Numerical calculation of expansion induced by alkali silica reaction

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HIGHLIGHTS

- A model to predict alkali silica reaction (ASR) induced expansion was developed.
- The model took into account the influences of different factors on ASR expansion.
- Volume of gel was calculated in the model by using solid state reaction theory.
- Validation of the model shows that the model can predict ASR expansion very well.

ARTICLE INFO

ABSTRACT

This paper proposed a model to predict alkali silica reaction (ASR) induced expansion. The model can estimate the influential factors on ASR expansion, such as the aggregate sizes, mechanical properties of composite materials, and initial alkali concentration. Chemical reactions were described by solid state reaction theory. Concrete was considered to include aggregates, crack region and uncracked region. Alkali silica gel was considered to be the main reason of expansion, and the gel volume was calculated according to the alkali-silica reactions. The model was validated by an experiment of ASR-affected concrete specimens containing glass aggregate. The comparison of calculation results with experimental results showed good applicability of the model.

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1. Introduction

Alkali silica reaction (ASR) is one of the most important topics about concrete durability. Alkalis contained in the cement, mineral admixtures, and superplasticizers, releases into the pore solution and reacts with the reactive component of aggregate. The generated alkali silica gel causes a high expansive pressure in the presence of water. As a result, cracks occurs, providing intrusion paths for other aggressive agents into concrete.

ASR is a complicated phenomenon involving both chemical and mechanical process. Modeling of ASR has been widely investigated, such as UFO model [1,2], Sellier/Poyset model [3,4], Suwito/Xi model [5,6], and Bažant model [7]. In these models, the macro expansion processes and the degradation of concrete mechanical properties were simplified, while the chemical ions diffusion processes and the generated gel diffusion within matrix, aggregate were emphasized. These models can be described as chemical model. In these models, a relative elementary volume (REV) was studied, and the ASR processes were described mainly by mathematical methods. For example, UFO model was proposed by Uomoto, Furusawa in 1992. The method adopted in this model was wildly used in other models for ASR expansion. In this model, alkali ion diffusion, which is the key problem for ASR, is described by Fick's law. ASR chemical reactions are assumed to take place in transition zone between aggregates and mortar matrix and the generated products deposited surrounded the aggregate. The expansion process was considered to be controlled by diffusion process.

This paper aims to propose a calculation method to predict the expansion induced by ASR, in which both the chemical process and mechanical process were considered. The amount of generated alkali silica gel and cracks within mortar matrix were the key parameters influencing the ultimate expansion obviously. The relationship between the amount of generated gel and consumption of alkali was determined based on solid state reaction theory. The generated cracks were considered by separating concrete into cracked zone and uncracked zone. Geometry of the composite structure and chemical assumptions were presented firstly. The amount of generated gel was calculated according to alkali consumption. The strain caused by ASR generated gel was used as parameter to calculate ultimate ASR induced expansion.

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The calculated results were compared with experimental data to validate the applicability of the model.

2. Modeling of ASR

2.1. Mechanism and geometry of ASR

Alkali silica reaction always take place at the interface of reactive aggregate and the generated gel deposits within the surrounding pores. Expansion stress is caused and induces deformation of mortar matrix. When the tangential stress is larger than the tensile stress of mortar matrix, cracks generates in the mortar. Actually, this problem is quite similar with the rebar corrosion of reinforcement concrete. Suwito [8] studied reinforcement corrosion within concrete in plane strain condition. The corrosion product volume is larger than the consumed rebar volume. Expansion stress was generated within the interface of rebar and concrete, and finally caused concrete cracking. In his model, the composite structure was composed of rebar, crack zone, and uncrack zone. Within the crack zone, fracture mechanics was used to model the cracks propagation, while within uncrack zone, the concrete can be seen as elastic materials and thus can be described by elastic theory.

Since the ASR problem is quite similar with the rebar corrosion situation, the idea of dealing with corrosion expansion in reinforcement concrete is adopted to model the ASR expansion and cracking. As seen in Fig. 1, a relative elementary volume (REV) contained reactive aggregate was selected and assumed to be spherical. The REV was composed of reactive aggregate, cracking zone and uncracking mortar. An interface pressure P_1 would firstly generated at the interface of aggregate and cracking zone, and then a pressure P_2 generated at the interface of cracking zone and uncracking zone, and finally caused the expansion of REV.

According to the existing ASR mechanisms, the chemistry of ASR and the details of the reaction processes are still not completely understood. However, three basic aspects are contained in ASR expansion processes. They are the diffusion of the water and chemical ions into reactive aggregate, and induced the dissolution of silicon-oxide tetrahedron. Then the chemical reaction takes place and alkali silica gel is formed causing expansion stresses. Obviously, it is difficult to consider all procedures of ASR in modeling. Simplified assumptions should be proposed as:

- The effect of sodium ions is similar as potassium ions in ASR, and the diffusion of sodium ions and water into reactive aggregate will induce the dissolution of Si–O bond. (The research of Cong demonstrated that the effect of sodium ions is quite similar as potassium ions in ASR processes, except that some differences on reaction rate).
- The generated gel will first deposit surrounding reactive aggregate, and then induce pressure at the interface between aggregate and mortar.
- The diffusion is the controlling process of ASR expansion, which means that the ASR expansion mainly depends on the diffusion of chemical ions into reactive aggregate.

2.2. The calculation of alkali silica gel volume

ASR processes contained diffusion of chemical ions, the chemical reaction between chemical ions and solid reactive aggregate. In accelerated curing conditions, the alkali concentration within mortar pores becomes saturation, i.e. equilibrium state, in short time. If we assumed aggregate particles to be spherical, the reactant and product layer can be seen as uniform spherical shell. Besides, the alkali ions distributed uniformly around the reactive aggregate, and react with reactive substances within aggregate quickly, since the high concentration of alkali ions. Within this process, the reaction rate is larger than the diffusion rate of alkali ions into reactive aggregate, which assures the prompt reaction between alkali and reactive aggregate and the generation of product gel.

Considering the system showed in Fig. 2, after a curing time t, some reactive aggregate was consumed by ASR and converted to alkali silica gel. Then, the conversion rate of reactive aggregate can be described as,

$$G = \frac{R_a^3 - (R_a - x)^3}{R_a^3} = 1 - \left(1 - \frac{x}{R_a}\right)^3 \tag{1}$$

Because of the volume difference of reactant and product, Carter estimated the conversion degree of solid state reaction as

$$f(G) = [1 + (\eta - 1)G]^{2/3} + (\eta - 1)(1 - G)^{2/3}$$
$$= \eta + 2(1 - \eta)\frac{2DuC_0}{R_0^2 \rho n} \cdot t \tag{2}$$

In which, G represents conversion degree of the reaction, D represents the diffusion coefficient of alkali ions, C_0 represents initial concentration of alkali ions, R_a represents the initial radius of aggregate, t represents curing time, η represents the volume ratio of product and reactant, n represents the number of alkali molecules within product gel, μ and ρ represent the molecular weight and density of product gel, respectively. If all parameters
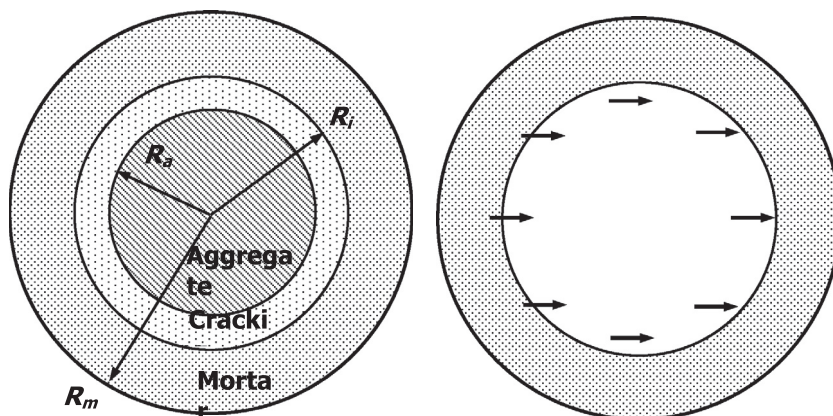

Fig. 1. Schematic of ASR calculation.