C-S-H Globules Clustering on Nano-scale Simulated by Discrete Element Method for Pore Structure Exploration

K. Li, M. Stroeven, P. Stroeven, L. J. Sluys
Faculty of Civil Engineering and Geosciences, Delft University of Technology,
Stevinweg 1, PO Box 5048, 2600 GA Delft, the Netherlands
E-mail: K.Li-1@tudelft.nl

Abstract

To numerically simulate hydrating cement paste, the vector approach is a well-known method that has been around for two decades [1]. In this method, it is assumed that the reaction products of the cement particles evenly precipitate on the surface of cement particles (or nucleate into the free pore space). And because the volume of the reaction products exceeds that of the reactants, particles "grow" in size, thereby invading pore space as the hydration progresses in time. Most commonly these methods assume the cement particles to be spherical because the interaction between hydrating (= growing) spherical particles becomes increasingly more complex for non-spherical particles. Recent research however demonstrated that this "precipitation onto the free surface" process of C-S-H formation poorly represents the actual situation [2]. Hence, Jennings suggested the C-S-H structure to be better described as a clustering of brick shaped globules on nano-scale [3]. The difference between the precipitation model and the approach described by Jennings is that the globules are not growing in size, but are increasing in numbers. Hence, allowing for/requiring a different approach of simulation.
This paper will highlight a possible approach to simulate the structural development of hydrating cement by modeling the interaction between globules using a DEM approach. Compared to the "traditional" hydration simulation on a micro-level using the spherical vector approach (that reveals an overestimation of the pore size distribution of several orders), a more realistic capillary pore network structure is expected with this method. So, the simulation presented in this paper has the potential to bridge the gap between experimental observations and simulated data.
It is expected that the double random multiple tree structuring (DRaMuTS) and star volume measuring [4], developed for quantitative evaluation of the pore network structure simulated by the vector approach on micro-level, can also be applied to assess pore network characteristics on nano-level.

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