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Effective diffusivity of hardened cement paste from 3D microstructures: A critical comparison of real and virtual microstructures

NEWS: **“Effective diffusivity”**

Diffusivity is a key durability indicator for assessing the penetrability of aggressive substances (e.g., chlorides) and designing concrete cover depths for corrosion resistance. Predicting concrete diffusivity remains challenging because it requires a good understanding of the mechanisms related to the concrete microstructure.

Our newest study conducted together with TU Tokyo, Japan, compares experimentally obtained hardened cement paste microstructures from µCT and virtual microstructures generated by two hydration models, namely CEMHYD3D and HYMOSTRUC. Several microstructural features (phase volume fractions, connectivity, pore size distribution, and two-point correlation functions) were cross-validated among the microstructures on the basis of image analysis. In addition, the corresponding effective diffusivities in a fully saturated state were compared. The simulated effective diffusivities of the µCT and CEMHYD3D microstructures agree well with the experimental data, where HYMOSTRUC overestimates. However, none of the virtual microstructures can fully capture the actual microstructural features. HYMOSTRUC produces realistic pore size distributions but overly connected capillary pores, whereas CEMHYD3D generates excessive scattering of small pores with low connectivity. The impact of the differences in the pore structure on the output diffusivity is presented.

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