Nano-XCT cementitious materials sub-microstructure influence on species transport and corrosion of reinforcement

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***Intro/purpose*.—**Modern descriptions of concrete properties probe at the smallest length, but structural and chemical behavior are manifested at greater scales, thus nanoscale models must be integrated with macroscopic ones. We present a model based on a real microstructure morphology where microscale geometry 3D is reconstructed from the nano-scale X-ray computed tomography data. Included are: ions (Fe^{2+}, OH^-, Na^+, Cl^-) and O_2 transport in sub-micro scale XCT-based geometry; analysis of exchange current distribution, concrete conductivity/polarization on rebar corrosion; comparison with simplified models; 3D vs. 2D computations.

***Materials/methods*.—**X-ray computed tomography data of a Portland cement sample were obtained as a series of 601 images (512px x 512px); voxel size was 129 nm^3. Using Simpleware® four phase segmentation was obtained (gel pores, capillary pores, light grains, dark grains (Figure 1) and 3D meshes were created (~2,300k tetrahedral elements) for numerical simulation using COMSOL Multiphysics®.

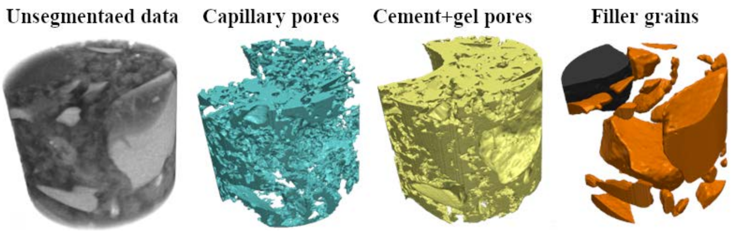

Figure 1: Unsegmented XCT data and results of phase segmentation.

Equations implement mass conservation law, Nernst–Planck fluxes, and embedded electroneutrality conditions (with Na^+ elimination). Depending on phase different material parameters are used:

$$\sum_{i=\mathrm{OH^-},\mathrm{Fe^{2+}},\mathrm{Cl^-}} \left(z_i - \frac{z_{\mathrm{Na^+}} D_{\mathrm{Na^+}}}{D_i}\right)\frac{\partial c_i}{\partial t} + \nabla\cdot \mathbf{J}_{\mathrm{Na^+},\varphi} = R_{\mathrm{Na^+},\varphi}, \ \frac{\partial c_i}{\partial t} + \nabla\cdot\mathbf{J}_i = R_i, \ i = \mathrm{OH^-},\ \mathrm{Cl^-},\ \mathrm{Fe^{2+}},\ \mathrm{O_2} \quad (1)$$

$$\mathbf{J}_{\mathrm{Na^+},\varphi} = -(z_{\mathrm{OH^-}} - z_{\mathrm{Na^+}})D_{\mathrm{Na^+}}\nabla c_{\mathrm{OH^-}} - (z_{\mathrm{Fe^{2+}}} - z_{\mathrm{Na^+}})D_{\mathrm{Na^+}}\nabla c_{\mathrm{Fe^{2+}}} - (z_{\mathrm{Cl^-}} - z_{\mathrm{Na^+}})D_{\mathrm{Cl^-}}\nabla c_{\mathrm{Cl^-}},\ \mathbf{J}_i = -D_i(\nabla c_i + z_i \tfrac{F}{RT} c_i \nabla\varphi)$$

while boundary conditions were in the form of Tafel kinetics, $i_k = i_k^0 \cdot \exp\left(\pm\frac{\alpha_k F}{RT}(U_{rebar} - \varphi - E_{eq,k})\right)$.

***Results*.—**Example of distributions of electrical potential and concentrations of ions and oxygen in a sample with real microstructure are presented in Figure 2.

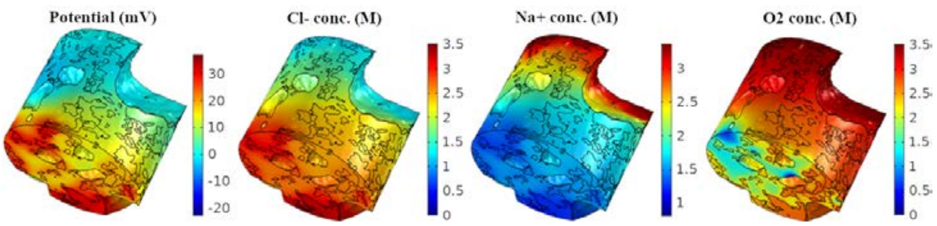

Figure 2: A 3D calculation of potential and concentration of species in real nano/micro structure for t = 10 s.

***Discussion/Conclusion*.—**The model shows that description involving real micro-morphology of concrete coupled with transport of multi-ion system and charge transfer reactions on the rebar surfaces is feasible using modern equipment and computational tools. It allows full description of current, potential and species distribution paving a way for the predictive diagnosis of rebar corrosion.

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