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Multiscale Computational Methods for Cement and Concrete Research

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ABSTRACT

Cementitious materials, such as concrete, cement, and mortars, play a pivotal role in modern society as the foundation of infrastructure development. With an increasing rate of urbanization and the continuous ageing of existing infrastructure worldwide, there is an urgent need for improving the sustainability, durability and performance of these materials. Virtual laboratories can harness modern computational methods to not only provide deeper insights into the complex behavior of the material during production, processing and service but also help design durable and high-performance materials while reducing carbon emissions e.g. during cement production. However, attempts at developing an accurate and comprehensive virtual laboratory for these materials is still at an early stage. Cementitious materials such as concrete are multiphase materials whose properties in the fresh and hardened state are governed by chemical and physical (multi-physics) properties and processes that range over multiple size scales (µm – cm) and additionally change with time (seconds - years). Thus, even the state-of-the-art models and simulation methods are limited in scope due to this immense complexity. The current focus of the scientific community is not only in incorporating additional physics (multiscale, multiphase, multiphysics) but also using reduced order strategies and materials informatics. This mini-symposium will focus on recent advances, challenges, and ongoing research in the computational modelling and simulation of building materials. Among others, the following topics will be covered by the mini-symposium:

- Multiscale and multilevel models (continuum micromechanics, computational multiscale models)
- Reduced-order modeling strategies
- Data-driven methods, materials informatics, AI and Machine Learning tools for building materials
- Methods for simulating damage, fracture, transport and physico-chemo-mechanical processes (creep, shrinkage, chemical dissolution, chemically expansive processes)
- Rheological modelling and classification of fresh cementitious composites
- Simulation of concrete flow and additive manufacturing processes (e.g., DEM, SPH, PFEM, CFD etc.)