Polymer Physics and Modeling of Polycarboxylate-based Superplasticizers

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The tendency of developing urban areas brought a great demand for building materials in the last few decades. The innovation of new chemical admixtures has an increment in industry improving the rheology and early strength of cement-based material [1,2]. The use of modified polycarboxylate-based (PCE) superplasticizers in ready-mix or precast concrete cuts off required energy for construction decreasing the curing temperature and cost of building material. Moreover, the addition of superplasticizers results in a significant reduction to the annual worldwide CO_2 emissions. Therefore, a continuous development of the PCE superplasticizers would be benign for us all if one considered the big picture of reducing the consumption of natural resources and energy.

The research is a computational study, and our objective is to explore the polymer physics of PCE superplasticizers in aqueous solution and at liquid/solid interfaces using both the all-atom Molecular Dynamics (aaMD) and the Coarse-grained Molecular Dynamics Simulation (CGMD) simulation methods. More specifically, we are going to study (i) the interactions between PCE fragments and the various ions in a cement pore solution and how ions distribute around those PCE fragments; (ii) interactions of C-S-H surfaces with ions and calculations of the surface zeta potential [3]; and (iii) interactions between PCE fragments and C-S-H surfaces in the presence of ions using the aaMD simulation method. The aaMD method has a spatial resolution on the scale of a single atom, which is a great advantage when studying the physics of interfaces. However, it is rather computationally demanding to simulate polymers using the all-atom model, and that's why we choose to work with PCE fragments instead of the entire macromolecule. The downside is that this choice may limit us from studying the polymer physics of PCE polymers [4].

In order to simulate the actual PCE polymers used in industry, we apply the CGMD simulation method by first developing coarse-grained models for PCE polymers in aqueous solution and then apply the same polymer model to study their conformational and adsorption properties at liquid/solid interfaces. We are particularly interested in exploring the physics of PCE polymers, which are comb-shaped copolymers with negatively charged backbones and neutral side chains, in the vicinity of a negatively charged surface with the presence of multi-valent cations [5].

References

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