Characterization of C-A-S-H gels of different alkalinity and chemical composition: a comparative study

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Introduction

- Cement manufacturing is composed of many complex systems whose exact mechanisms are very convoluted and could not be analyzed with preexisting techniques.
- Modern methods and instruments enable the observation of the molecular structure of synthetic CASH gels.
- Monitoring the evolution of CASH gels allows for a further understanding of the naturally occuring CASH gels in cement and the modification of certain parameters that could potentially reduce the environmental impact of cement production. Using current methods, 1 tonne of portland cement generates 1 tonne of CO_2 in the atmosphere[1].

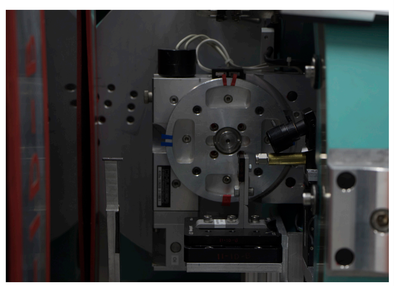
Methods

- The characterization of CASH gels is made via:

1. Thermogravimetric analysis (TGA);
2. X-ray diffraction data from theBRUKER XRD and the Advanced Photon Source at the Argonne National Laboratory;
3. Attenuated Total Reflectance in conjuction with Fourier Transform Infrared Spectroscopy (ATR-FTIR)

for all combinations of 0.6 and 1.2 Ca/Si ratios with a 0.1 Al/Si ratio across all samples and 0.5M and 5M NaOH alkalinities over the course of three months.

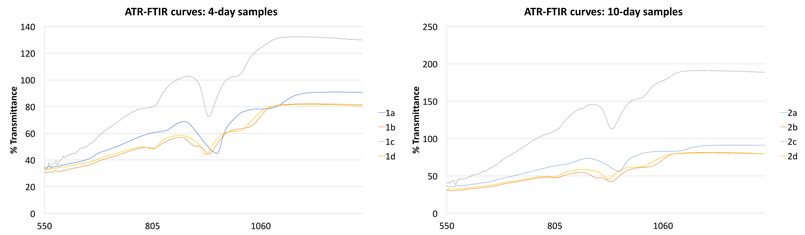
Intermittent steps occur at 4 and 10 days and 1, 2, 3 months.



Workstation and beamline apparatus at the Argonne National Laboratory, 2016.

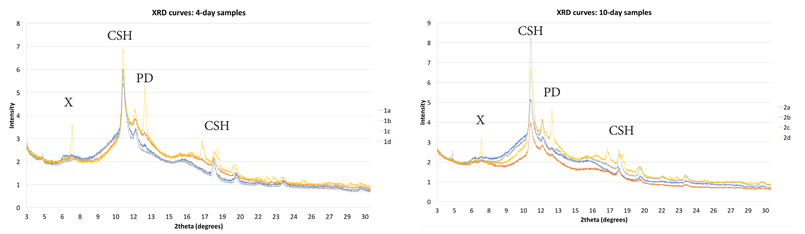
Results

The 4 day and 10 day sample data from the ATR-FTIR, TGA and XRD instruments accordingly is as follows:



- We notice a horizontal shift to the left in the silica peaks, indicating depolymerization of the silica in the mix.

- TGA: We observe ever-decreasing water content levels in the samples across all alkalinity and Ca concentrations.



- XRD: The braggs peak of both samples correspond to CSH (CSH) and Portlandite (PD) phases across the matrix.
- Characteristic peaks were compared against a braggs peak database to identify the type of phase existing in the mix.

Discussion

ATR data:
The ATR-FTIR results emphasize on the area indicating the polymerization of silica in the mix. The full graph expressed interesting behavior at approximately 2000 cm^{-1} for the samples with higher alkalinity and calcium content. We also observe changes brought by the NaOH content in the mix. One potential explanation is that the depolymerization of silica by the NaOH drives the modification of the CASH gel [1].

TGA data:
We also observe that the TGA curves are not perfectly flat after the 100 °C point, indicating the evaporation of something other than water from the mix. It is worth noting that the gas flown through the chamber for drying was oxygen. Future iterations will incorporate Nitrogen into the model, in order to avoid any spontaneous synthesis of new materials in the sample under consideration.

XRD data:
The diffraction of CSH and portlandite phases across the matrix is evident from the first braggs peak and the subsequent, shorter ones occuring across the full 2theta range, as expected in the evolution of the CASH gels. However, interesting phases before the main braggs peak occur, indicating the existence of some intermittent phase in the mix (marked in “X”, see graph).

References

1. I. García Lodeiro, D.E. Macphee, A. Palomo, A. Fernández-Jiménez, Effect of alkalis on fresh C–S–H gels. FTIR analysis, Cement and Concrete Research, Volume 39, Issue 3, March 2009, Pages 147-153, ISSN 0008-8846, http://dx.doi.org/10.1016/j.cemconres.2009.01.003.
2. Ibid