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# Modeling Chloride Transport in Cracked Concrete --- a 3-D image–based microstructure simulation

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# BACKGROUND

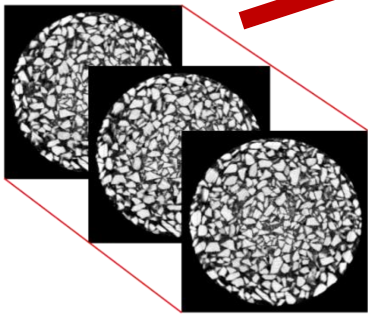
- The prediction of the service life of concrete materials is difficult, because of their complex heterogeneous microstructure and their random nature. Real multiphases microstructure is desirable for simulating chloride transport in multiphase cementitious materials.
- Crack always appears during the service life. Cracks with different widths and depths reduce the effective cover thickness and accelerate the migration of chloride ions. It is desirable to develop a model predicting the chloride diffusion in cracked concrete while considering the real microstructure, e.g. paste, voids, and aggregates.
- A 3-D image-based microstructure simulation procedure was developed to model the chloride ingress in cracked mortar.

# Outline

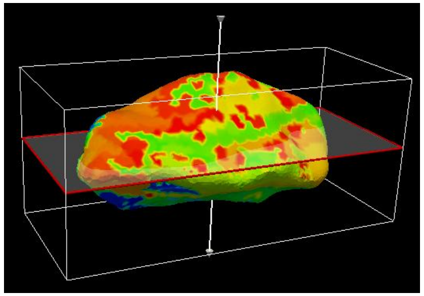
- Background
- Image-based microstructures
  - X-ray CT image based 3-D microstructure
  - Spherical harmonic based virtual microstructure
- Transport and binding model
- Results
  - Micro-XRF measurement validation
  - X-ray CT microstructure simulation
  - Virtual concrete microstructure simulation
- Conclusion

# Image-based microstructures

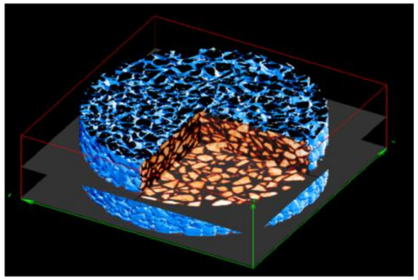
- Engineering Materials
  - Cementitious materials, asphalt concrete
- Fractured rocks in geological systems
  - Subsurface fractured rocks, damaged sediments
- Medical
  - Bones, teeth, bio-tissues
- Two different representations of microstructures, X-ray CT image-based and spherical harmonics-based, with cracks were employed to compute transport and absorption binding effects.



Raw 2-D sequential images



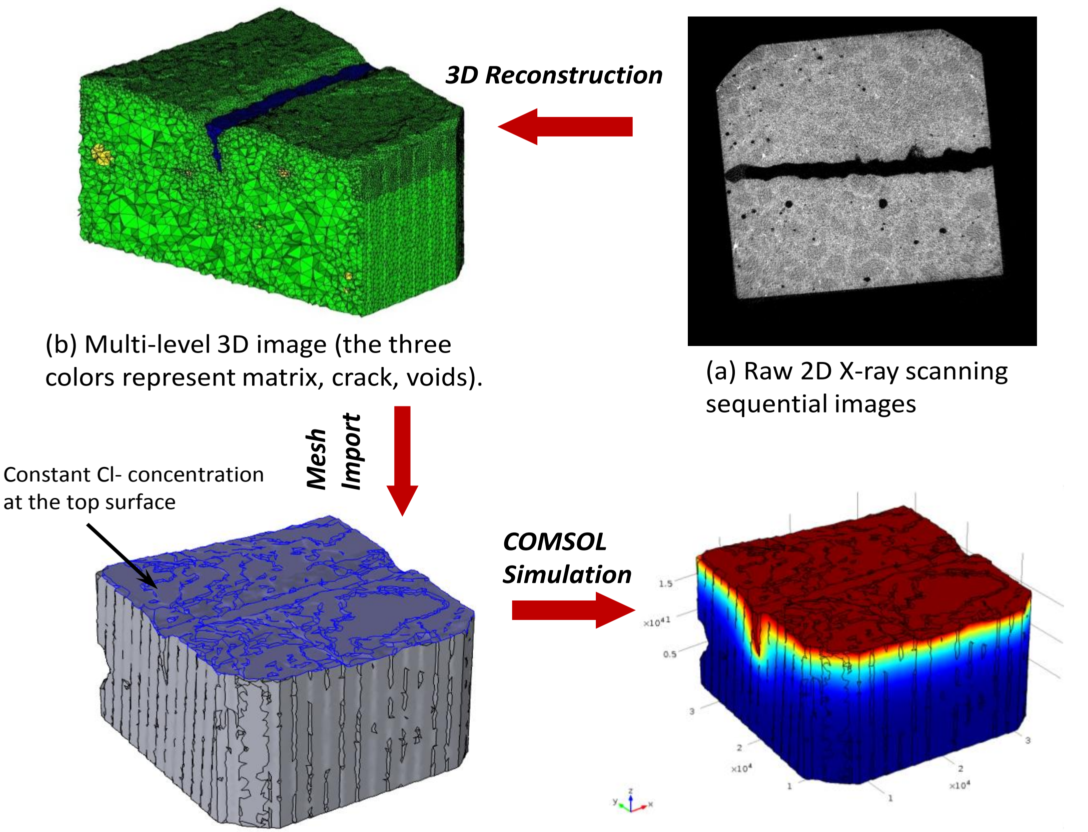
Extract individual aggregate and perform 3-D characterization



Multi-level segmentation on raw grey images and 3-D reconstruction

# X-RAY CT MICROSTRUCTURES

- Based on recent 3-D meshing procedures ([Lu and Garboczi]), the microstructures with a crack could be generated.




(b) Multi-level 3D image (the three colors represent matrix, crack, voids).

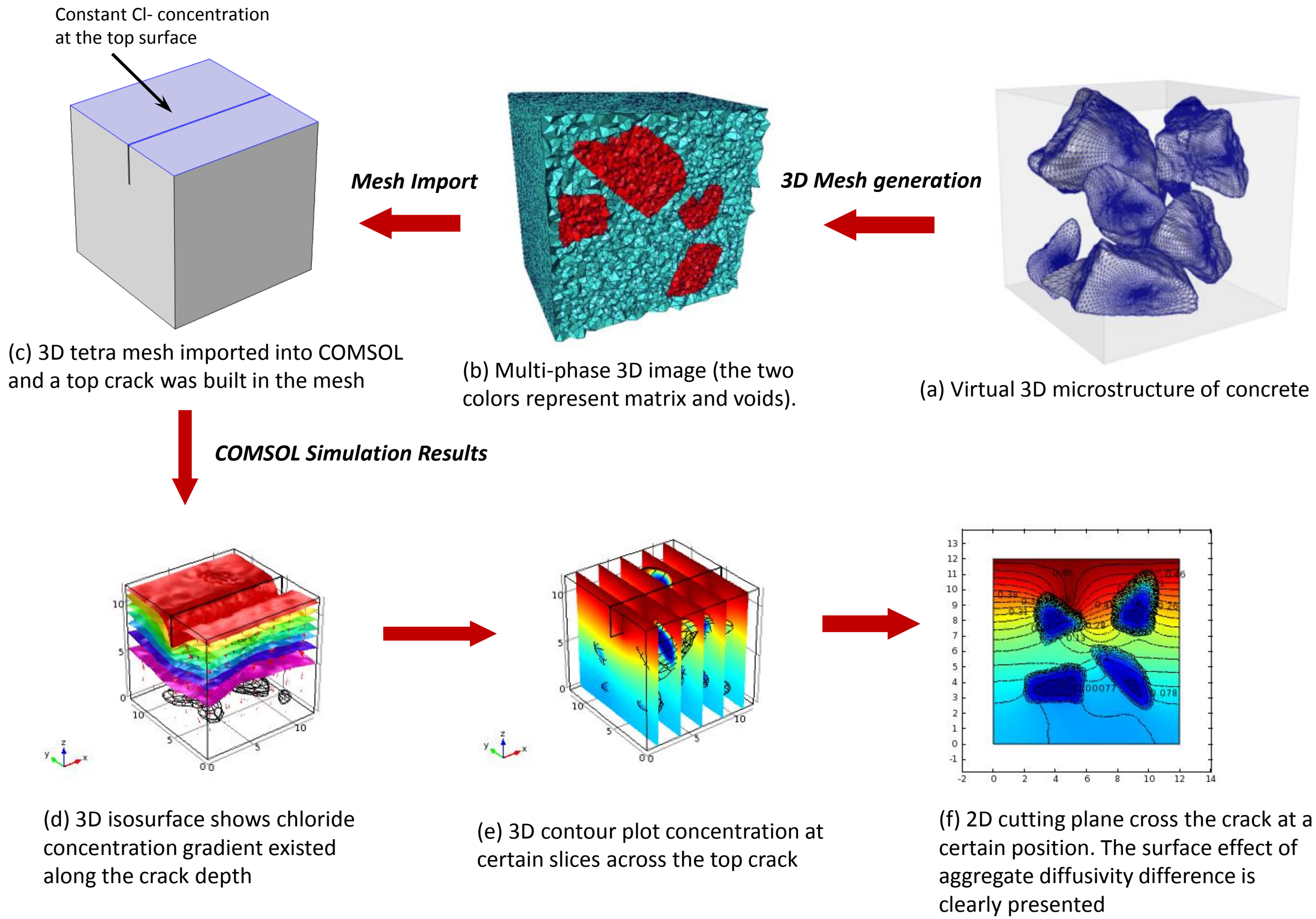
(a) Raw 2D X-ray scanning sequential images

(c) 3D tetra mesh imported into COMSOL, then boundary and initial conditions are applied

(d) Simulated concentration contour of the X-ray CT microstructure

Three-dimensional diffusion and binding simulation procedure with an X-ray microtomography image set; cubic specimens were 25 mm on a side.

# Virtual concrete microstructures




The 3-D virtual microstructure was made by real aggregates represented in spherical harmonic analysis. The virtual concrete model was built using a random particle placement program (Qian 2012). The virtual concrete model has 12 irregular shape aggregates from the VCCTL database, and a built-in crack, located on the top surface.

# Chloride transport and binding model

- The basic chloride diffusion equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left( D\frac{\partial C}{\partial x} \right)$$

$$\frac{C(x,t)}{C_s} = 1 - erf\left( \frac{x}{2\sqrt{Dt}} \right)$$

Where:

C - the chloride concentration and t is time,
D - the effective diffusion coefficient

- Chloride binding capacity

$$C_{total} = C_{bound} + C_{free}$$

$$C_{bound} = \alpha C_{free}$$

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

α - fitting parameter, here taken to be equal to 4, obtained by fitting the experimental data

Relationship between free and bound chlorides and equilibrium

k - the sorption rate constant in bulk mortar

# Simulation approach

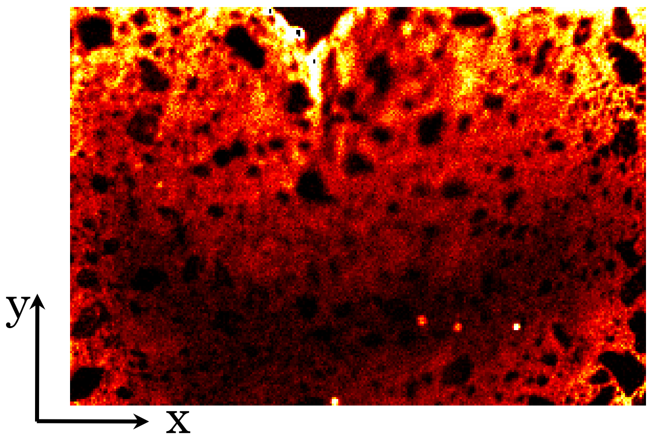
- Employing a constant concentration chloride source fixed at the sample top surface, we simulated a ponding test of chloride ingress.
- For chloride transport in both of the models, the top surface of the specimen was kept at a constant chloride concentration of 1170 $mol/m^3$. The other surfaces were assumed to be impermeable, experimentally by using an epoxy layer coating, designed to block chloride diffusion during the measurement. Therefore, we specified a zero flux boundary condition at the bottom surface and at side surfaces.
- Since binding only takes place within the mortar/concrete part, no reactions take place within the crack area. The initial concentration in the crack was set to 1170 $mol/m^3$, the constant ponding value, because the concentration in the crack will be quickly made equal to the ponding value via convection.

# Parameters used in COMSOL simulations

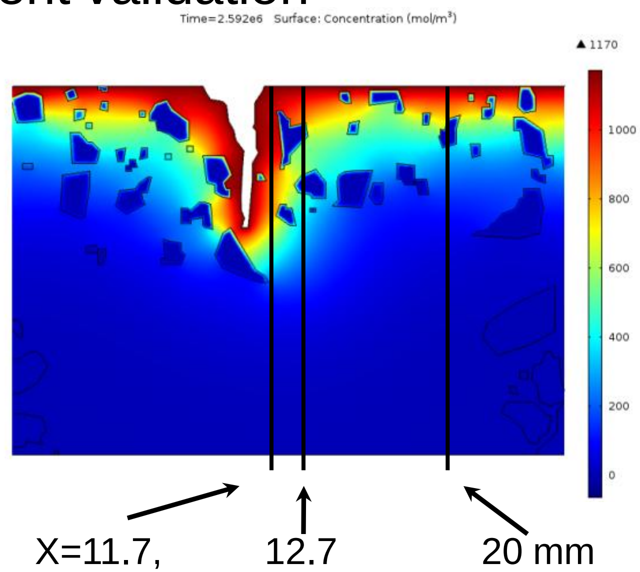
| Parameter | Calibrated value |
|---|---|
| Diffusion coefficient of bulk mortar | $6x10^{-11}$ $m^2/s$ |
| Sorption rate constant in bulk mortar | $3x10^{-7}$ $s^{-1}$ |
| Diffusion coefficient in crack | $2x10^{-9}$ $m^2/s$ |
| Diffusion coefficient in voids | 0.001 $m^2/s$ |
| Diffusion coefficient in non-diffusive aggregates | 0.001 $m^2/s$ |
| α parameter in linear isotherm | 4 |
| External chloride concentration | 1170 $mol/m^3$ |
| Assumed porosity of mortar | 0.1828 |

# Verification case study

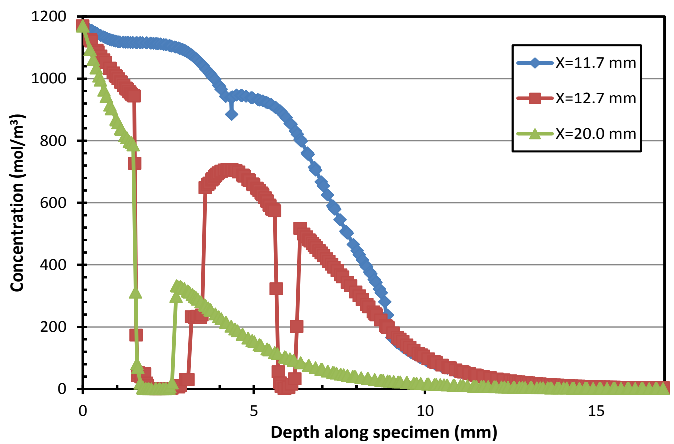
- Micro-XRF technique measurement validation




(a) Micro-XRF measurement plot for chloride

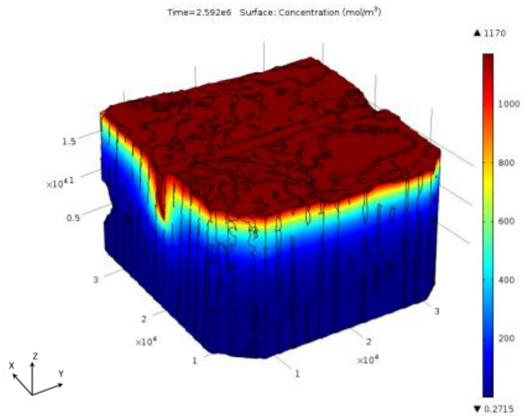



(b) 2-D chloride ingress contour

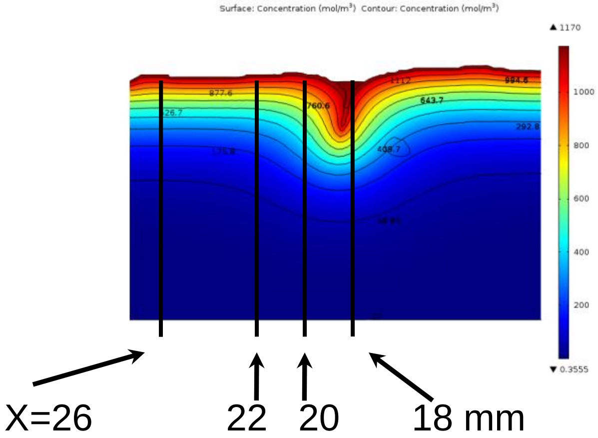



(c) The concentration data was sampled at 3 fixed values of X direction, X=11.7, 12.7, and 20.0 mm of 30 days

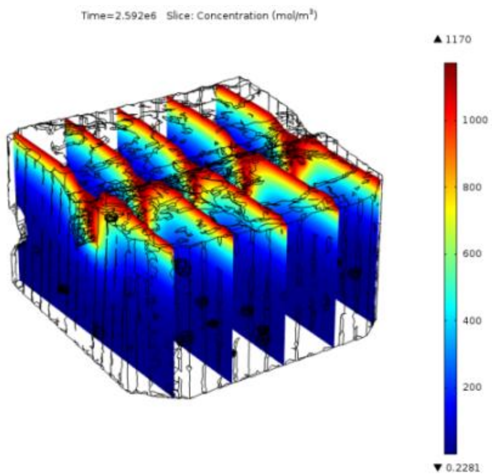
# X-RAY CT MICROSTRUCTURE RESULTS



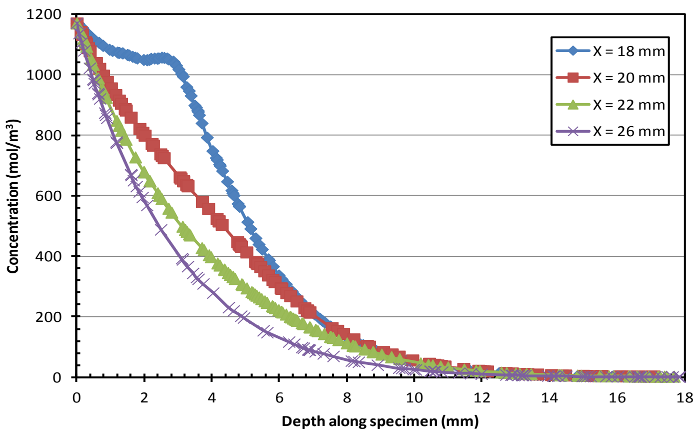

(a) Concentration contour plot of 3-D X-Ray image-based model at 30 day




(b) 2-D cutting surface at Y = 5 mm

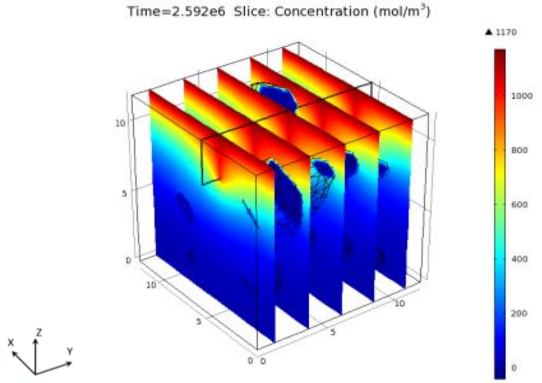



(c) 3-D sliced surfaces

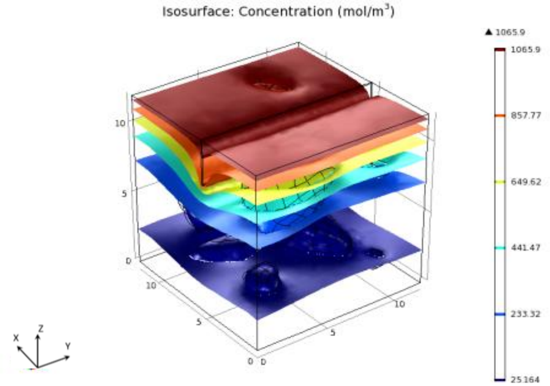



(d) Concentration profile along the crack depth, (data sampled at X=18 mm, 20 mm, 22 mm, 25 mm

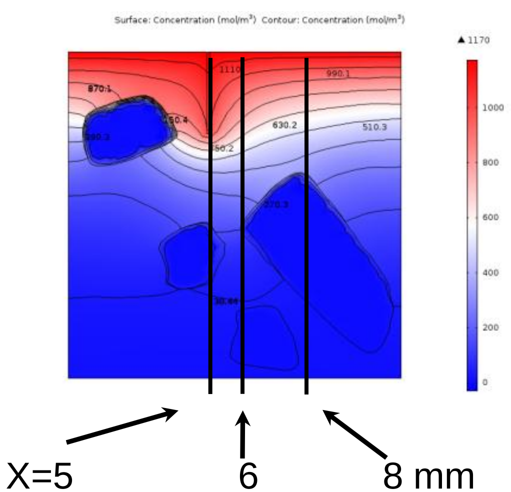
# VIRTUAL CONCRETE MICROSTRUCTURE RESULTS



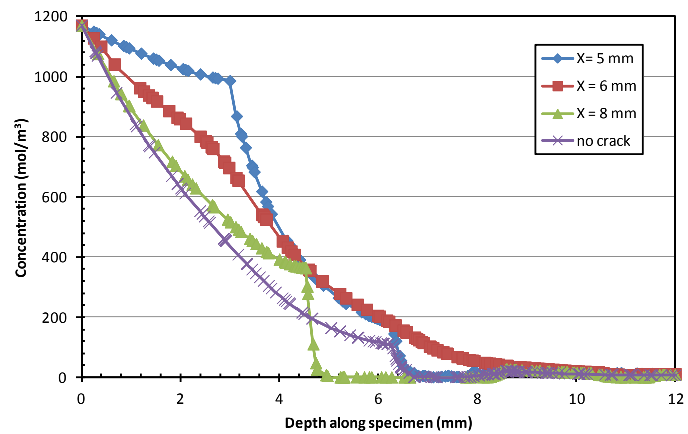

(a) Sliced concentration contour




(b) Isosurface concentration




(c) 2-D concentration contour at a cutting plane




(d) Concentration profile data sampled at (X=5 mm, 6 mm, and 8 mm), comparing non-cracked specimen at sampling point (Y=5 mm, X=5 mm)

# CONCLUSION

- We presented one µXRF measurement and three examples of chloride ingress simulations. Both X-ray CT image-based and spherical harmonic based microstructures were successfully applied to build heterogeneous cracked concrete models. Chloride ingress processes in these cracked heterogeneous concrete microstructures were accurately simulated with the COMSOL Multiphysics.
- Comparison to micro-XRF measurement data indicates that the contributions of the crack play a significant role in the chloride ingress.
- Cracks in concrete can have an accelerating effect on the chloride diffusion, while the sorption binding generally retards the chloride penetration. In other words, the cracks would act as an accelerator (conductor), while binding would act as a moderator. Hence, the behavior of chloride transport in cracked concrete media depends strongly on whether there is a crack and on the inherent binding capability of the concrete.

# References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- 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.
- Lu, Y., and Garboczi, E. "Bridging the gap between VCCTL based CAD and CAE using STL files." ASCE Journal of Computing in Civil Engineering (under review).
- Qian, Z. (2012). "Multiscale Modeling of Fracture Processes in Cementitious Materials."PhD thesis, Delft University of Technology.

*Thank you for your attention!*