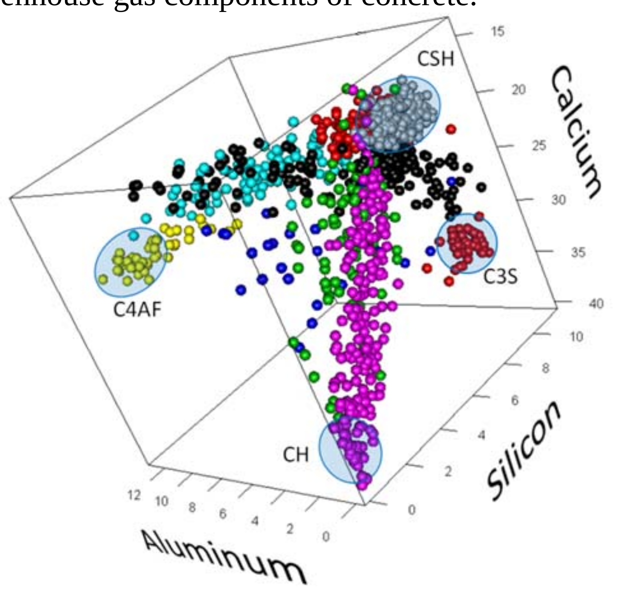
What's in Your Concrete? (Part 1)

Problem

Concrete is defined by its properties in the hardened state. However, these are known to depend strongly on the chemical make-up created by the tens of chemical hydration reactions that take place when cement clinker phases react to form this cohesive liquid stone. The difficulty in reliable assessment of this chemical signature stems from the many possible combinations and spatial distributions of different elements (Si, Ca, Al, Fe, Mg, S, Na, etc.) that make up the multiple phases within the cement paste. These phases include calcium-silicate-hydrates (C-S-H), portlandite (CH), aluminates, and unhydrated clinker. Additions of slag, fly ash, silica fume, limestone, and other chemically complex phases significantly add to this challenge. To relate the *in situ* chemistry to the mechanical performance of the binding phase of concrete, new experimental and analytical tools are required. Such capabilities will afford control and validation of new models and prototype cements to attain industry-wide goals including lowering the greenhouse gas components of concrete.



In situ assessment of cement chemistry by statistical cluster analysis of wavelength dispersive spectra for a specific Portland cement (OPC). Colors represent different phases in hardened cement paste as identified by this analysis. Units in atomic percent (number of atoms/total number; except H).

Approach

We employ a statistical clustering algorithm to translate experimental measurements into a chemical signature of each cement paste. These experiments employ an electron microprobe to collect X-ray wavelength dispersive spectra (WDS) at many points on the sample surface. Each point in this array is a three-dimensional pixel of μm-scale volume, or a voxel, and a massive array is acquired (e.g., >1000 voxels over ~1mm^2). The results are then analyzed via a clustering algorithm. This approach employs expectation maximization to assign each voxel to the most probable cluster. Each cluster is representative of a chemically distinct phase within the hardened cement or concrete. The number of unique clusters is identified via Bayesian statistics, and the cluster volume fraction is determined from the number of voxels comprising that phase.

Findings

This cluster analysis quantifies chemical composition and volume fraction of cement paste phases, as a function of mixture design and environmental exposure.

Impact

This research combines *in situ* X-ray spectra and multivariate statistics to characterize quantitatively the chemical signature and volume fraction of phases in hardened cement paste. The comparable size of voxels in this chemical analysis and our nanomechanical characterization now provides both an indispensible tool to link cement chemistry to nanoscale mechanical properties and engineering performance of cement and concrete.

More

Research herein conducted by Muhannad Abuhaikal, graduate student in the CSHub, in collaboration with Drs. K.Stewart and J.A. Ortega, and supervised by Profs. K.J. Van Vliet and F-J. Ulm.

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