Strategy for exploring the pore structure of cementitious materials based on a DEM approach

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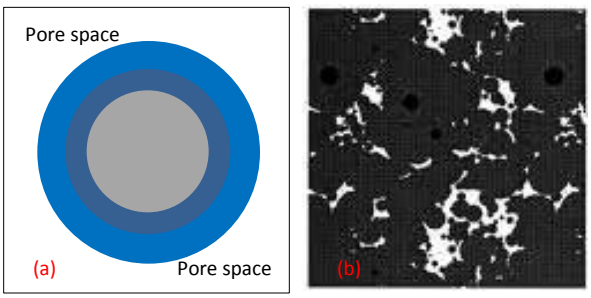
Problem statement



Problem: Assumption of poreless hydration products leads to the overestimation of pore space in simulations.

Figure 1: (a) Partly hydrated cement particle;
(b) Fully hydrated particle system [1].

What do we see in practice

On the basis of the latest finding by Jennings, as shown in Fig. 2, we can see that the major hydration product (calcium silicate hydrate, CSH) consists of brick-like nano-globules, together with large gel pores (LGP) and small gel pores (SGP). Moreover, a very strict boundary between CSH and pore-space is not obvious. In contrast to a homogenous substance, CSH is classified as CSH-in and CSH-out in practice. The density of CSH-in is much higher than CSH-out. Therefore, modelling of CSH that includes the structure at nano-level seems more realistic and may give us a solution to the "overestimation" problem.

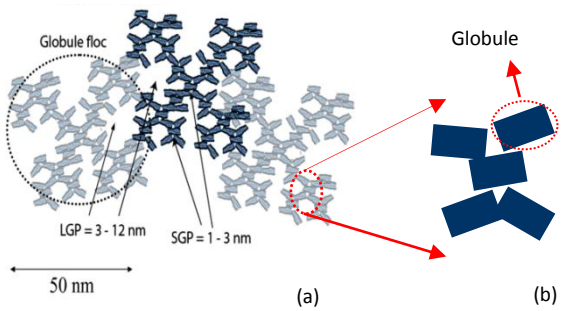


Figure 2: (a) Model proposed by Jennings, taken from [2];
(b) Illustration of globules.

Numerical approach

It is assumed that the reaction between cement grains and water results in non-porous CSH-in and a number of CSH-out globules. Globules either attach to the current globule structure or nucleate in pore space. Therefore, the free space is filled gradually as hydration goes on. The numerical model should precisely describe this process. The sizes of cement grains remain unchanged during calculation.

However, far too many nanoparticles are required to represent CSH as a structure of globules. The number of globules can be diminished by reducing the total space into typical representative volume element (RVE) regions. Only these RVE regions are considered for simulation of cement hydration. According to Jennings, globule flocs grouped by globules will be used to describe the structure in the RVE. A multi-scale approach will be employed to connect the structures obtained at different scales. The RVE of a single cement particle is given in Fig. 3. A possible RVE is given in Fig. 4, red circles represent CSH globules.

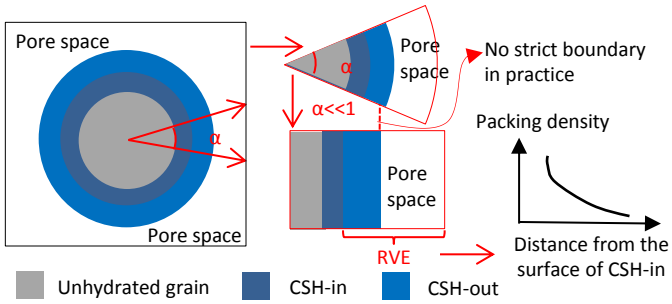


Figure 3: The RVE of a single cement grain.

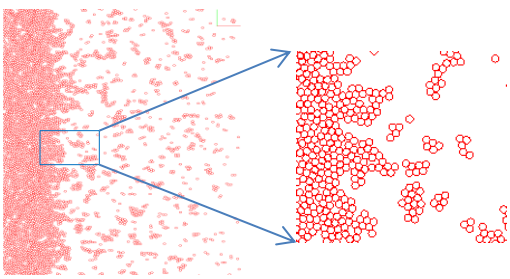


Figure 4: Illustration of a possible RVE with the interface on the left side.

In addition, the contact area of products between neighboring grains should also be considered when choosing a suitable RVE, illustrated in Fig. 5.

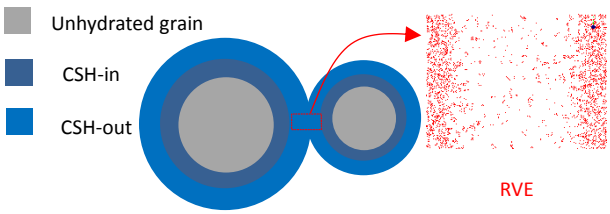


Figure 5: The RVE of two interacting grains.

References

[1] Stroeven. M., Stroeven. P., 'SPACE system for simulation of aggregated matter application to cement hydration', *Cem. Concr. Res*. 29 (8) (1999) 1299-1304.

[2] Jennings, H.M., 'Refinements to colloid model of C-S-H in cement: CM-II', *Cem. Concr. Res*. 38 (3) (2008) 275-289.

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