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## X-ray CT characterization and fracture simulation of ASR damage of glass particles in alkaline solution and mortar

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#### A B S T R A C T

The alkali-silica reaction (ASR) damage in reactive aggregates affects the long-term durability of the concrete infrastructure. The generated ASR gel can expand by imbibing water from the pore solution and the resulting expansion pressure causes the aggregate fracture. This study aims to simulate the development of ASR damage in glass particles of two types of samples (glass in alkali solution and glass mortars). The dynamic micro X-ray CT technique was conducted to monitor the crack propagation in glass aggregates at different reaction stages (up to 64 h). The Boundary Element Method (BEM) and Displacement Discontinuity Method (DDM) were used to efficiently simulate the crack propagation within irregular glass particles under gel expansion pressures. The aggregate boundaries were built with the BEM elements and the initial cracks were meshed with the DDM elements. The estimated expansion pressure was applied to the initial crack surfaces. The discontinuous displacements and stresses were calculated along the crack path and crack tip. The mixed-mode Stress Intensity Factors (SIFs) were calculated based on plane stress conditions. The maximum circumferential stress criteria were used to simulate the propagation of cracks along a specific angle. The simulation results include the simulated crack path and the combined SIFs changing with the increments. With the estimate expansion pressure, the glass particle damages were simulated within conditions of alkali solution and confined mortar samples. The predicted crack propagation path was compared with the X-ray CT imaging data. The comparison results demonstrate the DDM has the ability to predicting the ASR damage propagation inside aggregates.

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#### 1. Introduction

The alkali silica reaction is a serious durability issue in concrete infrastructure [\[1\]](#page--1-0). The ASR gel generated from the reaction between active aggregate and alkaline concrete pore solution can expand significantly in moist conditions [\[2\]](#page--1-0) and crack the surrounding aggregate and cement paste [\[3\]](#page--1-0). It is important to characterize the crack caused by ASR damage for the understanding of its development mechanism [\[4\]](#page--1-0) and the corresponding damage mitigation.

The non-destructive micro X-ray computed tomography  $(\mu\text{CT})$ tests can monitor the in-situ dynamic microstructure revolution and crack development [\[5,6\]](#page--1-0). This technique has been also applied to study the ASR damage in concrete  $[7]$ . Marinoni et al.  $[8]$ immersed the prepared mortar samples in 1 M NaOH solution for 14 days and then analyzed the sample with the  $\mu$ CT technique.

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The development of microcracks caused by ASR damage was tracked with the built 3D mortar structure. Marinoni et al. [\[9\]](#page--1-0) applied  $\mu$ CT to investigate the mortar samples with reactive chert aggregate. The dissolution of quartz was observed when ASR dam-age took place. Hernandez-Cruz et al. [\[10\]](#page--1-0) studied the ASR in fiber reinforced mortar samples with the µCT method. Through 136 days of scanning, the dissolution of aggregate, the propagation and the gel swelling in crack were observed. The fiber reinforcement effect of ASR was also determined.

The observed crack propagation process in cement caused by ASR can be further analyzed with the fracture mechanic model. The current study mainly employed the Finite Element Method (FEM) for the crack simulation. Bazant et al.  $[11]$  built a micro fracture mechanical model to evaluate the size effect of the glass aggregate in concrete. Both of the size effects on the surface area-based chemical reaction rate and the expansion potential were considered in the model. Charpin and Ehrlacher [\[12\]](#page--1-0) investigated a ring-shaped fracture induced by the ASR gel swelling inside cement paste. The incremental energy criterion was used to build the fracture simulation model. The size effect of the active

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aggregates was also observed through the finite element analysis. Reinhardt and Mielich [\[13\]](#page--1-0) studied the crack propagation in aggregate caused by ASR gel pressure. The critical stress intensity factors (SIFs) were calculated at different reaction times.

Besides the application of FEM, the fracture mechanics simulation has been conducted with the Discrete Numerical Method (DEM) [\[14,15\],](#page--1-0) Discontinuous Deformation Analysis (DDA) [\[16\],](#page--1-0) Numerical Manifold Method (NMM) [\[17\],](#page--1-0) Peridynamic (PD) Method [\[18,19\]](#page--1-0), General Particle Dynamics (GPD) Method [\[20\]](#page--1-0) the Boundary Element Method (BEM) [\[21–24\]](#page--1-0) and etc. Among them, Cundall and Strack [\[14\]](#page--1-0) built the DEM to describe the mechanical performance of the system in terms of discs and spheres, which is based on the explicit numerical scheme. The DEM method was validated by comparing the force vector plots obtained from DEM simulation with the photoelastic analysis results. Shi and Coodman [\[16\]](#page--1-0) developed the forward numerical model DDA to analyze the rock block systems. The sliding and detachment between the blocks can be obtained, and particularly, the constraints of no inter-particle tension and penetration were considered in the simulation process. Shi [\[17\]](#page--1-0) built the NNM based on the displacement equations at different material domains, which aimed to investigate the material response to external and internal loadings. The FEM and DDA can be considered as the special cases of NNM. Silling et al. [\[18,19\]](#page--1-0) established the PD to describe the discontinuities of materials generated under external deformation. The stress wave propagation based on the PD theory was analyzed and the relationship between the material stability and wave dispersion was investigated. The PD theory [\[18\]](#page--1-0) was further generalized by considering that material response at one point collectively depends on all bonds connected to that point. The volume change and shear angle of materials under external loadings can then be obtained with the bond-based PD theory. Zhou and Shou [\[25\]](#page--1-0) further applied the bond-based PD theory to analyze the crack initiation and propagation inside the rock materials. The simulation outcome was found in accordance with the exper-imental results. Wang et al. [\[26\]](#page--1-0) further developed the nonordinary state-based PD (NOSB-PD) theory to investigate the crack growth and coalescence in the rock materials with pre-existing flaws. The effect of flaw length, ligament angle and confining stress on crack propagation was analyzed with the built NOSB-PD model. Zhou et al. [\[20\]](#page--1-0) proposed the GPD method to study crack development in heterogeneous rock material containing initial damage under uniaxial compressive loadings. The tensile, compressive, shear and mixed type coalescence modes can be observed from the simulation results. Among these methods, the simulation with the BEM [\[27\]](#page--1-0) theory only needs to mesh the boundaries of the studying area as boundary elements, which is particularly suitable for the analysis of random-shape-particles. Mi and Aliabadi [\[21\]](#page--1-0) built the numerical approach for three-dimensional fracture mechanics problems. Particularly, the discontinuous quadrilateral quadratic elements were applied to model the crack. The model was verified by analyzing the fracture problems within boundaries and embedded cracks. Aliabadi [\[23\]](#page--1-0) further developed dual boundary element methods to solve the crack propagation problem. Both the displacement and traction integral equation were used in this method and the method can solve the problem under the mixedmode crack. Lewandowski and Rozumek [\[28\]](#page--1-0) analyzed the crack propagation in steel specimen under cyclic moment loading with the boundary element methods. The crack propagation was found to be influenced by the existence of weld and heat-affected zones.

Based on the boundary element method, the Displacement Discontinuity Methods (DDM) [\[27\]](#page--1-0) were first proposed by Crouch [\[29\]](#page--1-0) to analyze the fracture mechanics problems. The two coinciding surfaces of crack were considered as finite line segments with constant discontinuity on displacement. Based on that assumption, the relationship between the discontinuous displacement and stress

field along the crack was also built by Crouch [\[29\]](#page--1-0) based on the solution to Kelvin's problem [\[29\]](#page--1-0). Olson [\[30\]](#page--1-0) further built the equation to calculate the stress intensity factor based on the displacement discontinuity. The equation is based on the relationship between the driving stress (the difference between remote stress and crack tip stress) and the SIFs  $[31]$ . By combining the DDM theory built by Crouch [\[29\]](#page--1-0) and the SIFs calculation equation proposed by Olson [\[30\]](#page--1-0), Cooke et al. [\[32–34\]](#page--1-0) developed the FRIC 2D Code for the fracture simulation of rock materials. The FRIC 2D Code was designed based on the plane strain condition. Particularly, the frictional slip and the crack propagation process can be analyzed by defining the frictional interfaces.

This study aims to analyze the ASR damage in glass aggregate through micro fracture mechanics. The micro X-ray CT experiment was first conducted to capture the process of crack propagation inside glass particles. The simulation model was built based on the captured aggregate images and applied to simulate crack propagation with BEM and DDM. Particularly, the aggregate boundary and crack tip was built with BEM elements and DDM elements, respectively. The expansion pressure estimated from gel volumetric strain and the bulk modulus was input on the initial crack surface. The crack starts to propagate when the fracture criterion is satisfied. Then the simulated crack paths were compared with the observed crack path from X-ray CT tests for the validation. This study provides the micro fracture characterization and simulation tools to study ASR damage in aggregates under different reactions or environmental conditions.

#### 2. Fracture simulation with BEM and DDM

#### 2.1. Elastic formulation for displacement discontinuity method for crack

The DDM theory is based on the boundary element method [\[35\]](#page--1-0), which is convenient for the fracture analysis [\[36\].](#page--1-0) When dealing with irregularly shaped objects [\[37\]](#page--1-0), using the boundary elements can save time for model simulation compared to finite elements [\[38\]](#page--1-0). As most aggregates have irregular boundaries [\[39\]](#page--1-0), the DDM is very suitable for simulating aggregate fracture.

Normally, a crack has two coinciding surfaces with a certain separation distance between them  $[40]$ . The DDM  $[29]$  considers the crack as a one-surface element with displacement discontinuity. The demonstration of DDM with a 2a length crack is shown in Fig. 1. The displacement discontinuity is determined by the displacement difference between the upper and lower crack surface as denoted by the surfaces at  $y = 0_+$  and  $y = 0_-$ , respectively. The relationship between displacement discontinuity and displace-





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