**IACIP Webinar (January 29 [8:30 pm US] / 30 [9:30 am China], 2022)**

# Analytical investigation of phase assemblages of alkali-activated materials in CaO-SiO2-Al2O3 systems: The management of reaction products and designing of precursors

Rui Xiao, University of Tennessee

**Abstract:** This study presents an analytical investigation based on thermodynamic simulation aimed at achieving a holistic management of the phase assemblages of alkali-activated materials (AAMs) and gaining insights into the designing of precursors. Gibbs free energy minimization method was conducted on AAMs spanning the compositional envelopes at (metastable) thermodynamic equilibrium. The stability regions and quantities of simulated phases were identified in the SiO2-CaO-Al2O3 ternary contour diagrams, yielding the overall relationships between the chemical components of precursors, phase assemblages and pH in pore solution. The analytical results are in good agreement with the available experimental observations that the main stability regions of C-(N-)A-S-H appear at CaO/SiO2 = ~1.0 and relatively low Al regions while N-A-S-H phases generally dominate the Ca-deficient regions of the contour diagrams. Strätlingite mainly occurs at intermediate levels of Si, Al and Ca. Katoite and AFm phases form at Al2O3/CaO = ~3.0 under Si-deficient conditions. The findings also suggest the stability regions of a product may span a range of pH of aqueous solution, making it possible to simultaneously control pH and maintain the amount of precipitated phase. The application of this work in designing precursors can achieve a more precise control of the phase assemblages for AAMs.

**Bio:** Rui Xiao is currently a PhD student in Dr. Baoshan Huang’s group at the University of Tennessee. He received his B.E. in structural engineering from Tongji University and M. Sc. from Pennsylvania State University. He also worked as a structural engineer at China Railway Shanghai Design Inst. Co., Ltd. His current research interests include cement chemistry, image processing and moisture damage in asphalt mixture. Up to now, Rui has published 25 research papers in prestigious international journals. His PhD project is the multiscale investigation of interaction between moisture and asphalt-aggregate systems.

**Date and Time:**

 8:30 pm - 09:30 pm, January 29th (Saturday), 2022 (Eastern Time at New York)

9:30 am - 10:30 am, January 30th (Sunday), 2022 (Beijing Time in China)

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