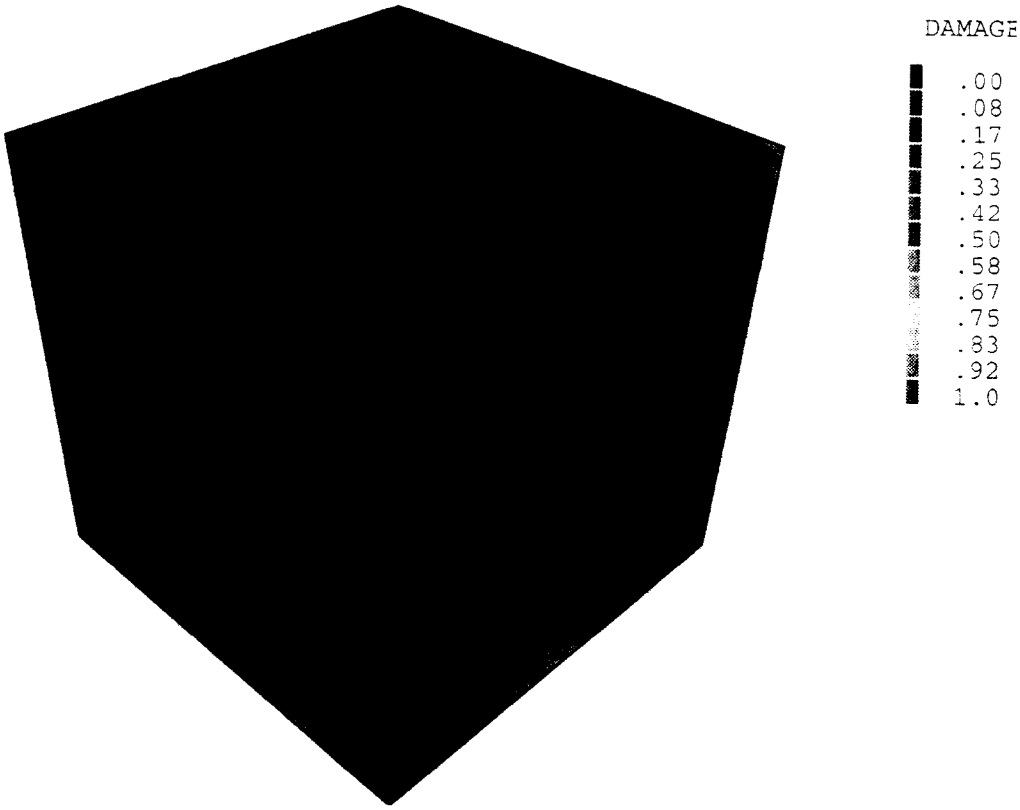


Fig. 10. Three-dimensional simulation of AAR damage. Lighter zones are more damaged than the dark ones.[20]

$$\sigma_{eq}(t) = \beta.\varepsilon_o^{aar}(t) \qquad (13)$$

$\sigma_{eq}(t)$ is the local pressures developed by the gel swelling and β is the coefficient of proportionality. The local pressure developed by the gel is proportional to the global variable easily measured: the free expansion. The crack opening is controlled by fracture mechanics and the crack propagation occurs when $K_I > K_{IC}$ with K_I the stress intensity factor and K_{IC} the critical stress intensity factor. In a linear elastic material and a bi-dimensional representation, K_I is a function of the two principal stresses and the pressure inside the crack. Details of calculation are presented at this conference[23] and show that a uniaxial compression σ_1 (5 MPa) reduces the strain largely in the direction of the load ε_1, but less in the perpendicular direction ε_2(Fig. 11).

Simulations of AAR

In order to simulate the behaviour of a site structure like a dam the following equation uses the different parameters previously studied.

$$\varepsilon^{aar}(H,T,\sigma,t) = H^m.\,\frac{\varepsilon_o}{A_o}$$

$$\left(1 - A_o - e^{-k_0 exp\left(\left(\frac{E_a}{RT}\right).t\right)}\right) f(\sigma) \qquad (14)$$

$f(\sigma)$ is the relation between strain and stress, ε^{aar} and σ are the strain and stress tensors. The inelastic and anisotropic properties and the damaging behaviour will simulate the comportment of concrete structures. First results appear as confident and bring real progress in the knowledge of structural effects induced by AAR. They will be compared to experimental tests in progress and to site structures.

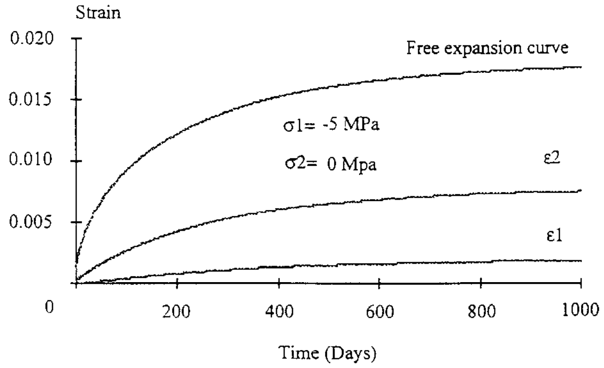


Fig. 11. Evolution of the free expansion in a uniaxial compression case ($\sigma < 0$) vs time.[22]

Numerical models

Numerical modelling of affected concrete [26, 27]

A numerical analysis is performed through a non-linear finite element calculation by an incremental approach. The development of the AAR expansion is simulated by a large number of small increments of free expansion. The free expansion corresponds to the expanded concrete free from any restraint. In the concrete structure, a local restraint expansion is a function of the free expansion and stress development. An incremental approach is used due to the interaction between expansion and induced stresses. The mechanical behaviour of concrete is represented by a constitutive model based on the theory of plasticity. The uniaxial stress–strain is derived from that of AAR affected concrete cylinders. This analytical approach is able to assist site investigations. New developments are presented at this conference.[28, 29]

Numerical model for dams [30]

This numerical model, is close to the 'numerical concrete' developed by Roelfstra *et al.*[31] and representing the heterogeneity of the material by discretization, has been applied to two gravity dams by Lopez *et al.*[30]. The finite element model uses 525 nodes and 698 standard elements of which 383 represent mortar and 155 joint elements correspond to the aggregate–mortar interface. A volumetric expansion of aggregates alone shows that without confinement pressure, tensile stresses around aggregates can generate fracture and damage in the matrix.

Parametric model [32, 33]

The parametric model is a finite element structural analysis of dams altered by AAR. Parameters influencing the concrete expansion are confinement C, temperature T, moisture M and reactivity R (Fig. 12). Factors F_C, F_T, F_M and F_R are computed over 1 year in different zones of the dam. These normalized expansion factors are then associated in a 'CTMR rule' which simulates the anisotropic non-uniform

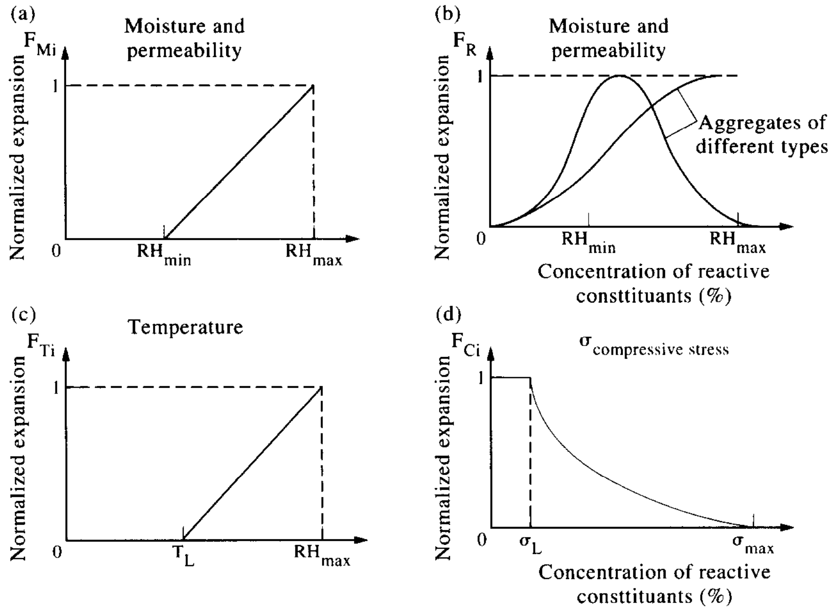


Fig. 12. Factors influencing AAR related concrete expansion.[32]

three-dimensional distribution of AAR expansion. For a given point x, y, z in the mass of concrete, the law is:

$$CTMR_m(x,y,z) = |\Sigma \beta_{nm} F_{nm}(x,y,z)| \qquad (15)$$

$m = x$, y, z; $n = C$, T, M, R; b = calibration factors adjusting computed displacements and measured displacements; F is the normalized expansion factors. The displacements in the mth direction are:

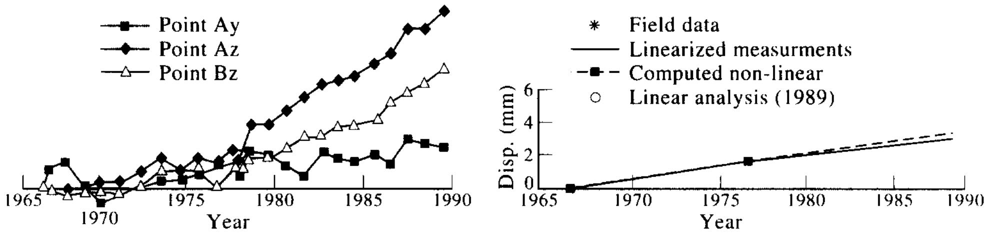
$$D_m(x,y,z) = D_m^{\max} \times \mathrm{CTMR_m}(x,y,z) \qquad (16)$$

$D_m^{\max}$ is the maximun swelling in the mth direction. The CTMR rule is expected to be used in the prediction of the altered concrete structure and of the effect of remedial works. The model has been applied to the spillway pier of a hydroelectric complex in Quebec. The state of stress was estimated in two ways: (1) linear elastic analysis with fictitious temperatures; and (2) the CTMR law. In the non-linear analysis two events were considered: (i) concrete cracking simulated by an elasto-brittle smeared cracked model; and (ii) the reduction in AAR expansion with an applied/induced compressive stresses. Figure 13 shows the good agreement between measured and calculated displacements The CTMR method has been found more reliable for tensile stresses than the linear analysis and more reproductible for profiles of cracking. Numerical simulations have been improved in the last years, but they emphasize the complexity of the concrete response to the different strains and more particularly to AAR. Calculations remain heavy with a large number of parameters, they are different from one concrete structure to another one.

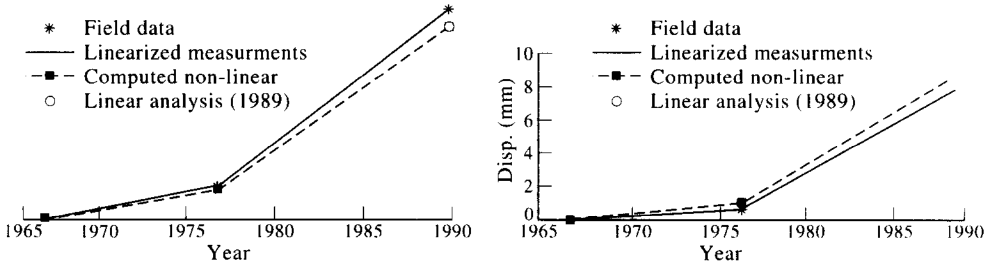
CONCLUSION

Since the last conference on Alkali–Aggregate Reaction (London 1992), progress has been made in simulating mechanical effects induced by the chemical reaction between reactive silica and Na^+, K^+, OH^- ions in concrete. New models consider concrete a heterogeneous material with a connected porosity and randomly distributed reactive sites. Local and global concentrations of alkalis are determined by an apparent diffusion law through the pore solution. Capillary pressures generated by the gel after water absorption result in cracking treated by the fracture mechanics. Confinement, temperature, moisture are parameters characterising the anisotropy of the AAR. So the simultaneous use of chemistry, physics, thermodynamics, probabilistics, kinetics and mechanics is able to model expansion. These new models will be improved, taking into account recent results, on the composition of gels and their water content more particularly.

Numerical simulations of AAR expansions by finite elements have also acquired advancement



(a) Measured displacements (b) Horizontal displacement (Point Ay)



(c) Vertical displacement (Point Az) (c) Vertical displacement (Point Bz)

Fig. 13. Measured and calculated displacements for three points Ay, Az, Bz in zone II, emerged part of the pier.[33]

compared to equivalent thermal loads. The anisotropic non-uniform character of AAR is taken into consideration in a new CTMR law, which calls for a closer combination with physical processes involved.

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APPENDIX

Probabilistic model[5,19]

Local chemical reaction
Diffusion law

$$\frac{\Delta Prob(Na^{+}_{local})}{(\Delta t)}$$

$$= -D\,\frac{Prob(Na^{+}_{local}) - Prob(Na^{+}_{max})}{\sqrt{\pi \mathrm{Dt}}} \qquad (1)$$

D is the diffusivity coefficient in the cement paste; t is time; Δt is time increment; Prob ($\mathrm{Na}^{+}_{\mathrm{local}}$) is the local probability of presence of alkalis related to the presence of reactive silica; and Prob($\mathrm{Na}^{+}_{\mathrm{max}}$) is the global probability of alkalis.

The formation of gel is possible if all the elements (reactive silica, OH^-, Na^+, K^+) are present in the ECRV. This is expressed as:

$$Prob(I_{gel} = 1) = Prob\{(I_{Na^+} = 1) \cap (I_{sir} = 1)$$

$$\cap (I_{OH^-} = 1)\} \qquad (2)$$

Sir is reactive silica and I_i is the presence indicator of element i. As the medium is always alkaline, the probability of the presence of OH^- ions is taken equal to 1. So the new formula is:

$$Prob(I_{gel} = 1) = Prob\{(I_{Na^+} = 1) \cap (I_{sir} = 1)\} \qquad (3)$$

Gel pressure
Widening of a crack: volume of a crack

$$vf = \frac{K_I.(k+1)}{\mu}\sqrt{2\pi}\left(\mathrm{af}\,\frac{2}{3}\,(\mathrm{af} - \mathrm{ri})^{3/2}\right.$$

$$-\frac{2}{5}(af-ri)^{5/2}\Bigg) \qquad (4)$$

where *af* is the radius of the crack considered as circular and plane (Fig. 6); *ri* is the radius of the reactive site; K_I is the stress intensity factor; and k and μ are the elasticity coefficients of concrete.

The gel penetration characterized by the variable A is written as:

$$A=\max\left[(\mathrm{af}-2\pi\left(\frac{\mu\dfrac{2\sigma\cos\theta}{\mathrm{P_g}}}{\mathrm{K_I(k+1)}}\right)^2),\mathrm{ri}\right] \qquad (5)$$

where *af* is the half-length of the crack. The gel volume in the crack is V_{gf}.

$$V_{\mathrm{gf}}=\frac{\mathrm{K_I(k+1)}}{\mu\sqrt{2\pi}}\left[\frac{2}{3}\,af.(r\mathrm{max}^{3/2}-r\mathrm{min}^{3/2})\right.$$

$$\left.-\frac{2}{5}(r\mathrm{max}^{5/2}-r\mathrm{min}^{5/2})\right] \qquad (6)$$

$r\mathrm{min}=af-A$ and $r\mathrm{max}=af-ri$. If $ks=vf/V_{\mathrm{vo}}$: increasing in the connected porosity due to cracking and $\gamma=V_{\mathrm{gf}}/vf$: partial filling up of cracks by the gel. The gel pressure is:

$$P_g=\frac{E_g}{3}\left[1-\frac{V_{vo}}{V_{gel}}\,\phi\left(\frac{-ln(2\sigma cos(\theta)/P_c)-\bar{lnr_p}}{\bar{\bar{lnr_p}}}\right)\right] \qquad (7)$$

Thermodynamical model of reactive porous materials[15]

Free energy

$$\Psi=\Psi(\varepsilon,T_o,\xi)=\frac{1}{2}K\varepsilon^2-\alpha K\varepsilon\xi-\Im_o\xi+\frac{1}{2}L\xi^2 \quad (1)$$

where K is the tensor of elastic characteristics; T is the temperature; α is the coefficient of coupling between chemistry and mechanics; and $\Im_o$ the initial chemical affinity of the reaction. The state laws are:

$$\sigma=\frac{\partial\Psi}{\partial\varepsilon}=K(\varepsilon-\alpha\xi) \qquad (2)$$

where σ is the stress tensor.

$$\Im_a=\Im_o+\alpha K\varepsilon-L\xi \qquad (3)$$

The kinetics of chemical reactions is considered as linear and follows the Arrhenius' law

$$\Im_o=\eta.exp\left(\frac{E_a}{RT}\right)\xi \qquad (4)$$

where E_a is the activation energy; R the perfect gas constant; T the temperature; and η a constant of kinetics. If the reaction in the pore solution is controlled by a diffusion mechanism, it is also possible to involve cracking in η.

The swelling is, by coupling eqns (B2)–(B4)

$$\varepsilon=\varepsilon_\infty\left(1-exp\left(-\frac{t}{\tau}\right)\right) \qquad (5)$$

ε_∞ and t are constants expressed in relation to variable and intrinsic parameters K, α, $\Im_o$, η, E_a.