Modeling of Chloride Transport in Cracked Concrete: A 3-D Image–based Microstructure Simulation

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Introduction: It is desirable to develop a model predicting the chloride diffusion profile in cracked concrete while considering the real microstructure including cement paste, voids, and aggregates. In this study, a 3-D image-based microstructure [1] simulation procedure was developed to model the chloride ingress in cracked mortar of two microstructures [3]. A micro-X-ray fluorescence (XRF) test was conducted to measure the chloride concentration profile of a mortar sample.

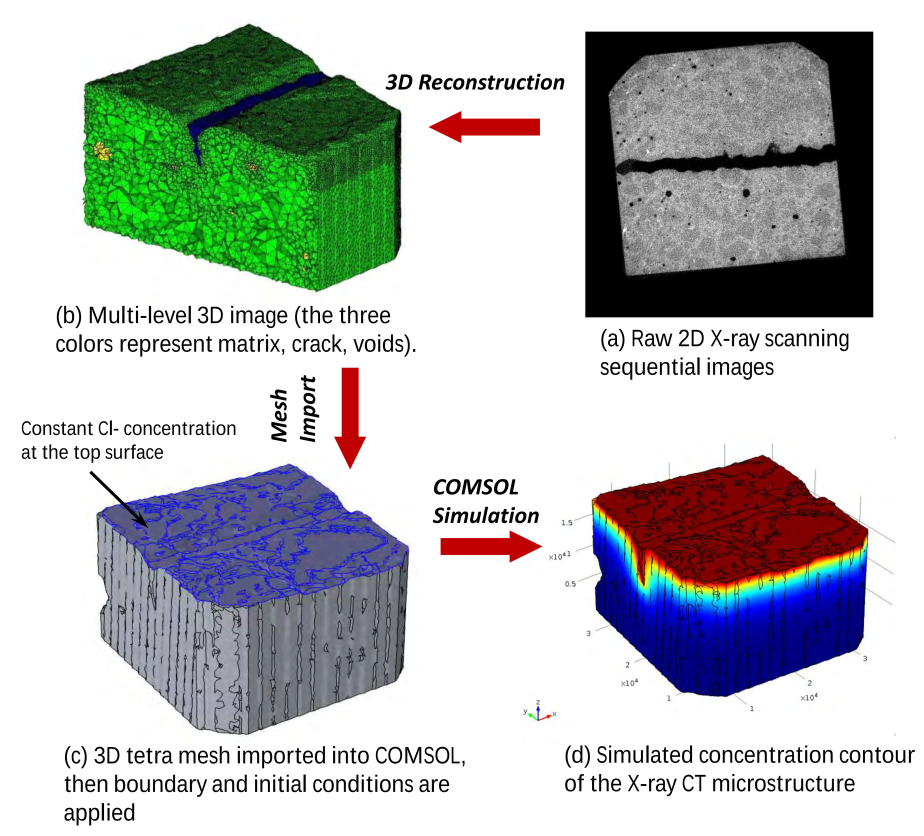


Figure 1. Microstructure #1: Three-dimensional diffusion and binding simulation procedure with an X-ray microtomography image set [3].

Transport and binding model: Chloride binding is significant to the chloride transport process, and can be an important factor in predicting the service life of concrete structures. In these simulations, a simple linear isotherm was utilized to express the relationship between free and bound chlorides: $C_{bound} = \alpha C_{free}$

This binding sorption/reaction is implemented in COMSOL Multiphysics by adding a reaction term to the standard diffusion equation, resulting in:

$$\frac{\partial C}{\partial t} = \nabla \cdot \left(D \nabla C \right) + k(C_{bound} - \alpha C_{free})$$

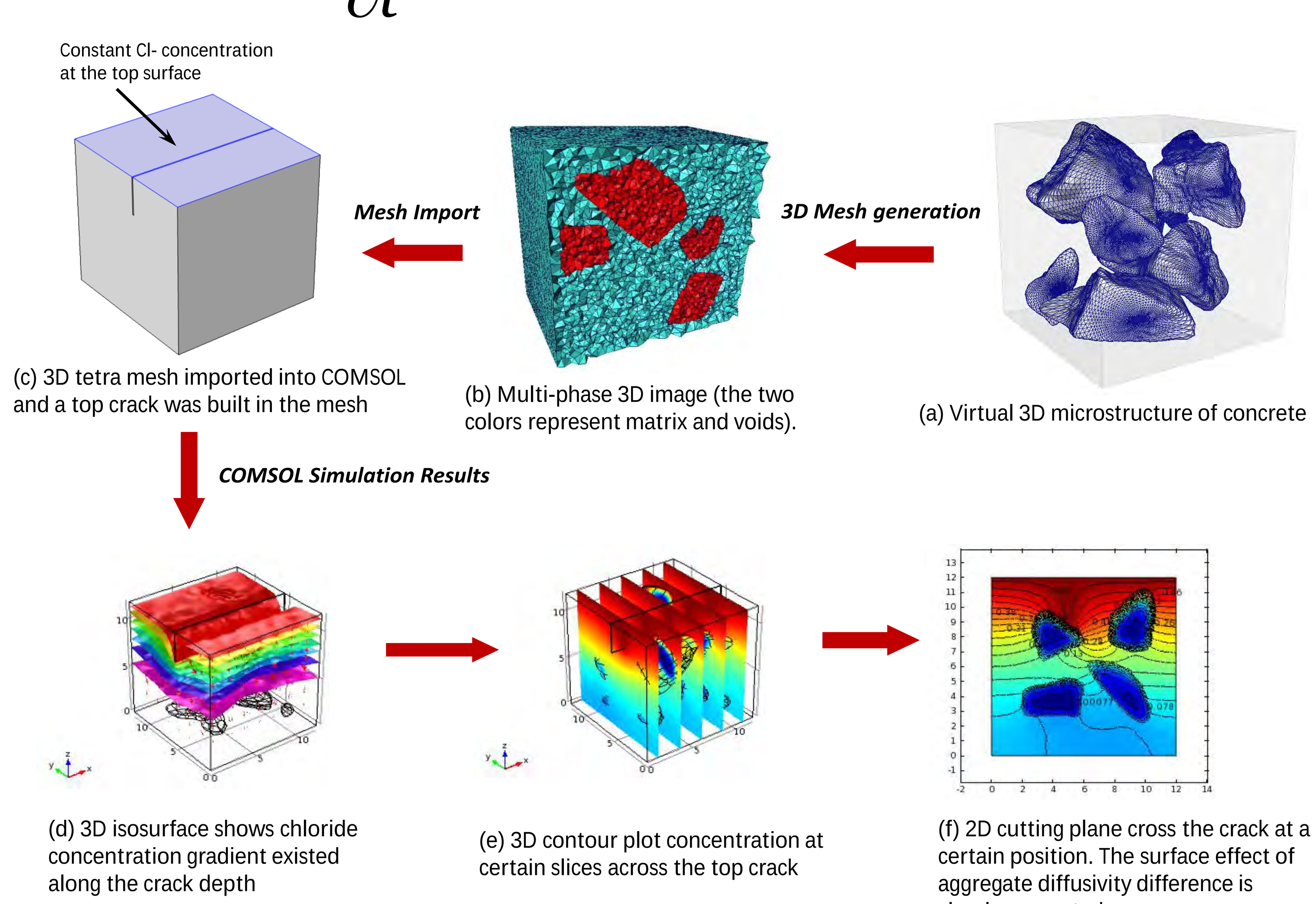
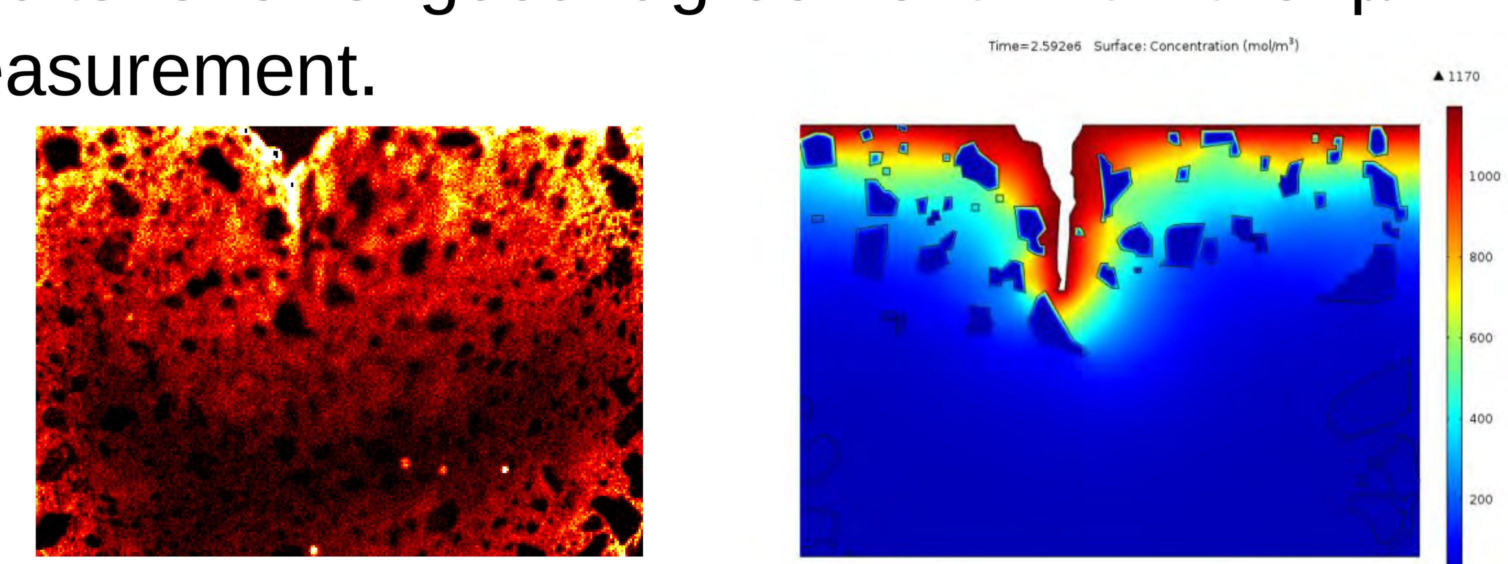


Figure 2. Microstructure #2: Three-dimensional virtual concrete simulation made by real aggregates represented in spherical harmonic analysis [2]. The virtual concrete model has 12 irregular shape aggregates from the VCCTL database, and a built-in crack, which is located on the top surface of the sample.

Results: The µXRF technique rapidly measures the elemental composition of a sample by irradiating it with a thin beam of X-rays without disturbing the sample. Using µXRF, we detected the chlorine concentration on the concrete sample as a function of spatial location with a resolution of about 20 µm. COMSOL simulation results shows good agreement with the µXRF measurement.



(a) Micro-XRF measurement plot for chloride; (b) 2-D chloride ingress contour

Figure 3. Micro-XRF measurement result of chloride concentration contour plot and the 2-D chloride ingress simulation contour comparison

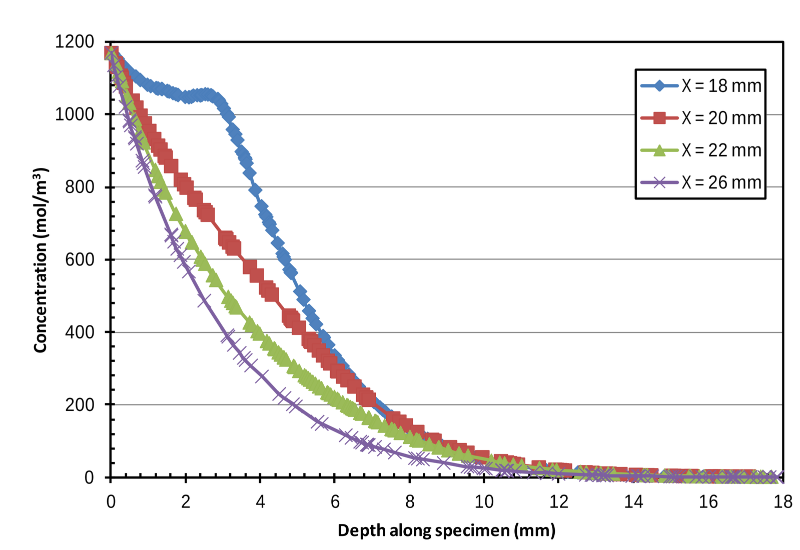


Figure 4. Microstructure #1: Concentration profile along the crack depth, the straight cutline arranged from the closest to the farthest away from the crack, (Y=20 mm, X=18 mm, 20 mm, 22 mm, 26 mm, Z= cross depth)

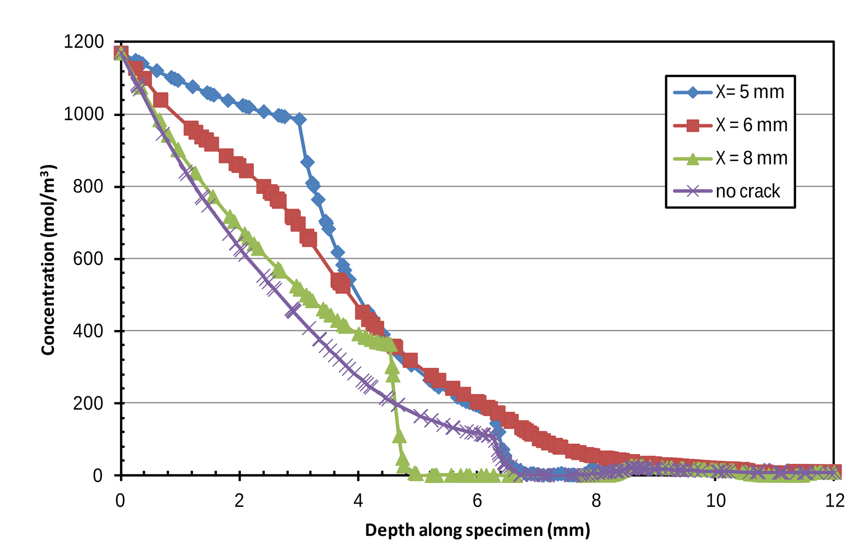


Figure 5. Microstructure #2: Concentration profile plot at cutting line long (Y=5 mm, X=5 mm, 6 mm, and 8 mm, Z = cross depth), comparing non-cracked specimen at cutting line long (Y=5 mm, X=5 mm, Z = cross depth)

Conclusion: Chloride ingress processes in these cracked heterogeneous concrete microstructures were accurately simulated with the COMSOL Multiphysics. It was observed that cracks in concrete can have an accelerating effect on the chloride diffusion, while the binding generally retards the chloride penetration. The behavior of chloride transport in cracked concrete depends strongly on whether there is a crack and on the inherent binding capability of the concrete.

References:

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2. Garboczi, E. J. (2002). "Three-dimensional mathematical analysis of particle shape using X-ray tomography and spherical harmonics: Application to aggregates used in concrete." *Cement and Concrete Research*, 32(10), 1621-1638.
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