Potential and Limitations of Multiscale Modelling
Lessons learnt in a European cement research project

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Collaboration between experimentalists and modelers both from industry and academia is vital in cement and concrete research for advancing understanding and technology development. However, there are several potential conflicts due to different methodologies and priorities. Experimentalists rely on empirical data. Modelers use theoretical simulations. Industrial researchers face real-world challenges. Academics tend to oversimplify material systems in order to isolate effects. Overcoming these potential conflicts requires open-minded collaboration, mutual respect, and interdisciplinary training. When modelers interact with experimentalists and non-modelers, it is essential to clearly communicate the purpose of modeling and the idealizations the model introduces compared to real-world observations. Since models can rarely capture the full complexity of a system, experimental validation is crucial. Where data exists, it must be used for comparison. Additionally, we must critically examine key assumptions and assess how the model aligns with or challenges existing literature. Within the MatCHMaker project [1] we focus on deciphering the relation between microstructure and macroscopic strength of eco-friendly cementitious materials in which part of the traditional cement is replaced by powders of limestone and heat-treated clay. The purpose of multiscale modeling is to facilitate the understanding regarding the relation between microstructure and macroscopic strength of cement pastes produced by mixing cement and water. Rather than accounting for the full complexity of cementitious materials, scale transition methods of continuum micromechanics account for key features of the microstructure: the hierarchical organization, the interaction between different material constituents, their characteristic shapes, volumetric dosages, and mechanical properties. In the MatCHMaker project [1], we have extended a validated multiscale strength model for traditional cement paste [2,3] by including limestone and clay as additional material constituents. Comparing upscaled strength values with actual strength values and interpreting the differences based on (i) micrographs showing the actual microstructures, and (ii) results from calorimetry providing insight into chemical reactions at early material ages has helped to understand that particle size distributions of cement replacement materials matter when it comes to microstructure-macrostrength relations.

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[1] EU project MatCHMaker: https://he-matchmaker.eu/

[2] B. Pichler, C. Hellmich, Upscaling quasi-brittle strength of cement paste and mortar: A multi-scale engineering mechanics model, Cement and Concrete Research 41 (2011) 467–476: https://doi.org/cvh9zh

[3] M. Königsberger, M. Hlobil, B. Delsaute, S. Staquet, C. Hellmich, B. Pichler, Hydrate failure in ITZ governs concrete strength: A micro-to-macro validated engineering mechanics model, Cement and Concrete Research 103 (2018) 77–94: https://doi.org/ch9n