

Modeling the alkali aggregate reaction expansion in concrete

Sekrane Nawal Zahira* and Asroun Aissa

Department of Civil Engineering, Djillali Liabes University, Civil Engineering
and Environment Laboratory, Sidi Bel Abbés 22000, Algeria

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Abstract. Alkali aggregate reaction affects numerous civil engineering structures and causes irreversible expansion and cracking. This work aims at developing model to predict the potential expansion of concrete containing alkali-reactive aggregates. First, the paper presents the experimental results concerning the influence of particle size of an alkali-reactive aggregate on mortar expansion studied at 0.15–0.80 mm, 1.25–2.50 mm and 2.5–5.0 mm size fractions and gives data necessary for model development. Results show that no expansion was measured on the mortars using small particles (0.15-0.80 mm) while the particles (1.25–2.50 mm) gave the largest expansions. Finally, model is proposed to simulate the experimental results by studying correlations between the measured expansions and the size of aggregates and to calculate the thickness of the porous zone necessary to take again all the volume of the gel created by this chemical reaction.

Keywords: simulation; alkali aggregate reaction; expansion; model; particle size

1. Introduction

Concrete is a building material that can suffer from chemical degradation mechanisms that can lead to premature failure of the structure. Alkali aggregate reaction (AAR) is one of the most famous pathologies of the material. This reaction can be visualized as two-step process. The first step involves the formation of the reaction product between the reactive silica and the alkalis of concrete. The real damages to the concrete, however, are caused by the second step. In this step, the reaction product, which is a gel, absorbs water and swells; this gel has a high affinity for the water imbibition. While it absorbs humidity, it causes increases of volume and swelling pressure in the concrete. This pressure is fairly intense to cause rupture of the internal microstructure of the concrete. AAR expansion depends on numerous parameters: amounts of alkali, reactive silica and water present, aggregate size...etc.

One of the main difficulties is to measure the gel volume formed by this reaction. Microscopic models could be one method of doing this (Sellier *et al.* 1996, Bazant and Steffens 2000 and Poyet *et al.* 2007). Such models should be able to predict the differences of expansions with the variation of all influential parameters such as a size of aggregate and have to be compared with experimental results (Multon *et al.* 2010 and Sanchez *et al.* 2014).

* Corresponding author, Ph.D. student, E-mail: n.sekrane@gmail.com

Many papers deal with the effect of particle size of reactive aggregates on the expansion due to alkali aggregate reaction (Diamond and Thaulow 1974, Hobbs and Gutteridge 1979, Zhang *et al.* 1999, Kuroda *et al.* 2004, Multon *et al.* 2008, Gao *et al.* 2012 and Dunant and Scrivener 2012). Experiments have been performed on several types of aggregates such as the greywacke, chert, mylonite, quartzite, silica glass, andesite, siliceous limestone, flint and sandstone (Diamond and Thaulow 1974, Hobbs and Gutteridge 1979, Zhang *et al.* 1990, Hasni *et al.* 1993, Wigum *et al.* 1996, Kuroda *et al.* 2004, Ramyar *et al.* 2005, Duyou Lu *et al.* 2006, Multon *et al.* 2010, Gao *et al.* 2013 and Yuksel *et al.* 2013).

Our work aims at developing model who studies the correlations between the measured expansions and the size of aggregates. For this reason, Experimental results from Duyou Lu *et al.* (2006) studies were used for serve them as the basis of experimental data in numerical simulation.

Three mix-designs were studied containing one reactive size distribution (0.15-0.80 mm), (1.25-2.50 mm) and (2.50-5.0 mm). First, the paper presents the experimental conditions of the tests; then, the measurements of AAR-expansions are presented. Finally, model is proposed to simulate the experimental results by studying correlations between the measured expansions and the size of aggregates.

2. Materials and method

In order to determine the potential alkali reactivity of aggregate more quickly and accurately to comply with the fast growing infrastructure construction in China, a new test method (Chinese accelerated mortar bar method-CAMBT) was used by the authors (Duyou Lu *et al.* 2006). This method was developed recently in China by combining the advantages of the Chinese autoclave method and the Accelerated mortar bar test method (AMBT) (ASTM C1260, CSA A23.2-25A, RILEM TC191-ARP-02 and Zhongzi *et al.* 1998) with some modifications on the method by the authors. The main parameters in the new method, the AMBT and the autoclave method are compared in Table 1.

In the CAMBT, a single size fraction of fine aggregate (0.15-0.80 mm) and a high-alkali system of 1.5% Na₂O_{eq} (obtained through the addition of KOH to a low-alkali cement) are used, which are the same as in the Chinese autoclave test. Three series of tests were performed with cement-to-aggregate ratios of 10:1, 2:1 and 1:1. The water-to-cement ratio was fixed at 0.33. The mortar bar size was 40x40x160 mm. The storage conditions and testing procedures are similar to the AMBT method, except that the initial length measurement (or zero reading) is made after 4 h of immersion in 1 M NaOH at 80°C.

The common approaches to accelerate the reaction process in these accelerated procedures are using large proportion of fine aggregate particles and high temperature, high-alkali regime, but with significant difference in the mix compositions, such as specimen size, aggregate gradation etc. (Table 1). The five graded aggregate fractions used in the AMBT are derived from ASTM C227, the standard mortar bar test, while the 0.15-0.80 mm aggregate fraction used in the CAMBT follows the Chinese autoclave method. Previous study showed that, for (25 x 25 x 285 mm) mortar bars cured at 38°C and high humidity environment, there exists a pessimum particle size that could induce largest mortar expansion (Hobbs and Gutteridge 1979). However, little work has been reported on the effect of particle size on (40 x 40 x 160 mm) mortar bar expansion in 1 M NaOH solution at 80°C.

Table 1 Parameters in accelerated tests for alkali-silica reactivity

Parameters	AMBT	Autoclave method	CAMBT
Water-to-cement ratio	0.47	0.30	0.33
Cement alkalis ($\text{Na}_2\text{O}_{\text{eq}}$)	$1.0 \pm 0.1\%$ ^a	1.5% ^b	1.5% ^b
Aggregate size (mm)	0.15–5.0 ^c	0.15–0.80	0.15–0.80
Bar size (mm)	25x25x285	10 x 10 x 40	40x40x160
Cement-aggregate ratio	1:2.25	10:1, 5:1, 2:1	10:1, 2:1, 1:1
Curing temperature	80°C	150°C	80°C
Storage solution	1.0M NaOH	10% KOH	1.0M NaOH
Zero length	24 h in water @ 80°C	24 h moist @ 23°C	4 h in 1 M NaOH @ 80°C
Criteria	0.10 % @ 14 days	0.10 % @ 6 h	0.10 % @ 7 days

^a Use high-alkali cement.^b Use low-alkali cement, add KOH to mix water.^c Five required size fractions.

2.1 Materials

The aggregates selected were the quartzitic sandstone of Montreal, Canada (PO) and the quartzite of Norway (NQ). They were crushed and sieved to the following three size ranges: (0.15–0.80 mm), (1.25–2.50 mm) and (2.50–5.0 mm). The aggregate-to-cement ratio was 1:1.

In the proposed new test procedure, low-alkali cement was to be used, with the cement alkali content adjusted to 1.5% $\text{Na}_2\text{O}_{\text{eq}}$ by adding KOH to the mixing water. Low-alkali cement (0.58% $\text{Na}_2\text{O}_{\text{eq}}$) was first tried at the CANMET laboratory, but the paste was very harsh at the water-to-cement ratio of 0.33 when adding KOH. Therefore, high-alkali cement with 0.91% $\text{Na}_2\text{O}_{\text{eq}}$ was used without the addition of KOH in this study.

2.2 Mixing and moulding procedure

For each test, a mould of three prismatic sample of (40x40x160) mm was used. The mixing and moulding procedures followed the requirements of CSA A23.2-25A. The mixing water and cement were placed in the bowl and mixed at slow speed for 30 s; the entire quantity of aggregate was then added slowly over 30 s, while mixing at slow speed. The mixture was then mixed for 30 s at medium speed and then allowed to stand for 90 s with the bowl covered with a wet towel to avoid moisture loss. The mixture was then mixed again for 60 s at medium speed (Oberholster and Davies 1986, Lu *et al.* 2006)

The mixture was compacted into the molds with a tamper. The molds, covered with plastic sheet, were stored in a fog room at 23°C for 24 ± 2 h. The bars were then demolded and immersed in water in sealed plastic containers, which were then placed in an oven at 80°C for 24 ± 2 h.

The initial length measurement is then taken, the bars transferred in containers filled with a 1 M NaOH solution at 80°C and the containers returned to the oven maintained at 80°C. The length changes of the bars were measured at 1, 3, 5, 7, 10, 12, 14 and 28 days, respectively.

The expansion result is the average of three measurements.

3. Experimental results and discussion (Lu *et al.* 2006)

The expansion results for the Potsdam sandstone (PO) and Norwegian quartzite (NQ) are presented in Table 2. The expansions for bars with a single fraction of reactive aggregates are shown in Figs. 1 and 2, they indicate that the expansion of bars with (0.15-0.80 mm) aggregate particles basically increases linearly with time at least up to 14 days. For specimens with (1.25-2.50 mm) and (2.5-5.0 mm) particles, the expansion curves are generally linear, with a slow-down after about 14 days.

Measurements of mass change of the bars at 14 days showed that the aggregates gained some weight. Mass gain for specimens of these aggregates varies from 0.2–1.0% of their initial weights (1 day in water at 80°C) (Lu *et al.* 2006).

Figs. 3(a) and 3(b) shows the effect of aggregate particle size on expansion at different ages. Using 0.10% as a criteria for expansion, the bars with the finest fraction of aggregate (0.15-0.80 mm) did not give the largest expansion in this test condition, especially at early ages, they showed AAR-expansion lower than about (0.057%) for PO and about (0.104%) for NQ. It clearly indicates that, the aggregates give the largest expansion at the (1.25-2.50 mm) size fraction throughout the test period (0.239% for PO) and (0.243% for NQ), for bars with (2.50-5.0 mm) aggregate particles AAR-expansion measured is (0.183% for PO) and (0.185% for NQ) (Lu *et al.* 2006).

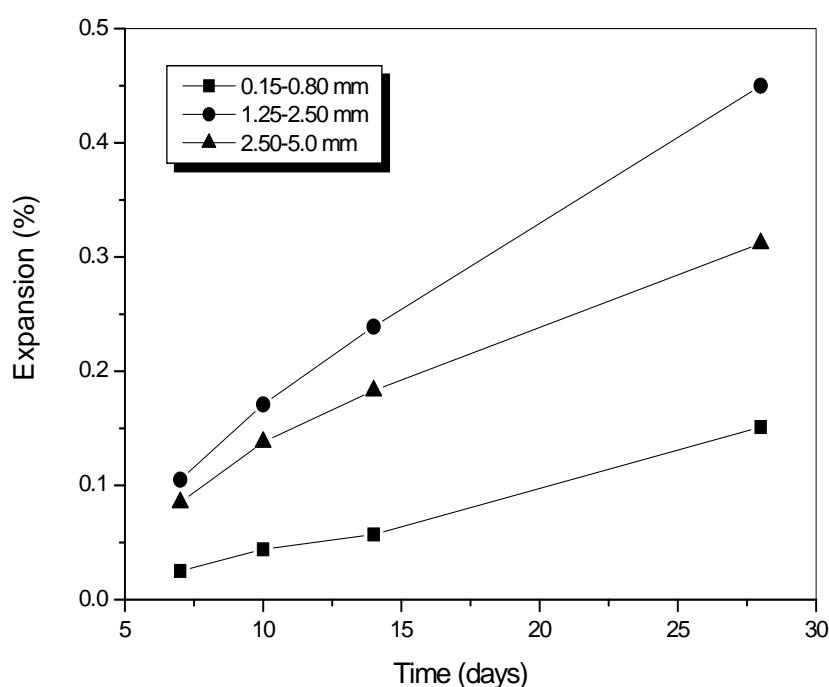


Fig. 1 Expansions of mortars containing reactive particles of size (0.15-0.80) mm, (1.25-2.50) mm, (2.50-5.0) mm measured for (PO) (Lu *et al.* 2006)

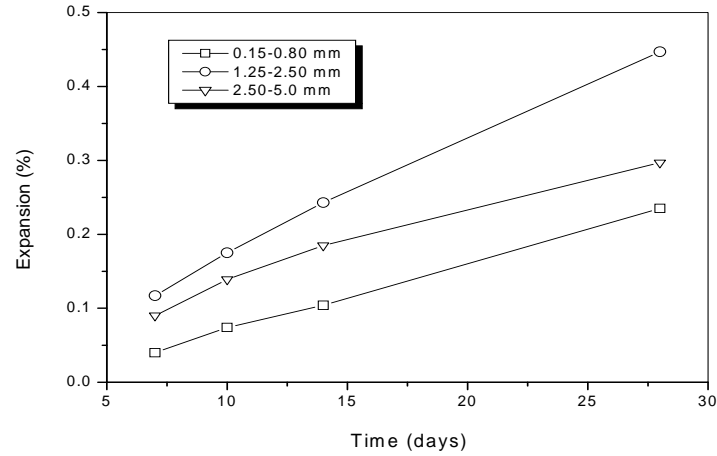
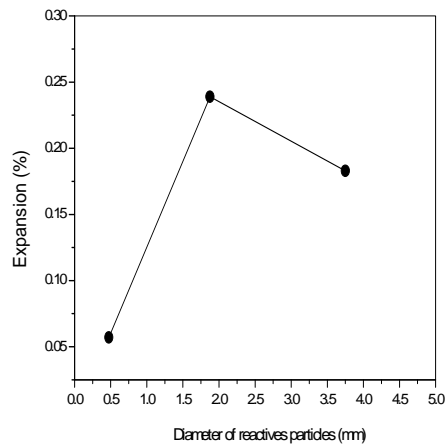
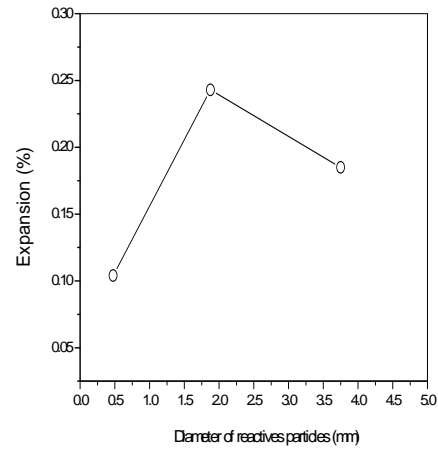


Fig. 2 Expansions of mortars containing reactive particles of size (0.15-0.80) mm, (1.25-2.50) mm, (2.50-5.0) mm measured for (NQ) (Lu *et al.* 2006)



(a) PO



(b) NQ

Fig. 3 Relationship between expansion and reactive particles size

Table 2 Expansion results for the reactive aggregates (Lu *et al.* 2006)

Aggregate	PO			NQ		
	0.15-0.8 mm	1.25-2.5 mm	2.50-5.0 mm	0.15-0.8 mm	1.25-2.5 mm	2.50-5.0 mm
07 days	0.025	0.105	0.085	0.040	0.117	0.090
10 days	0.044	0.171	0.138	0.074	0.175	0.139
14 days	0.057	0.239	0.183	0.104	0.243	0.185
28 days	0.151	0.450	0.312	0.235	0.447	0.297

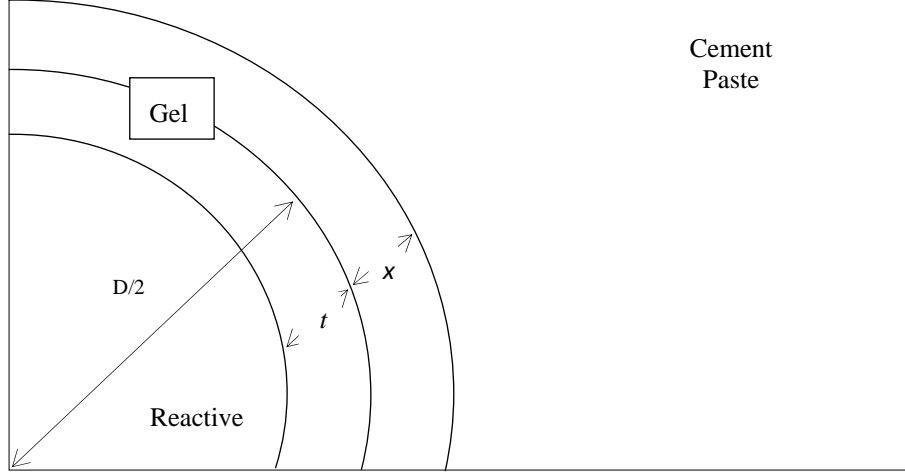


Fig. 4 Schematic of a reactive particle after the reaction

4. Expansion and model and discussion

The model presented in this section aims to improve the understanding of the experimental results obtained in the first part and calculate expansion of mortars containing only one size.

The various assumptions constitutive of the models are (Fig. 4)

- The siliceous aggregates are spherical of diameter D_i
- A volume of silica produced “ n ” volume of gel ($n>1$)
- The small and coarse aggregates are attacked on an identical thickness “ t ”
- There exists a porous zone of thickness “ x ” surrounding the aggregates in which the products are formed.

The expansion of the mortar is caused by the expansions of the AAR-gels. It can be assumed that this expansion is caused by the volume variation of the aggregate (in presence of gel). For the sake of simplicity, it is assumed that the mortar expansion due to AAR (ε_{AAR}) is proportional to the aggregate expansion (Eq. (1)). For several sizes of reactive particles, the aggregate expansion is the sum of the expansions of all the reactive aggregates (Multon *et al.* 2010).

$$\varepsilon_{AAR} = k \cdot \sum_{i=1}^N \phi_i \varepsilon_i \quad (1)$$

Where

ε_i : The expansion of one reactive aggregate of class i .

ϕ_i : The volume fraction of reactive aggregates of class i relative to the mortar volume (total volume of reactive aggregate of class i / total volume of the mortar).

N : The number of classes of reactive aggregates.

k : The fraction of expansion due to AAR related to the expansion of reactive aggregates.

The mortar expansion is assumed to be due to the aggregate expansion. If $k=1$, the mortar expansion is equal to the aggregate expansion. In reality, k has to be equal to or lower than 1, since the mortar expands less than the aggregate due to the mechanical effect of cement paste. During the reaction, at a given moment, the aggregate is attacked on a thickness “ t ” and it produces a volume of the gel equal to V_i^g

$$V_i^g = n \left[\frac{\pi D_i^3}{6} - \frac{\pi (D_i - 2t)^3}{6} \right] \quad (2)$$

During the formation of the AAR-gel, a part of the gel can migrate through the porosity close to the aggregate. Therefore, the aggregate expansion for one aggregate i can be described by Eq. (3).

$$\varepsilon_i = \frac{\langle V_i^g - V_i^p \rangle^+}{V_i} \quad (3)$$

With:

V_i^p : The volume of the porosity close to the reactive aggregate in which the AAR-gel can migrate without causing expansion.

V_i : The volume of one reactive particle, it is given by the following formula

$$V_i = \frac{\pi D_i^3}{6} \quad (4)$$

Where:

D_i : The diameter of the reactive particle.

$$\langle X \rangle^+ : \text{The positive part of } X, \text{ If: } \begin{cases} X < 0, & \langle X \rangle^+ = 0 \\ X > 0, & \langle X \rangle^+ = X \end{cases}$$

Assuming that the gel can migrate along the same distance of the aggregate “ x ” whatever the size of the aggregate (simplifying hypothesis), the volume of the porosity is given by Eq. (5)

$$V_i^p = \left[\frac{\pi (D_i + 2x)^3}{6} - \frac{\pi D_i^3}{6} \right] \cdot p \quad (5)$$

Where:

p : is the porosity of the mortar.

The combination of Eqs. (1)-(5) for only one class of reactive particles leads to the Eq. (6).

$$\varepsilon_{AAR} = k \cdot \phi_i \cdot \left[\left\langle n \left(1 - \frac{(D_i - 2t)^3}{D_i^3} \right) - p \left(\frac{(D_i + 2x)^3}{D_i^3} - 1 \right) \right\rangle^+ \right] \quad (6)$$

In order to carry out this calculations and in order to obtain expansions comparable to measured

expansions on mortars, the porosity of the mortar (p), the thickness of attack of the aggregates (t), the voluminal coefficient of the gel (n) and the distance (x) which gel must diffuse in the cement paste are fixed (see Table 3). These calculations are performed using the technical computing software Maple 12. The calculated expansions are plotted in Figs. 5(a)-5(b).

Figs. 6 and 7 compares experiment results of AAR-expansion of mortars containing one size of reactive particles with the results calculated by the expansion model; they have a similar shape of expansion curve. It is observed that the model simulates the experimental data well. The finest fraction of aggregate (0.15-0.80 mm) did not give the largest expansion, they showed AAR-expansion equal to (0.060% for PO) and (0.104% for NQ). The (1.25-2.50 mm) size fraction give the largest expansion (0.249% for PO) and (0.264% for NQ), for bars with (2.50-5.0 mm) aggregate particles AAR-expansion measured is (0.162% for PO) and (0.174% for NQ).

To sum up, the model developed in this article is similar to other models (such as Sellier, Poyet and Multon) in the assumptions constitutive (spherical aggregates, taking into account the influence of the diameter of reactive aggregates, calculating the expansion is done for a single granular class except Poyet model which is the only applied to simulate the swelling of a material containing different granular classes). However, the difference is in the fact that these models simulate the expansion by a probabilistic description of the mechanisms governing the alkali-silica reaction and take into account the probable mean concentration around the reactive aggregate, and our model simulates the expansion with a description of effects induced by the swelling of the gel. The volume of gel was calculated according to Eq. (2) and the volume of porosity to be filled around each particle of diameter D_i before the expansion starts is given by Eq. (5). The expansion of mortar was then taken as the volumetric change of the aggregate due to the gel volume not contained in the porous zone Eq. (3). This simple relation allows the final expansion to be plotted against the reactive aggregate. The small reactive particles, because of their uniform distribution in the paste, could create gel distributed regularly in all the mortar. This gel would migrate in the matrix and to be easily adapted by the porosity of the cement paste, without creating expansion of the mortar. However, the gel produced around the coarse grains could generate considerable pressures leading to important macroscopic swellings if the thickness of porosity was little.

Using this model, the thickness of the porous zone can be estimated according to the diameter of the reactive particles in order that gel created could be completely adapted by the porosity of the mortar. In this case, the volume for the gel created is equal to the sum of the volume of the gel produced by the aggregate during its reaction and of the volume of the porosity in which the gel can diffuse

$$V_i^g = \left[\frac{\pi D_i^3}{6} - \frac{\pi (D_i - 2t)^3}{6} \right] \cdot n + \left[\frac{\pi (D_i + 2x)^3}{6} - \frac{\pi D_i^3}{6} \right] \cdot P \quad (7)$$

From Eq. (7), the distance “ x ” is calculated

$$x = \frac{\sqrt[3]{\left[\left(\frac{n-1}{P} \right) \cdot (D_i^3 - (D_i - 2t)^3) \right] + D_i^3 - D_i}}{2} \quad (8)$$

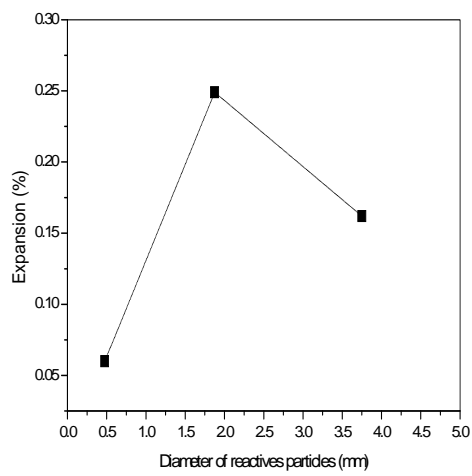
The results of calculations with the technical computing software Maple 12 are plotted in Fig. 8.

Fig. 8 gives the evolution of “ x ” and shows that the gel produced in the small aggregates needs less distance to be adapted by the porosity of the paste, however the thickness become important

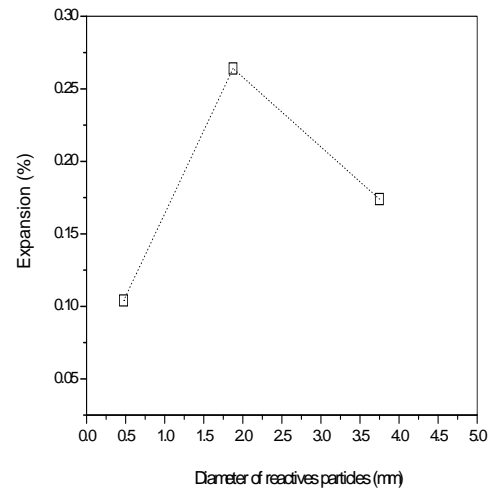
for aggregates greater than 1 mm. Therefore, the results of calculations by this model indicate that, if there is a lot of gel, “ x ” has to be large to prevent expansion for the reactive particles.

Table 3 Model parameters

parameters	k	n	t	x	P
PO	0.2	2	0.25mm	0.35 mm	25%
NQ	0.2	2	0.25 mm	0.38 mm	25%



(a) PO



(b) NQ

Fig. 5 Expansion of the mortars against the diameter (D_i) of the reactive particles: calculated by the expansion model

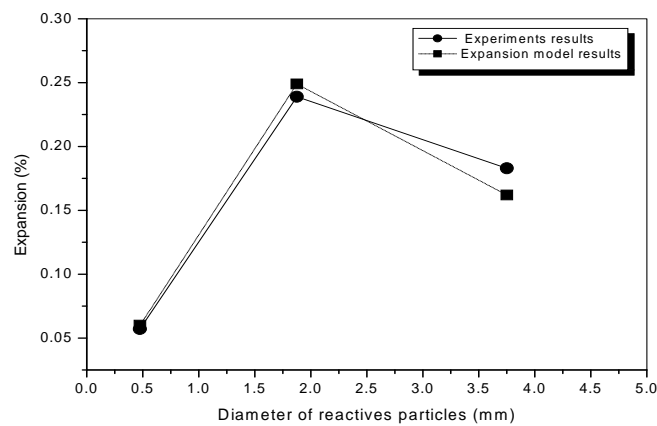


Fig. 6 Expansion of the mortars against the diameter (D_i) of the reactive particles: Comparison between the experiments and the expansion model for (PO)

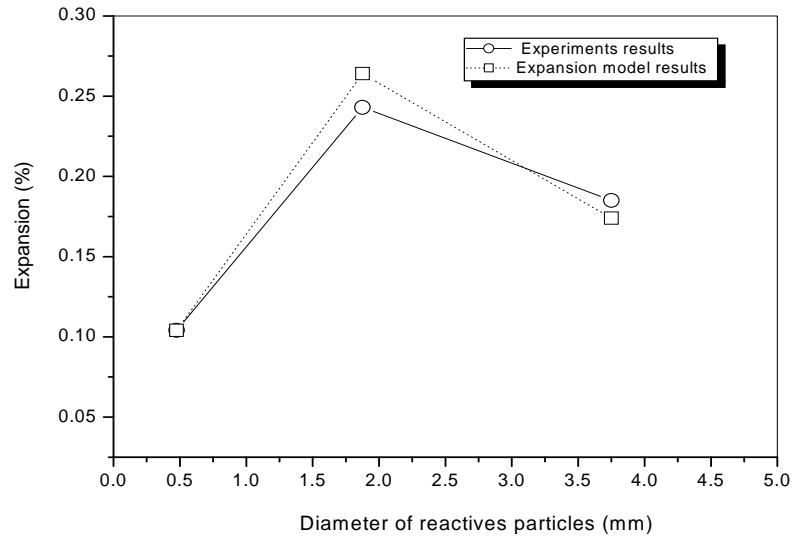


Fig. 7 Expansion of the mortars against the diameter (D_i) of the reactive particles: Comparison between the experiments and the expansion model for (NQ)

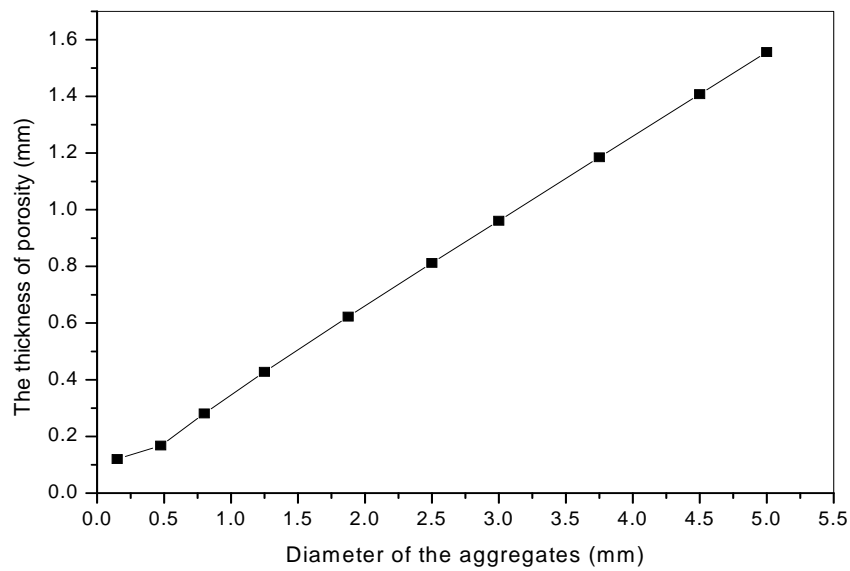


Fig. 8 The distance “ x ” in which the gel must diffuse in the paste to be completely adapted by the porosity according to the diameter(D_i) of the aggregates (PO) and (NQ).

5. Conclusions

In this paper, a combination of experiments and modelling was used to study the size effects of the reactive aggregate on AAR-expansions. For this reason, three particle size fractions for two aggregates were studied in mortars and the experimental measurements has presented. The results indicate that, for the (40x40x160) mm specimen cured in the 1M NaOH solution at 80°C, no AAR-expansion was measured for the mortar bars containing 0.15-0.80 mm size range while the mortar bars containing 1.25-2.50 mm size range show the largest expansion, especially at early ages and for bars with 2.50-5.0 mm aggregate particles, the AAR-expansion measured is (0.183% for PO) and (0.185% for NQ).

The expansion model developed simulates the experimental results well and sums up the main experimental observations; it allows some important phenomena related to the size of reactive aggregate to be interpreted easily. The smallest reactive particles did not cause expansion, but the largest ones expanded greatly. Moreover, it computes the thickness of the porous zone necessary to take back all the volume of the gel created by the reactive aggregates in the cement paste according to the diameter of the grains. The results indicate that the thickness increases with the diameter of the reactive aggregates.

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