Sixth International Conference on Durability of Concrete Structures **Paper Number DSM11**
18 - 20 July 2018
University of Leeds, Leeds, West Yorkshire, LS2 9JT, United Kingdom

A Novel Multiscale Modelling Approach for Evaluation of the ASR in Concrete Structures

M. Jalal, M. Mirsayar and A.K. Mukhopadhyay
Texas A&M Transportation Institute, Texas A&M University, TX, USA

ABSTRACT

This paper presents a new multiscale approach for evaluation of the volume change in concrete structures due to the alkali-silica reaction (ASR). A practical step by step approach that can be applied to the real structures is developed based on combined experimental and numerical assessment by considering the most influential ASR parameters at different scales. In the first step, the ASR expansion is measured using accelerated concrete cylinder test (ACCT) for different concrete mixtures covering different variables of important factors such as mix design (e.g., w/cm, fly ash type and replacement percentages), aggregate reactivity, alkali loadings, temperature, and relative humidity etc. All measured expansion data are then modelled using artificial neural network (ANN) modeling approach in the second step. In the third step, finite element (FE) model is utilized at different scales to analyze the real structures and representative volume element (RVE) taking into account the ASR gel expansion and structural boundary conditions. Finally, the effects of the structural constraints are taken into account by introducing correction factors to the predicted free expansion (i.e. no constraints) of the RVE by ANN model. It was found that a combined effect of both internal gel pressure and structural constraints determines the net volume expansion in a concrete structure. In order to show the applicability of the proposed approach, the model is employed for evaluation of the ASR-induced net volume expansion at different locations of a dam structure under realistic in-service conditions. The microstructural study was also done by using X-ray CT that can be used to estimate the ASR progress in concrete structure and validate / support the FEM based predictions.

Keywords: Alkali- Silica Reaction (ASR), a novel multiscale approach, concrete structures; expansion prediction

1.0 INTRODUCTION

Nowadays, durability of infrastructures in general and concrete structures in particular, is a highly demanding concern inasmuch as it can be considered as a key to Sustainable construction. It is more perceivable considering the fact that concrete is the most widely used man-made material in the world. Alkali- silica reaction (ASR) is one the most complex durability issues of concrete structures which is a detrimental reaction between the alkaline pore solution in concrete and various metastable forms of silica in aggregates (Pool, 1992; Hobbs, 1988) leading to formation of ASR gel. In the presence of sufficient moisture (> 80% RH), the gel swells through moisture absorption and generate tensile stresses. When these stresses exceed the tensile strength of concrete, cracking in concrete structures initiate (Chatterji, 1989; Diamond, 1976; Garcia-Diaz *et al.*, 2006; Hanson, 1944; Ichikawa and Miuri, 2007; McGowan and Vivian, 1952; Powers and Steinour, 1955; Rodrigues *et al.*, 1999; Farnam *et al.*, 2015; Kagimoto *et al.,* 2015).

Since the pioneering work of Stanton (1940), much has been done to identify, mitigate and model the ASR over the past years. Regarding durability of concrete structures, test methods durability enhancement through supplementary cementitious materials (SCM) and development of prediction models have been evolved among which ASR has been a challenging topic (Malvar *et al.,* 2002; Shehata and Thomas, 2002; Pan *et al.*, 2012; Saouma and Perotti, 2006; Alnaggar *et al.,* 2012).. Challenges pertaining to ASR can be generally outlined as development efficient performance tests, applicability to field structures, taking into account the influencing parameters and development of a comprehensive model addressing scale effect which are separately reflected in different research studies (Lindgard *et al.,* 2012; Multo and Sellier, 2016). However since these factors are somehow interrelated having interactions on each other, individual studies without fitting into a comprehensive paradigm or framework may not get much success to resolve the problem, which is the main drawback of the current studies and models (Bazant and Zi, 2000; Wenk and Monteiro, 2008; Bazant and Steffens, 2000; Goltermann, 1994; Goltermann, 1995) With this respect, it is of great importance to keep in mind that this framework is not about predicting an exact level of deterioration with the specific materials and design , but to estimate a relative level of performance with acceptable range of criteria to ascertain acceptable field performance (Goltermann, 1995).

In the present paper, a new multiscale modeling plan for ASR is presented to cover a variety of influencing parameters and scales. Even though this modeling plan is intended to be applied to dam structures, nevertheless, it is still under progress to be an extendable modeling platform to accommodate different structures with different variables.

2.0 Methodology

The new modeling approach briefly presented here is in fact a comprehensive assessment and modeling paradigm taking into account various parameters and scale effects and combines the experiment and modeling techniques at different scales of micro and macro in order to be able to connect the laboratory and modeling results to the filed performance for dam structures. Indeed, this approach tried to correct and cover the gaps of other available models that focus on some aspects in details and thereby missing the total picture and compound effect in ASR assessment. This is especially momentous about ASR which is complicated and has several parameters involved. Another noteworthy aspect is that in this approach, an engineering estimate with acceptable error is sought by seeing the total picture instead of very accurate prediction with just focusing on very limited aspects which can be defective or impractical. However, description of the whole details and results is outside the scope of this paper.

2.1 Steps of the approach

This multi scale approach for ASR assessment and prediction is mainly composed of the following steps:

- Testing concrete mixtures using Accelerated concrete cylinder test (ACCT) method
- Artificial Neural Network (ANN) Model development – application of ANN model to predict the lab measured expansion and model calibration
- Use of Finite element (FE) modelling (small and large scale) and estimation of adjustment factors
- Microstructural assessment using X-Ray CT to validate or support the FE based fracture mechanics model
- Application of adjustment factors to correct the free expansion predicted by ANN and prediction of expansion matching with field conditions

A simple flowchart representing the steps and their connections is depicted in Fig. 1.

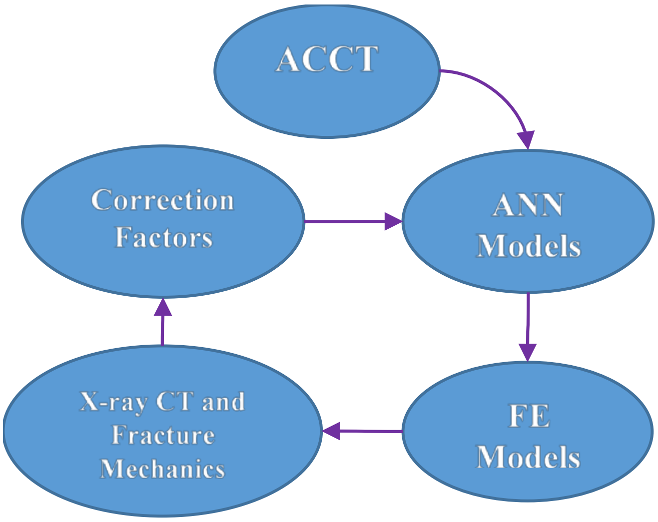

Fig. 1. Flowchart the multiscale approach

2.2 ACCT Testing

Accelerated concrete cylinder test (ACCT) was used to measure the ASR expansion in the concrete cylinder (Liu and Mukhopadhyay, 2015). In this test procedure, the concrete cylinder is cast with a threaded rod on top of the sample, on top of which an LVDT rod is assembled. The cylinder is then placed in a container with a soak solution similar to pore solution of the concrete. After that the container is placed in an oven with a specific temperature (such as 60˚C) and then expansion readings over time are recorded by an LVDT device connected to a computer.

2.3 Assessment of influencing parameters

Devising a comprehensive experimental and modeling plan requires both theoretical considerations and practical verification. Coming up with the influencing parameters in ASR whether of minor or major influence is a crucial part of the approach development which has been somewhat done in some studies (Lindgrad *et al.,*2012; Multo and Stellier, 2016a; Lindgrad *et al.,* 2011; Rajabipour *et al.,* 2015*)*. However these papers show some drawbacks such as parameters completeness, scale effects (molecular scale, lab scale and real structure scale), and lacking of good connections between the steps.

In this study which is under progress, it is tried to include as many influencing parameters as possible in the ACCT test in order to develop a more accurate ANN prediction model. The parameters include mix design parameters such as w/c ratio, fly ash (FA) Type, FA content, cement content, as well as temperature (T), relative humidity (RH), alkalinity and aggregate reactivity.

2.4 ANN Model

Artificial Neural Network (ANN) can be defined as a massively parallel distributed processor that has a natural propensity for storing experiential knowledge and making it available for use. It is categorized as Artificial Intelligence method which is very useful for behavior prediction of complex engineering systems [31-33]. A special feature of ANN model is that it can take as many variables as possible even the qualitative parameters. Another facet is that the model can be flexible to be easily extended to accommodate more variables in case of need. This model was develop in MATLAM software. In this model, four parameters including FA type, FA%, Alkalinity, and time were used to predict ASR expansion over time. More details regarding the modelling technique and how to find the best model with the smallest error can be found in the earlier work published before [34, 35].

2.5 FE Model

FE models in this study can be used in two different scales; real structure scale and representative volume element (RVE). The effects of ASR gel production rate as well as the structural boundary conditions on the volume expansion in concrete are studied for a representative volume element (RVE). The effects of internal pressure induced by the gel production as well as the structural constraints (e.g. structural weight, external loads, etc.) are simulated by the finite element (FE) approach. It was found that a combined effect of both internal gel pressure and structural constraints determines the net volume expansion in a concrete structure. External pressure (P_{ex}) is determined from dam structure analysis for which Max/ Min pressures need to be considered. Internal pressure (P_{in}) can be obtained based on ASR degree (progress) in the structure for which Max/ Min should be determined. In this study, P_{in} was assumed higher than the maximum pressures found in the literature [36-38].

2.6 Microstructure assessment

The microstructure of the ASR affected concrete can be studied using petrography as a destructive procedure and X-Ray Computed Tomography (CT) as a non-destructive device. Microstructure assessment can be used as a measure to evaluate the ASR degree occurred in the structure and to find a correlation between this measure and expansion measured in the lab. An image of the X-Ray CT machine is illustrated in Fig.2.

Fig. 2. Image of X-ray CT machine

To be more specific in this approach, in order for ASR gel pressure to be estimated, degree of ASR in the affected structure should be evaluated. Then based on ASR extent, gel pressure (Pin) can be estimated. For example, if the ASR degree occurred is evaluated to be around 30%, then 30% of the maximum ASR gel pressure can be considered as the current P_{in}. Besides, 2D and 3D images of concrete lab samples and field core can be obtained to evaluate ASR situation.

3.0 RESULTS AND DISCUSSION

3.1 FA parameters

FA type can be characterized in terms of CaO and glass content for which the XRF can be used for the former and XRD can be utilized for the latter. As an example, the results of glass content quantification for available FAs in the lab for this study are presented in Table 1.

An example of XRD spectrum for FA1 is also presented in Fig. 3. The values obtained from FA characterization can be used as input variables to introduce FA type into the ANN model.

Table 1. FA parameter quantification

FA Class C	
Type	**Glass Content**
1	47.8
2	40.2
3	22.2
FA Class F	
Type	**Glass Content**
1	50.05
2	48.28

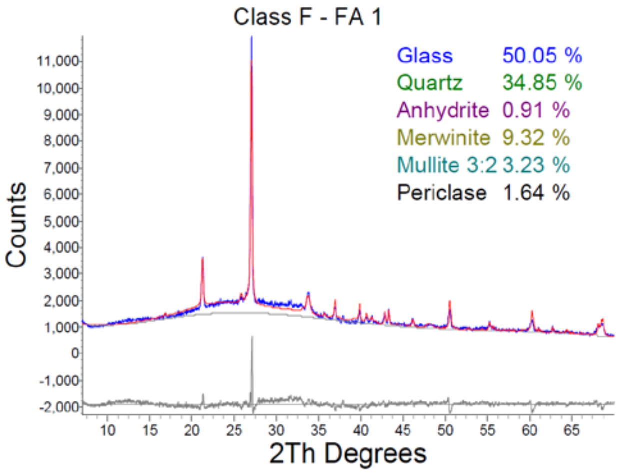

Fig. 3. XRD spectrum of FA type 1 used in this study

3.2 ANN model results

As mentioned earlier, several parameters can be included in ANN model. For the sake of brevity, results of model Performance along with parametric study of FA type effect on ASR expansion are presented in Figs. 4 and 5. Work related to show the effects of other parameters (e.g., alkali loadings, T and RH etc.) is under progress

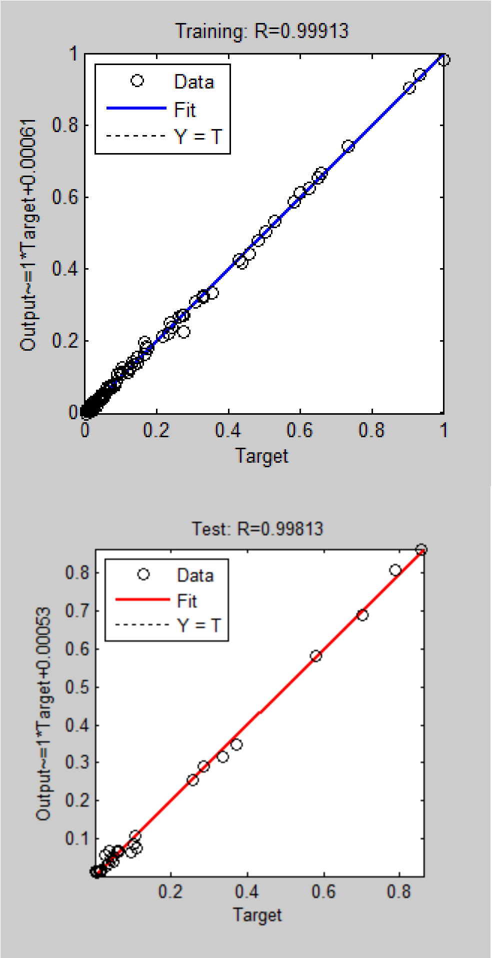

Fig. 4. Performance of ANN model for ASR prediction for train and test datasets

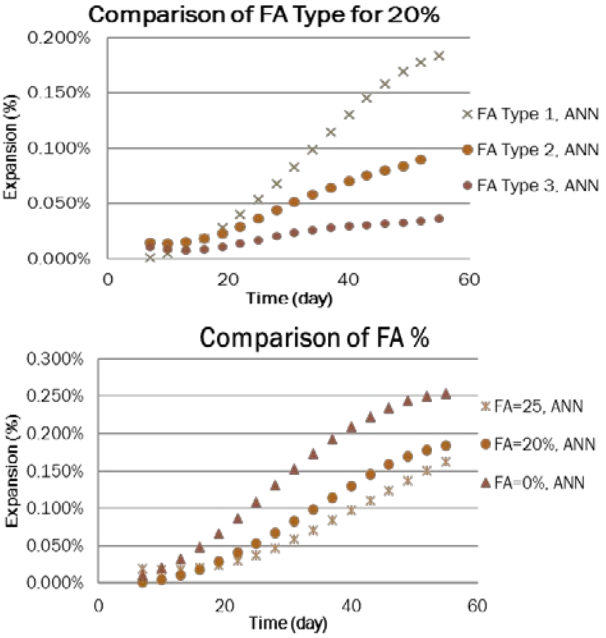

Fig. 5. ASR expansion prediction in terms of FA type and percentage

As can be seen from Fig. 4, very high correlation for train and test datasets are obtained from ANN model predictions. Effect of FA type and percentage can also be thoroughly distinguished from the plots in Fig. 5 indicating the capability of the model to capture the effect FA type and percentage parameters.

3.3 Summary of FE model results

In this study, the total structure of the dam was modeled with its loading and boundary conditions. It can be said that in this case, the main constraint for ASR expansion was the weight of the structure that was mainly consider in calculation of correction factors for ASR free expansion. However, in other cases such as reinforced concrete structure, reinforcement ratio can be considered as the main restraint that can be modeled and introduced in correction factor calculations in this approach. The details of correction factor calculation are outside the scope of this paper.

In order to show the applicability of the proposed approach, the model is employed for evaluation of the ASR-induced net volume expansion at different locations of a dam structure under realistic in-service conditions. The effects of the structural constraints are taken into account by introducing correction factors to the estimated free expansion (i.e. no constraints) of the RVE.

The structure of an RVE modeled in FE along with the results for strain contours are displayed in Fig. 6. It should be noted that at the time, perfect spherical aggregate was modeled and the model considered to be axisymmetric and thereby one eighth of the geometry was considered.

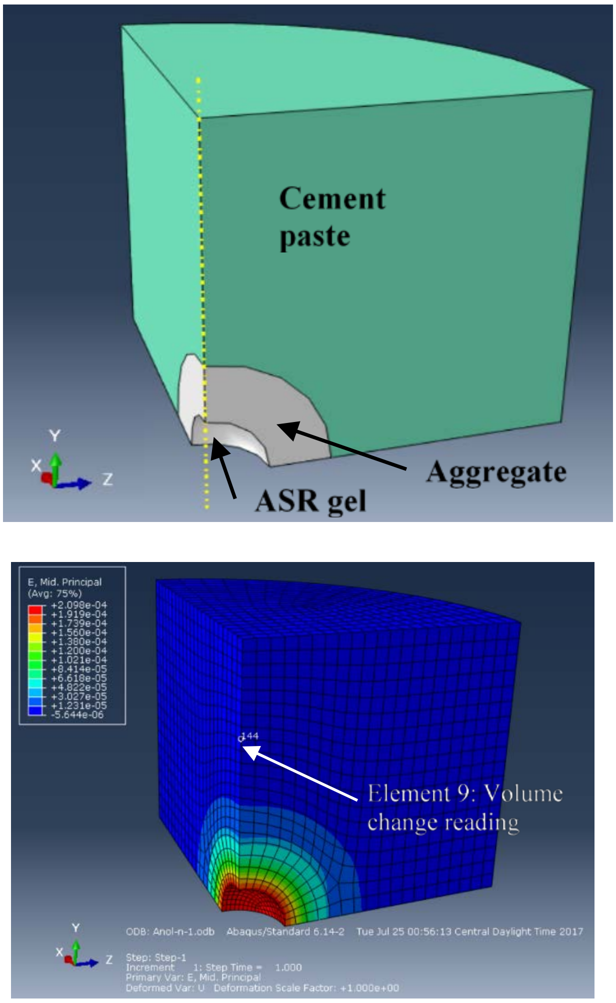

Fig. 6. RVE structure and strain distribution in FE

A series of correction factors calculated for different depth of the dam structure along with its corresponding P_{ex} and P_{in} is presented in Table 2. In this case, a combination of three P_{ex} and four P_{in} were used for correction factors calculation.

Table 2. correction factors for 12 combinations of P_{ex} and P_{in}

P_{in}	P_{ex}	Correction Factor (%)
7	0-0.03	67.98
7	0-0.06	36.15
7	0-0.09	4
9	0-0.03	75.1
9	0-0.06	50.3
9	0-0.09	25.45
11	0-0.03	79.72
11	0-0.06	59.45
11	0-0.09	39.06
13	0-0.03	83.01
13	0-0.06	65.7
13	0-0.09	48.54

Each correction factor corresponding to a P_{in} and P_{ex} in the real structure shows that the free expansion measured in the lab needs to be multiplied by that correction factor.

3.4 Microstructure with X-ray CT

Since X-ray CT is a non-destructive method, the details of ASR affected samples can be monitored and evaluated in macro and microscale. Aggregate change, ASR gel formation, crack initiation and propagation can all be investigated using X-ray CT. Top, front and side views of a sample scanned in x-ray CT machine is displayed in Fig. 7. As can be obviously noticed, a dark band has formed around the aggregate which can be considered as ASR gel and can be quantified through image processing technique which is going to be done as the next step in this study.

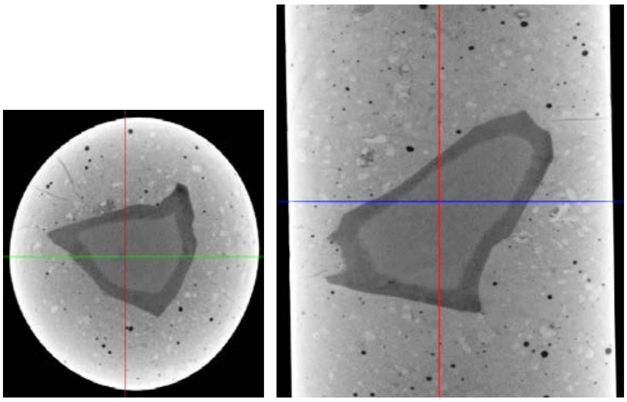

Fig. 7. X-ray CT image of ASR affected sample, the diameter of the cylindrical specimen is ~2.5cm

By using this technique, crack initiation and propagation can be assessed as well to find out whether crack starts inside the aggregate and then propagates into the paste or it may which is an unanswered question in ASR studies. The main purpose of using an X-RAY CT is to validate the prediction based on FEM to some extent and verify the effectiveness of FEM prediction.

3.5 Corrected ASR expansion

The steps of the approach are summed up here to better clarify the steps connection and the final outcome. As mentioned before, the ASR expansion is measured using ACCT method for different concrete mixtures covering different variables of the influencing parameters such as mix design (e.g., w/cm, fly ash type and replacement percentages, alkali loadings), aggregate reactivity, temperature, and relative humidity etc. All measured expansion data are then modelled using ANN modelling approach to predict the free ASR expansion. After that, using FE at different scales along with some supporting tools such as X-ray CT, the correction factors are derived. Correcting the free expansion

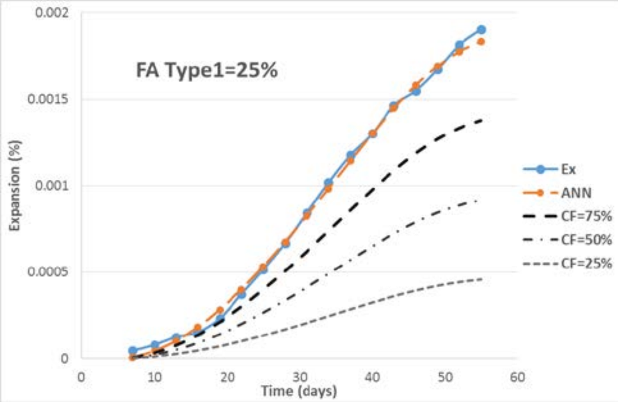

Fig. 8. Experimental, ANN predictions and corrected ASR expansion curves for a mix containing 20% of FA type 1.

predicted by ANN by applying these correction factors in order to predict the effective expansion matching with different locations in a dam is the final step of the proposed approach. Fig. 8 summarizes the final expansion curves for a dam structures based on this approach.

As can be seen from the figure 8, experimental and predicted ASR curve by ANN are in very good agreement. The other 3 curves are the corrected free expansion curved for different depth of the dam structure. As is noted, 3 levels of corrections have been presented as 75%, 50%, and 25%. CF 75% means reduction of the free expansion (predicted by ANN) by 25% to represent expansion at relatively upper level location in a dam. Similarly, CF 25% means reduction of the free expansion by 75% to represent expansion at relatively deeper level location. Herein, it can be seen that while the new multiscale approach can cover a variety of parameters, it can give different levels of expansion prediction for different scales and levels in a real structure.

4.0 CONCLUSIONS

In this study, a new multi-scale approach to evaluate and predict ASR in concrete structure was presented. This is a comprehensive approach which is under progress, based on what was developed so far, the following conclusions can be drawn:

- The new presented approach combines experimental and modeling techniques to predict ASR in concrete structures.
- Several parameters can be included in ANN model as a part of the approach which makes the model more robust compared to the available models.
- FE modeling was employed to analyze the ASR expansion in different scales.
- Microstructure assessment through x-ray CT was designed and performed to better identify the gel formation process.
- Correction factors were calculated to adjust the free expansion predicted by ANN model in order to predict expansion matching with real structure of dam.

References

Alnaggar, M., Cusatis, G., Di luzio, G., 2012. A discrete model for alkali-silica-reaction in concrete, VIII International Conference on Fracture Mechanics of Concrete and Concrete Structures, 1-12.

Bazant, Z.P., Steffens, A., 2000. Mathematical model for kinetics of alkali-silica reaction in concrete, Cement and Concrete Research, 30: 419±428.

Bazant, Z.P., Zi, G., 2000. Fracture mechanics of ASR in concretes with waste glass particles of different sizes, Journal of engineering mechanics, 226-232.

Chatterji, S. 1989. Mechanism of Alkali-Silica Reaction and Expansion," Proceedings, 8th International Conference on Alkali-Aggregate Reaction in Concrete,

Diamond, S. 1976. A review of alkali-silica reaction and expansion mechanisms 2. Reactive aggregates. Cement and Concrete Research 6(4): 549-560.

Farnam, Y., Geiker, M.R., Bentz, D., Weiss, J., 2015. Acoustic emission waveform characterization of crack origin and mode in fractured and ASR damaged concrete, Cement and Concrete Composites; 60: 135-145.

Ferraris, C.F., Clifton, J.R., Garboczi, E.J., Davis, F.L., 1997. Stress due to ASR in mortars, mechanisms of chemical degradation of cement-based systems, E&FN Spon London.

Garcia-Diaz, E., Riche, J., Bulteel, D., and Vernet, C. 2006. Mechanism of damage for the alkali–silica reaction. Cement and Concrete Research 36(2): 395-400.

Garmsiri K, and Jalal M, 2014. "Multiobjective optimization of composite cylindrical shells for strength and frequency using genetic algorithm and neural networks", Science and Engineering of Composite Materials, 21(4): 529-536.

Goltermann, P., 1994. Mechanical Predictions on Concrete Deterioration. Part 1: Eigen stresses in Concrete, ACI Materials Journal, 543-550.

Goltermann, P., 1995. Mechanical Predictions of Concrete Deterioration—Part 2: Classification of Crack Patterns, ACI Materials Journal, 58-62.

Hanson, W. 1944. Studies Relating To the Mechanism by Which the Alkali-Aggregate Reaction Produces Expansion in Concrete, pp. 213-228.

Hobbs, D.W., 1989. Alkali–Silica Reaction in Concrete, Thomas Telford, London.

Ichikawa, T., and Miura, M. 2007. Modified model of alkali-silica reaction. Cement and Concrete research 37(9): 1291-1297.

Jalal M, Ramezanianpour AA, 2012. "Strength enhancement modeling of concrete cylinders confined with CFRP composites using artificial neural networks". Composites Part B: Engineering; 43 (8), 2990-3000.

Jalal M, Ramezanianpour AA, Pouladkhan AR, Tedro P, 2013. Application of genetic programming (GP) and ANFIS for strength enhancement modeling of CFRP-retrofitted concrete cylinders, Neural Computing and Applications, 23(2): 455-470.

Jodaei, A., Jalal, M., Yas, M.H., 2012. Free vibration analysis of functionally graded annular plates by state-space based differential quadrature method and comparative modeling by ANN Composites Part B: Engineering 43 (2), 340-353.

Jodaei, A., Jalal, M., Yas, M.H., 2013, Three-dimensional free vibration analysis of functionally graded piezoelectric annular plates via SSDQM and comparative modeling by ANN, Mathematical and Computer Modelling; 57(5): 1408-1425.

K. Okada, S. Nishibayashi, and M. Kawamura, 1989. Eds., 8th ICAAR Local Organizing Committee, The Society of Materials Science, Kyoto, Japan, pp. 101-105.

Kagimoto, H., Yasuda, Y., Kawamura, M., 2014. ASR expansion, expansive pressure and cracking in concrete prisms under various degrees of restraint, Cement and Concrete Research, 59: 41-15.

Kawamura, M., and Iwahori, K., 2004. ASR gel composition and expansive pressure in mortars under restraint, Cement & Concrete Composites; 24: 47-56.

Lindgård, J., Andiç-Çakır, O., Fernandes, I., . Rønning, MDA Thomas, 2012. Alkali–silica reactions (ASR): Literature review on parameters influencing laboratory performance testing. Cement and Concrete Research, 42: 223–243.

Lindgård, J., Andiç-Çakır, O., Fernandes, I., Rønning, T.F., 2012. MDA Thomas, Alkali–silica reactions (ASR): Literature review on parameters influencing laboratory performance testing, Cement and Concrete Research;42: 223–243.

Lindgård, L., Andiç-Çakır, O., Borchers, I., Broekmans, M., Brouard, E., Fernandes, I., Giebson, C., Pedersen, B., Pierre, C., Rønning, T.F., Thomas, M.D.A., Wigum, B.J., RILEM TC , 2001. 219-ACS-P: Literature survey on performance testing, COIN project report 27, ISBN: 978-82-536-1209-6 p. 164.

Liu, K.-W., and Mukhopadhyay, A.K. 2015. Accelerated Concrete-Cylinder Test for Alkali–Silica Reaction. Journal of Testing and Evaluation 44(3): 1229-1238.

Malvar, L.J., Cline, G.D., Burke, D.F., Rollings, R., Sherman, T.W. and Greene, J.L., 2002. Alkali-Silica Reaction Mitigation: State of the Art and recommendations, ACI Materials Journal, Vol. 99, p.5.

McGowan, J., and Vivian, H. 1952. Studies in cement-aggregate reaction. 20. The correlation between crack development and expansion of mortar.

Morenon., P., Multon, S., Sellie, A., Grimal., E., Hamon., F., Bourdarot, E., 2017. Impact of stresses and restraints on ASR expansion, Construction and Building Materials, 140: 58-74.

Multo, S and Sellier, A, 2016. Multi-scale analysis of alkali–silica reaction (ASR): Impact of alkali leaching on scale effects affecting expansion tests, 2016; 81: 122–133.

Multo, S and Sellier, A, 2016a. Multi-scale analysis of alkali–silica reaction (ASR): Impact of alkali leaching on scale effects affecting expansion tests,; 81: 122–133.

Pan, J.W, Feng, Y.T., Wang, J.T.,Sun, W.C., Zhang, C.H., Owen, D.J.R., 2012. Modeling of alkali-silica reaction in concrete: a review, Front. Struct. Civ. Eng 6(1): 1–18.

Poole, A.B., 1992, Introduction to alkali–aggregate reaction in concrete, in: R.N. Swamy (Ed.), The Alkali Silica Reaction in Concrete, Van Nostrand Reinhold, New York.

Powers, T., and Steinour, H. 1955. An interpretation of some published researches on the alkali-aggregate reaction Part 1-The chemical reactions and mechanism of expansion, pp. 497-516.

Rajabipour, F., Giannini, E., Dunant, C., Ideker, J.H., Thomas, M.D.A, 2015. Alkali–silica reaction: Current understanding of the reaction mechanisms and the knowledge gaps, Cement and Concrete Research; 76: 130–146.

Rodrigues, F.A., Monteiro, P.J., and Sposito, G. 1999. The alkali-silica reaction: The surface charge density of silica and its effect on expansive pressure. Cement and Concrete Research 29(4): 527-530.

Saouma, V., Perotti, L.,2006. Constitutive Model for Alkali-Aggregate Reactions, ACI MATERIALS JOURNAL; 103: 194-202.

Shehata, M.H. and Thomas M.D.A. 2000. The effect of fly ash composition on the expansion of concrete due to alkali silica reaction, cement and concrete research, Vol. 30, pp. 1063-1072.

Stanton, T.E, 1940. Expansion of concrete through reaction between cement and aggregate, Proc. Am. Soc. Civ. Eng. 66 (10) 1781–1811.

Wenk, H.R., and Monteiro, M.J., 2008. Relationship between aggregate microstructure and mortar expansion. A case study of deformed granitic rocks from the Santa Rosa mylonite zone, J Mater Sci; 43:1278–1285.