Concrete Sustainability Hub@MIT – Research Profile Letter – August 2013

Controlling the Reactivity of Fly Ash

Problem

Silica fume, fly ash, and slag cements are common ingredients in the production of concrete. Although these materials are ubiquitous in industry, there remain various questions about their structure and the mechanisms by which they form C-S-H. To fully harness cementitious additives for engineered concrete a link must be found between microstructure and reactivity. In this study we look to understand why Class F fly ash does not react with water as well as Class C does.

Approach

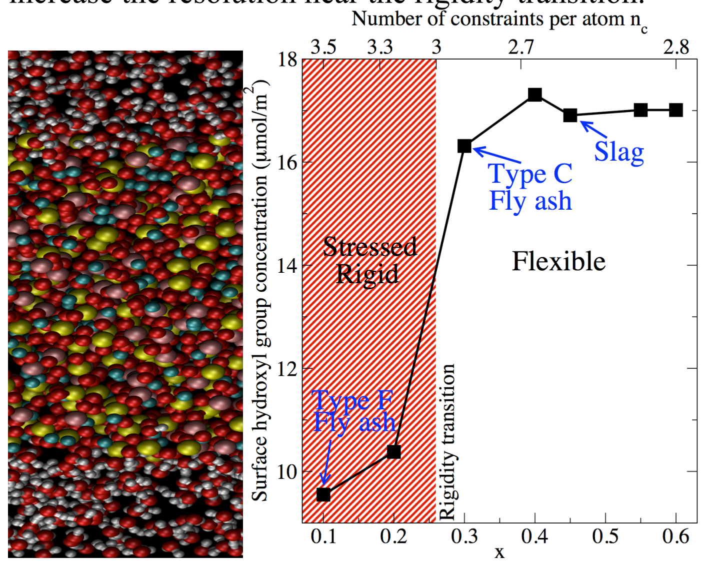
Molecular dynamics simulations have proven effective in the modeling of C-S-H systems. To model reactions with water, simulations require a reactive interatomic potential. Fly ash glasses have been simulated with compositions according to:

$$(SiO_2)_{0.65-x/2}\,(Al_2O_3)_{0.35-x/2}\,(CaO)_x$$

The respective microstructures of the different compositions have been analyzed in the framework of the rigidity theory. This method, in which a glassy network is seen as a simple mechanical truss, has been widely used in glass science. From the number of chemical constraints between the atoms, it can be determined whether a system is flexible, isostatic or stressed-rigid, which correspond to a number of constraints of less than, equal to or greater than 3 respectively (number of degrees of freedom per atom). Each glass is then exposed to water at which time we enumerate the number of hydroxyl groups formed on the surface.

Findings

The initial results of the molecular dynamics study support the predictions from rigidity theory. Over-constrained systems, those stressed-rigid, are less able to form OH groups when compared with those that are flexible. We present a rigidity transition at the isostatic case where x ~ 0.25, from stressed to flexible systems characterized by low and high x respectively. In other terms Class C fly ash and slag cement have favorable reactions with water compared to Class F fly ash. Further studies will increase the resolution near the rigidity transition.



Left: Cross Section of simulation for x=0.45 exposed to water.
Right: Connection between constraint theory and the number of hydroxyl groups formed on the surface.

Impact

The significance of structure and composition has been displayed in the context of cementitious additives including fly ash and slag. This work has provided a "formula" for model additives to provide the first systematic study connecting the number of constraints to the reactivity of fly ashes. This is direct evidence of a link between microstructure and reactivity, displaying that flexible systems are better able to form hydroxyl groups than stress-rigid systems. Finally, it provides a general recipe to predict which families of materials are reactive and can therefore be considered viable additives to improve cement

More

Research presented by D. Brommer, in collaboration with Drs. M. Bauchy, R. Pellenq, and M.J. Buehler.

This research was carried out by the CSHub@MIT with sponsorship provided by the Portland Cement Association (PCA) and the Ready Mixed Concrete (RMC) Research & Education Foundation. The CSHub@MIT is solely responsible for content.
For more information, write to CSHub@mit.edu.