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DNS of gas-liquid multiphase flow through FIB-SEM obtained cement-based microstructure

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Concrete is the world's most widely used building material, and its durability has an enormous environmental and economic impact. Cement-based structures are generally under unsaturated conditions, and among the different factors, moisture conditions are directly related to many durability issues, such as freeze-thaw or corrosion-induced damages [1], [2]. Nevertheless, traditional approaches for assessing moisture state and unsaturated transport characteristics typically rely on macroscale models that utilize macroscopic properties and simplified equations, including Lucas-Washburn and Richards' equations [3]. However, observations of the actual concrete structures often do not follow behavior predicted by the mentioned conventional models, meaning that more appropriate transport models are needed. Therefore, there is a need for a better fundamental understanding of essential processes at the pore level [4]. Despite considerable advancements in recent decades, current imaging techniques still fall short in achieving the spatial and temporal resolutions required to capture the intricate dynamics of water transport in complex, heterogeneous cement-based porous media.

This work uses an actual cement-based microstructure (imaged by FIB-SEM nanotomography [5]) as a computational domain. Extensive and computationally intensive 3D direct numerical simulations (DNS)[6] of air-water multiphase flow are carried out to obtain deeper insight and consistent explanations of different processes during a water absorption event. This work focuses on providing a detailed pore-scale insight into the full interface-resolved complexity of waterfront advancement (spatially and temporally), gaining a deeper understanding of an air-trapping mechanism, and exploring the complexities of pressure distribution of residual (non-wetting) gas phase. Obtained results and conclusions improve our fundamental understanding and could significantly impact the development of enhanced macroscale models needed for practical large-scale modeling.

[1] S. Mundra, E. Rossi, L. Malenica, M. Pundir, and U. M. Angst, "Precipitation of corrosion products in macroscopic voids at the steel-concrete interface – observations, mechanisms and research needs," Aug. 09, 2024, arXiv: arXiv:2408.05028. doi: 10.48550/arXiv.2408.05028.

[2] L. Malenica, Z. Zhang, and U. Angst, "Direct Numerical Modelling Of Capillary Driven Multiphase Flow at the Embedded Steel - Porous Media Interface," presented at the The 9th World Congress on Momentum, Heat and Mass Transfer, Apr. 2024. doi: 10.11159/icmfht24.175.

[3] Y. V. Zaccardi, N. Alderete, and N. D. Belie, "Lucas-Washburn vs Richards equation for the modelling of water absorption in cementitious materials," MATEC Web Conf., vol. 199, p. 02019, 2018, doi: 10.1051/matec-conf/201819902019.

[4] L. Malenica, Z. Zhang, and U. Angst, "Towards improved understanding of spontaneous imbibition into dry porous media using pore-scale direct numerical simulations," Advances in Water Resources, vol. 194, p. 104840, Dec. 2024, doi: 10.1016/j.advwatres.2024.104840.

[5] N. Ruffray, U. M. Angst, T. Schmid, Z. Zhang, and O. B. Isgor, "Three-dimensional characterization of the steel-concrete interface by FIB-SEM nanotomography," Oct. 06, 2023, arXiv: arXiv:2310.04322. doi: 10.48550/arXiv.2310.04322.

[6] J. Maes and S. Geiger, "Direct pore-scale reactive transport modelling of dynamic wettability changes induced by surface complexation," Advances in Water Resources, vol. 111, pp. 6–19, Jan. 2018, doi: 10.1016/j.advwatres.2017.10.032.

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