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Materials Today: Proceedings 17 (2019) 717–726

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RAMM 2018

Simulation of Alkali-Silica Reaction Model in a Concrete Gravity Dam at the Macroscale and Mesoscale

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Abstract

Alkali-silica reaction causes major problems in concrete structures due to the rapidity of its deformation. Factors that affect ASR include the alkali and silica content, relative humidity, temperature and porosity of the concrete, making the relationship a complex phenomenon to be understood. In investigating the mechanical deformation of the structure, the theory of continuum damage mechanics proves to be a suitable method. Damage mechanics can be used to predict the physical and chemical behavior of a structure, making it an appropriate method to study the behavior of the structure under the influence of alkali-silica reactivity. Therefore solution of the damage model is critically needed to overcome the concrete deformation problem. In this research, an engineering example of a thermo-chemo-hygro-mechanical model of a concrete gravity dam at the macroscale and coupled with the mesoscale will be studied for varying environmental conditions of temperature and relative humidity. The simulation was developed using the stochastic finite element software. Investigations found that temperature, as well as relative humidity influences the latency and characteristic time constants, which dictate the rapidity of ASR expansion into the structure, rendering heterogeneous values across the cross-section of the structure according to the relative humidity and temperature distribution.

Keywords: Alkali-silica reaction; diffusion; concrete; deformation.

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1. Introduction

Concrete has been the building block of construction for centuries, dating back to ancient civilizations like the Roman Empire. However, problems with concrete may arise not only from design errors like insufficient materials used in the construction, but also from the effects of environmental conditions like freezing and thawing, carbonation and alkali-silica reaction. Damage to concrete due to alkali-silica reaction, or ASR is a phenomenon that was first recognized in the United States of America in the 1940s by Stanton and has since been observed in many other countries. Since then, many studies on that matter have been published [5].

Factors that affect ASR vary greatly although it is unanimous that ASR occurs between deleterious silica from aggregates and hydroxide ions in the pore solution that result from cement hydration. Other factors include the relative humidity, temperature and porosity of the cementitious matrix. Temperature influences the reaction kinetics of silica disintegration and causes thermal stresses in the structure. Moisture provides a transport medium for external sources of alkali and works as a swelling agent for the gel which is hydrophilic in nature. The resultant gel flows into the voids or accumulates on the aggregate surface. The gel expands with the availability of moisture, thus exerting internal pressure onto the surrounding matrix and lowering the concrete stiffness, in extreme cases to the point ofcracking.

ASR deformation can be identified by a random network of crack patterns on its surface known as map cracking, leaching of the ASR gel and concrete spalling. ASR expansion in an affected concrete structure may happen rapidly and cause deformation to the structure well before its serviceability limit is reached, making the understanding of its process crucial. What sets apart ASR from other concrete damage models is its heterogeneity, occurring at different concrete regions at different rates depending on the concrete composition as well as external influences, making predicting its behaviour somewhat difficult. The heterogeneity of the process depends on the pore distribution in the concrete and the rate of water diffusion into the reactive sites. The rate of ASR expansion in turn depends on temperature and the availability of chemical substances from within the matrix or from external sources [3].

Despite the fact that ASR initializes in the mesoscopic regions of the concrete, the accumulative effects of its expansion escalates onto the macroscale level with the development of web cracking on the concrete surface. Once the extent of damage that ASR brings onto the concrete structure on the macroscale has been determined, the mesoscale model is then studied to gain a more explicit insight on what happens at the material level. Macroscopic material models are characterized by considering the heterogeneities and structural defects in an averaged sense and are therefore regarded as a homogeneous material. Modeling on the mesoscale level however, allows the matrix adjacent to the aggregate surface to be developed. This allows us to study the different phases separately, for instance, the effects of ASR gel expansion on the aggregates as well as the bulk matrix due to the difference in material and physical parameters of the different phases [1].

In investigating the mechanical deformation of the structure, the theory of continuum damage mechanics proves to be a suitable method. Damage mechanics can be used to predict the physical and chemical behavior of a structure, making it an appropriate method to study the behavior of the structure under the influence of alkali- silica reactivity. Therefore solution of the damage model, as well as simulation of the ASR phenomenon at both the macroscale and mesoscale level in order to provide better understanding, or even solving the problem is critically needed. Numerical simulation has enabled us to build models for the representation of different physical phenomena based on different theories and approximately solvable by the finite element methods in numerous occasions. The potential of ASR simulation in detecting the possibility of concrete expansion and cracking at a fine scale gives new perspective to this deleterious phenomenon. With a reliable finite element simulation, the generation of expansive pressures and damage propagation due to ASR is possible [2].

2. Alkali-Silica Reactivity

ASR expansion in an affected concrete structure may happen rapidly and cause deformation to the structure well before its serviceability limit is reached, hence understanding the process is crucial (Fig. 1). ASR deformation can be identified by a random network of crack patterns on its surface known as map cracking, leaching of the ASR gel and concrete spalling. The ASR process occurs when hydroxide ions in the pore solution interact with silica from the aggregates. Hydroxide ions, being alkaline in nature attack the reactive silica sites at the aggregate surface, producing a hydrophilic gel. This gel accumulates at the reaction sites and fills into adjacent voids, replacing the silica it consumed in producing the gel. When moisture diffuses into the affected concrete, this gel expands and migrates into the connecting porous medium resulting in an internal buildup of tensile stresses in the matrix. This will eventually lower the concrete stiffness. The amount of pressure exerted by the ASR gel expansion varies depending on a number of factors which include the relative humidity, temperature, the type and proportions of reacting materials and gel composition. This work briefs on the ASR mechanisms and factors affecting its reactivity. The most known literatures on ASR are from Dent-Glasser and Kataoka [6], Diamond [7], Swamy [8] and Larive [9], which are all referred to in this thesis. Then, the fundamental equations for ASR modeling are outlined. Previous works for ASR simulation can be found from the works of Capra [10], Ulm [11], Bazant [12], Bangert [13] and Fairbairn [14].

Fig. 1. Map cracking due to ASR deterioration on a concrete wall [2]

2.1. Factors Influencing ASR

2.1.1 Alkali Content

A major contributor of alkali in concrete is the Portland cement. Cement hydration produces metal alkali sodium, potassium and calcium hydroxides in the pore solution, which concentrations depend on the type and alkalinity of the Portland cement used. Additional sources of alkali can also be released by aggregates that naturally contain alkali. Swamy [8] explained that high alkali cements could produce a pH that range from 13.5 to 13.9, while low alkali cements produce a pH ranging from 12.7 to 13.1. Previous researches on ASR, for instance by Stanton [5] have discovered that the ASR process is only initiated if the alkali concentration in concrete is at a certain threshold value. He concluded from mortar bar tests conducted with cement content of over 600 kg/m^3 that expansion due to ASR does not occur when the cement acid soluble alkali content is less than 0.60% by mass, a threshold that is also recommended.

2.1.2 Silica Content

The alkali-silica reactivity depends on the stability of existing silica in the aggregates. Hobbs [15] explained that under normal circumstances, stable silica has an ordered arrangement of silicon oxygen tetrahedra making it more resistant to alkali attack while reactive silica has a random network of tetrahedra with voids between the groups of molecules making it susceptible to reaction. Minerals that are known for its reactive potency include silica minerals, opal, chalcedony and quartz, among others.

2.1.3 Relative Humidity

Water has dual role in the ASR process; firstly as a carrier of the alkali cations and hydroxyl ions and secondly, as a swelling agent for the ASR gel. Since all influencing constituents are still available in the initial state, ASR reaction rate is the highest at this point. The resultant gel is hydrophilic in nature; hence it absorbs water and increases in volume which is what causes the gel to have its expansive characteristic. It was suggested by Grattan-Bellew [16] that the optimum water/cement ratio for expansion of mortar bars containing alkali-reactive aggregates to be in the range of 0.4 to 0.6, depending on the physical and chemical properties of the aggregates. Experiments have also shown that a relative humidity of above 80% has a significant expansion effect due to ASR.

2.1.4 External Sources of Reactants

The ASR process needs both alkali and hydroxide ions in order to react. However, the initial contents of the constituents are rarely enough to promote major expansions before either constituent depletes. Therefore, ASR also depends on alkali obtained from other sources like mineral additions, mixing water and in cold climates, from deicing solutions. The Hawkin's Report (1999) suggested that if the external sources of alkali exceed 0.2 kg/m^3 of the concrete, it should be taken into account when calculating the total reactive alkali available. The age of the concrete during the time of introduction of the external sources of reactants also has an effect on the ASR process. Hobbs [15] presented an example that exhibits this effect.

2.1.5 Concrete Permeability and Porosity

Porosity and permeability control the movement and storage of fluid and air in concrete. Although the material packing, shape and sorting influence porosity and permeability, they both have different definitions. Porosity is the ratio of the volume of voids in the concrete to the total volume of the concrete itself. Permeability is a measurement of the ease with which a liquid or gas is able to travel through a porous solid material. Hence permeability of concrete also depends on the porosity. Although the concrete may be highly porous, if the voids are not interconnected, then the pore fluid is not free to flow, making the concrete impermeable. Permeability is often directional in nature. Pores can be filled with pore solution or entrained air. The availability of air voids enables the gel to migrate through undamaged concrete to fill air voids, hence reduce the risk of cracking. Porosity and permeability of the concrete also influences the absorption of alkali from external sources.

2.1.6 Temperature

Temperature influences the rate of water absorption by the ASR gel. Diamond, Barneyback Jr. and Struble [7] reported that ASR reaction and expansion rates are initiated early and develop rapidly when subjected to high temperature. However, as the reaction continues both reaction and expansion rates slow. When subjected to lower temperature, the reaction and expansion rates are slower in the initial state and continue until it reaches the same level of expansion as for the higher temperature. Hobbs [15] explained that this effect might be due to the migratory characteristics of the ASR gel for lower temperature having slower development rates, having more time to disperse into the porous medium without exerting pressure. On the other hand, gel at higher temperature is produced and dispersed throughout the porous medium rapidly and exerts pressure to the surrounding matrix. However, at a lower temperature the expansion exceeds the expansion attained at higher temperature. Hobbs [15] suggested that the gel reaches its maximum swelling pressure at a certain stage and at lower temperature, the period at which the gel exerts its maximum pressure is prolonged, causing higher expansions.

3. Macroscale Simulation of a Concrete Gravity Dam

Various experimental evidences for ASR deterioration can be found from literature, for example by Saouma and Perotti [17], and Comi [18]. Comi developed a chemo-thermo-damage model of a gravity dam that evaluates the local evolution of ASR swelling governed only by temperature, resulting in a damage model that is fully decoupled from the heat-diffusion problem. Saouma and Perotti worked on temperature and hydrostatic loading on a dam and its effects on the ASR process. Mostagh and Ghaemain [19] did an analysis of the Beauhrnois power plant gravity dam on how ASR reaction has a high dependency on stress, resulting in the vertical strains being smaller than the horizontal strains. Fairbairn [14] simulated the stress anisotropy of ASR swelling due to thermal and moisture dependency.

The numerical example presented here illustrates the performance of a two- dimensional decoupled thermo-chemo-hygro-mechanical model of a concrete gravity dam that evaluates the evolution of ASR resulting in a damage model for alkali-silica reactivity (Fig.2). The numerical simulation of stress anisotropy due to the ASR phenomena is performed by taking into consideration the thermoactivation of alkali-silica reactivity and its dependency on relative humidity. Considering the fact that damage caused by ASR is due to expansion, behaviour of the concrete gravity dam under compressive stress can be modeled as linear. Since the ultimate compressive strength value is not exceeded, damage due to compression is assumed negligible. Creep and shrinkage will not be considered in this simulation. The simulation was developed using the stochastic finite element software SLANG. The Newton-Raphson iterative method was adapted for this model.

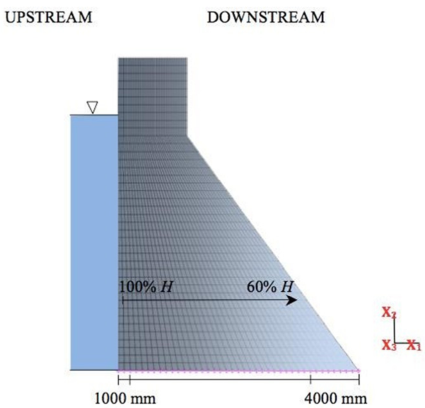


Fig. 2. Shaded zones depicting different relative humidity conditions ranging from 100% to 60%

Relative humidity influences the latency and characteristic time constants, which will in turn influence the ASR reaction rate. In this section, the effect of relative humidity will be presented for decreasing values of relative humidity values throughout the domain. Fig. 3 shows the concrete gravity dam with shaded zones reflecting the different values of relative humidity. Starting from the boundary which is exposed to water, the relative humidity of the region is set to 100% to represent submerged humidity conditions. The relative humidity gradually decreases to 60% moving towards to downstream, which is the minimum threshold value of humidity needed for ASR to initiate. The different zone sizes were calculated from the equation for moisture diffusion length, giving the moisture diffusion length in the 100% *H* zone as 1000 mm and the moisture diffusion length in the 60% *H* zone as 4000 mm.

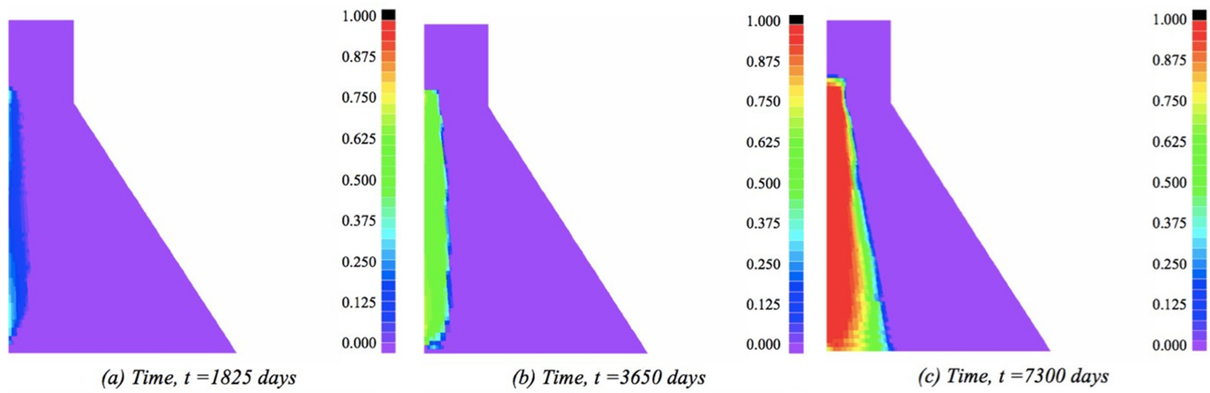


Fig. 3. Damage variable due to ASR and hydrostatic pressure for a constant temperature of 20°C and relative humidity ranging from 60% to 100%

It can be seen that the damage contours for the varying relative humidity is more localized to regions of higher relative humidity. Damage initiates at the zone where relative humidity is 100%, at the upstream region and continues inwards. There is no damage at the regions with the low relative humidity of 60%. However, as for the case of constant relative humidity, under these conditions, ASR reaction takes longer to occur and start causing damage to a structure.

Damage for the constant conditions start at approximately 3600 days while damage for the varying relative humidity start at approximately 1800 days, which is twice the time for the constant conditions case. However, after 7300 days damage in the constant conditions case is smeared throughout the dam while damage in the varying relative humidity case is localized at the higher moisture regions.

4. Mesoscale Simulation

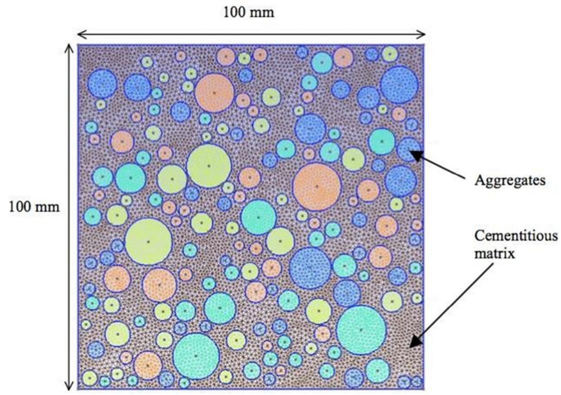


Fig. 4. Finite element model of the two-dimensional three-noded plane elements mesoscale model of a 100 mm x 100 mm concrete prism

Material models at the mesoscopic level help to gain insight into the origin and nature of concrete behavior. Previous works on ASR model concrete as a two-phase material which includes the homogenized skeleton with interstitial pores as a phase and the ASR gel as another. The model presented in this section is performed at the mesoscale where the model consists of two phases, the aggregates as one phase and the homogenized skeleton with interstitial pores as the other (Fig.4). Although the problems are not examined in full engineering detail, nor is the porosity of the matrix explicitly simulated, the model is sufficient to demonstrate the workability of the algorithm applied in this research. This has been proven feasible by a series of validation tests conducted with benchmark examples in the following section.

This section will touch on the fundamentals of mesoscale numerical simulation procedure for concrete, which is the take-and-place method, as well as the general ASR testing methods, and then extended to the ASR testing methods by the Finger-Institut Baustoffkunde. Results from the ASR testing will be numerically simulated and a comparison will be made. This is followed by a mesoscale model of ASR deformation for heterogeneous prism in order to study the effects of ASR on concrete at the mesoscale. Assume a two-dimensional mesoscale model of a concrete prism used for FIB testing measuring 100 mm x 100 mm. The mesoscale model is made up of a two-phased heterogeneous material consisting of aggregates as a phase and the cementitious matrix with interstitial pores as another phase.

Fig. 5 to 7 show the damage distributions for 80%, 100% and 60% relative humidity for the mesoscale model. It can be seen that although models with different relative humidity values have similar damage patterns, the time scale is longer for the lower relative humidity. Damage initiates at approximately 70 days for 100% relative humidity and 400 days for 80% relative humidity. For 60% relative humidity, which is the minimum condition for relative humidity required for ASR to initiate, it can be concluded that damage due to ASR expansion did not happen [1]. Damage initiation occurs at the interfacial zones in between matrix and aggregates due to ASR expansion and spreads throughout the whole matrix, which has lower stiffness than the aggregates. Since aggregates have larger stiffness values than the matrix, eventhough with a higher stress in the aggregates, the lower tensile strength value for the cementitious matrix causes the damage to initiate in the matrix. Damage in the aggregates initiates at a later time, afterthe tensile strength value for aggregates have been surpassed, which are approximately 1000 days for the 80% and 100% relative humidity, and no damage was seen in the aggregates with the 60% relative humidity [4].

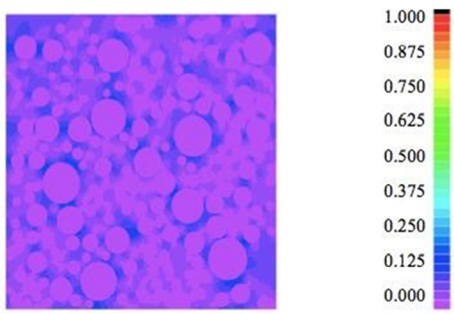
(a) Time =500 days

(b) Time =525 days

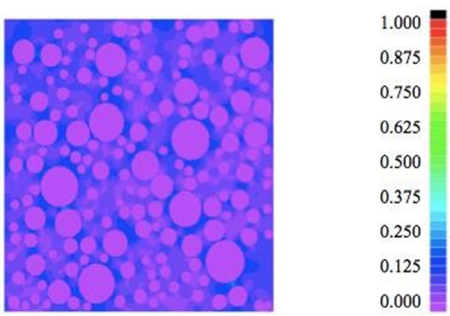
(c) Time =540 days

(d) Time =560 days

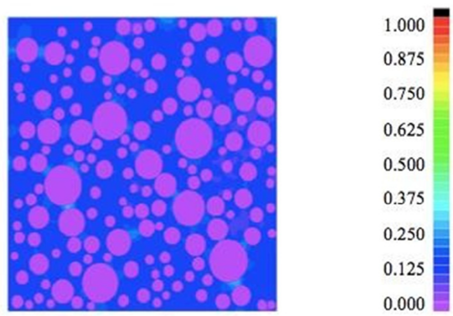
(e) Time =580 days



(f) Time =600 days



(g) Time =620 days



(h) Time =650 days

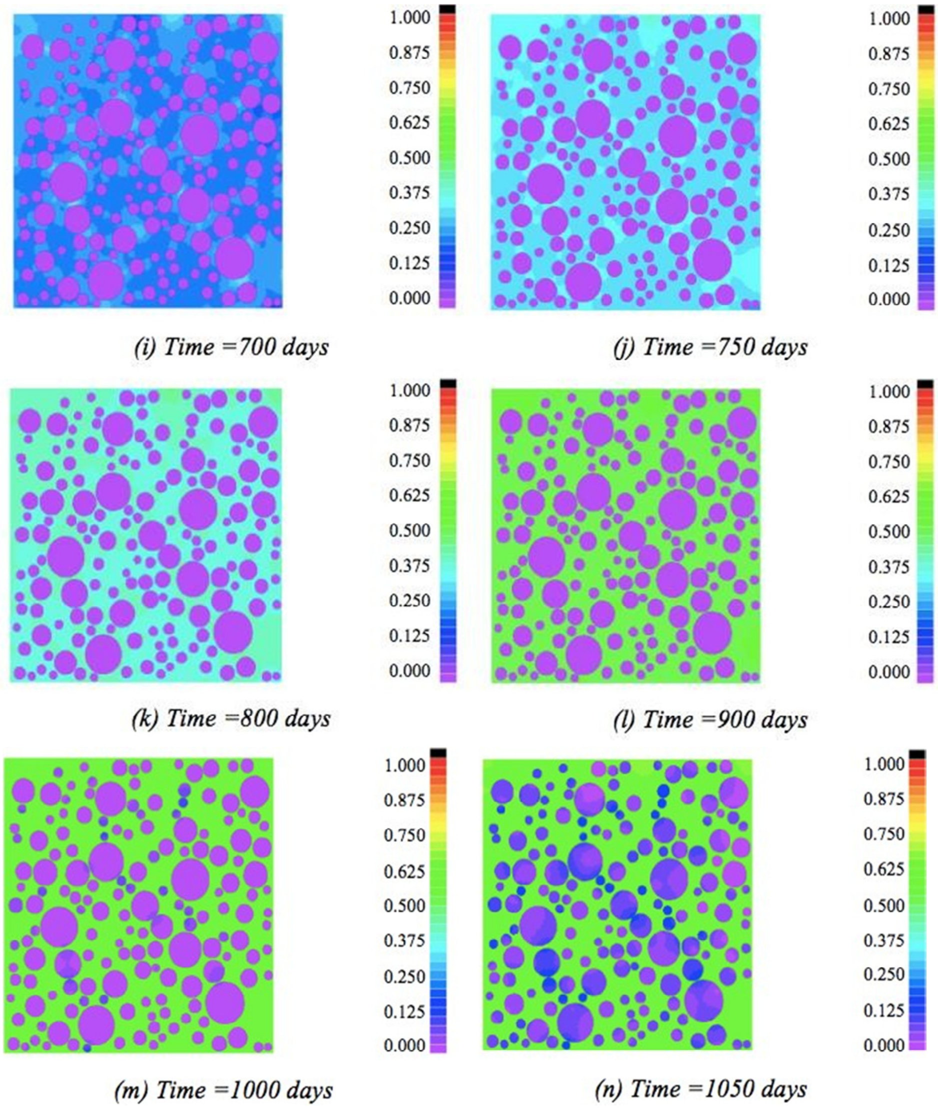


Fig. 5. Damage due to ASR expansion for an isothermal condition of 45°C and relative humidity of 80% for a mesoscale model with heterogeneous material properties [1]

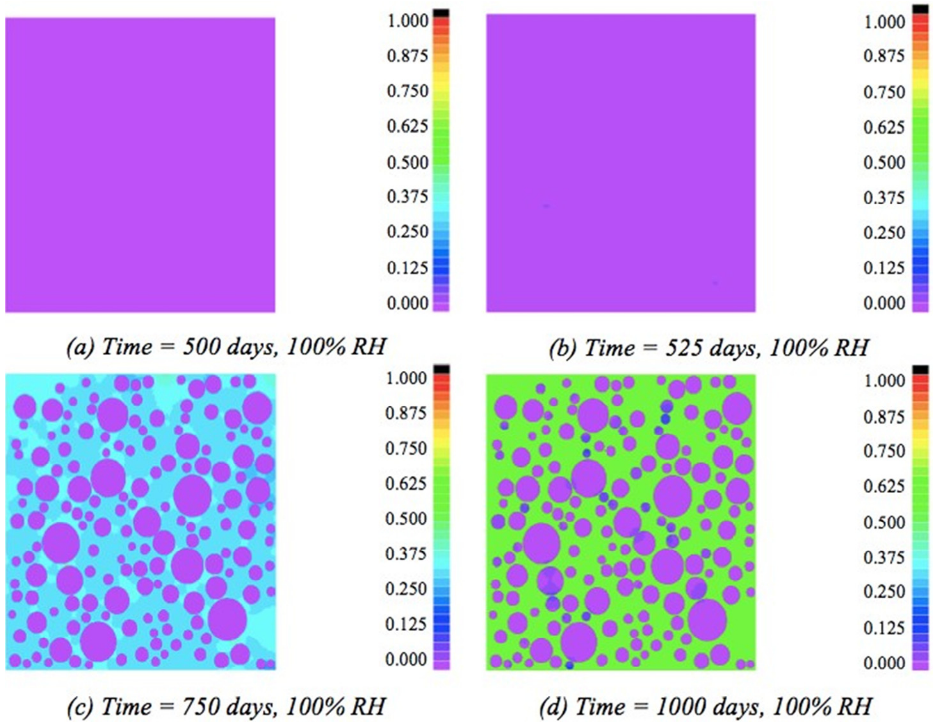


Fig. 6. Damage due to ASR expansion for an isothermal condition of 45°C and relative humidity of 100% for a mesoscale model with heterogeneous material properties [4]

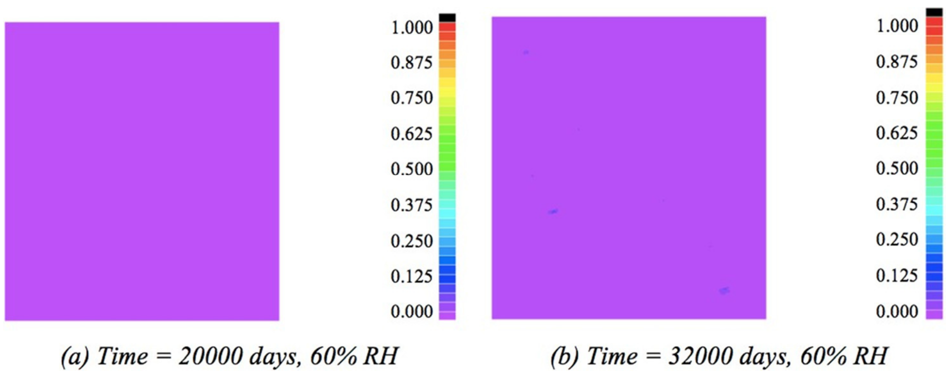


Fig. 7. Damage due to ASR expansion for an isothermal condition of 45°C and relative humidity of 60% Relative Humidity (RH)for a mesoscale model with heterogeneous material properties [3]

5. Conclusion

The engineering study of a macroscale concrete gravity dam incorporated with the effects of temperature, relative humidity and mechanical loading cases as isolated and combined cases in this work shows that individually, temperature, relative humidity and mechanical loading influence ASR expansivity and causes its own affects to the expansion or contraction of the structure. ASR has an increased effect due to moisture content. A higher relative humidity increases the characteristic and latency time constants, which means that a shorter time is needed before damage initiates.

The mesoscale model in this research was developed to have heterogeneous material properties for aggregates and the cementitious matrix. In order to study the sole effect of ASR chemoelasticity, any mechanical loading has been omitted. It has been found that damage initiates at the interfacial transition zones between the aggregates and the matrix and spreads within the matrix which has lower stiffness. Damage in the aggregates, which have higher stiffness and tensile strength, occurs at a much later time than for the cementitious matrix which has a lower tensile strength.

Therefore, it can be concluded that the intensity of damage in a concrete structure due to ASR expansion, be it on the mesoscale or macroscale, depends on a lot of factors, most importantly the temperature and relative humidity. Other external factors that play an influence on the damage orientation and structure deflection depend on material properties, boundary conditions and if applicable, external loading.

Acknowledgements

The authors would like to extend their acknowledgement to Universiti Tenaga Nasional especially to Innovation & Research Management Centre (iRMC) for funding the publication. Acknowledgements are also extended to Bauhaus-Universitaet Weimar, Germany for their great contribution and assistance to this work.

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