A Novel DEM-based Coupled 3D Thermo-Hydro-Mechanical Mesoscopic Model with Phase Changes for Modelling Concrete Behavior

M. Krzaczek*[1] and J. Tejchman[2]

[1] Gdańsk University of Technology
Narutowicza 11/12, 80-233 Gdańsk, Poland
e-mail: marek.krzaczek@pg.edu.pl

[2] Gdańsk University of Technology
Narutowicza 11/12, 80-233 Gdańsk, Poland
e-mail: jacek.tejchman@pg.edu.pl

KEYWORDS: *Concrete, DEM-CFD, Heat Transfer, Phase Changes, Fracture.*

Concrete is one of the most widely utilized construction materials, employed in several environmental contexts. The majority of concrete constructions are generally subjected to a temperature range that does not exceed that of the surrounding environment. They may, however, also be exposed to extremely high temperatures (e.g., during a fire) [1]. This work numerically examined the effect of increased temperatures on the uniaxial compressive and tensile behavior of plain concrete.

A unique DEM-based pore-scale 3D thermo-hydro-mechanical (THM) model of two-phase fluid flow and heat transfer in fluids and solids was employed to investigate the concrete behavior at the meso-scale. The model also accounted for phase transitions (evaporation/condensation) in the fluid. Heat transmission was associated with fluid dynamics (diffusion and advection), bound granular particles (conduction), and phase transitions. The model used a direct numerical simulation methodology, comprising two coexisting domains: a three-dimensional discrete (solid) domain and a three-dimensional continuous (fluid) domain. Both domains were discretized using a coarse tetrahedral mesh. The DEM-based THM model was put into the open-source software package YADE, utilizing the soft-particle technique [2]. The THM model's efficacy was demonstrated by a thermal contraction test utilizing a bonded particle assembly during cooling, leading to the formation of a macro-crack. Subsequently, numerical simulations of uniaxial compression and tension tests on concrete specimens were conducted. Concrete was regarded as a four-phase material comprising aggregate, mortar, interfacial transition zones (ITZs), and macropores. The concrete mesostructure was derived from laboratory micro-CT images [3]. The computations examined the influences of strain rate, temperature, aggregate fragmentation, fluid saturation, and viscosity. A technique termed clump breakage was utilized to simulate intra-granular disintegration of aggregates [3]. The numerical results were directly compared with relevant experiments in the literature [1], [4].

[1] D. J. Naus, The effect of elevated temperature on concrete materials and structures - a literature review, Report for the U.S. Nuclear Regulatory Commission Office, Office of Nuclear Regulatory Research (2005).

[2] M. Krzaczek, M. Nitka, J. Tejchman, A novel DEM-based pore-scale thermal-hydro-mechanical model for fractured non-saturated porous materials, *Acta Geotechnica* **18,** 2487–2512, 2023.

[3] M. Krzaczek, J. Tejchman, M. Nitka, Impact of strain rate, free water, and aggregate fragmentation on the dynamic behavior of concrete in compression regime using a unique coupled DEM/CFD technique, *Granular Matter* **27**, 79, 2025.

[4] J. Shen, Q Xu, Effect of elevated temperatures on compressive strength of concrete, *Construction and Building Materials* **229,** 116846, 2019.