July 8-10, 2013 | University of Illinois at Urbana-Champaign | Urbana, IL

4th Advances in Cement-based Materials: Characterization, Processing, Modeling and Sensing

FINAL PROGRAM

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MONDAY, July 8, 2013

Noon – 7:00 pm, Yeh Center Atrium
Registration

12:00 – 4:40 pm ♦ Yeh Center 1310
Tutorial: Probing the Structure of Hydration Products
Moderator: Paramita Mondal, Tyler Ley

12:00 – 12:05 pm
Welcome

12:05 – 12:55 pm
3-D Tomography
Erik Landis, University of Maine

12:55 – 1:45 pm
Fourier Transform Infrared Spectroscopy
Rohit Bhargava, Brad Deutsch, University of Illinois

1:45 – 2:10 pm ♦ FGH Atrium
Coffee Break

2:10 – 3:00 pm
Nuclear Magnetic Resonance Spectroscopy
Leslie Struble, University of Illinois

3:00 – 3:50 pm
Small Angle Neutron Scattering
Jeffrey Thomas, Schlumberger-Doll Research

3:50 – 4:40 pm
Lab Tour

5:00 – 7:00 pm ♦ Yeh Center Atrium
Poster Session and Opening Reception

Cleavage, Initial Hydration, Agglomeration and Interactions of Organic Molecules in Cement Clinker
Ratan Mishra, ETH Zurich; Robert Flatt, ETH Zurich; Hendrik Heinz, University of Akron

The 3-D shape of blasted and crushed rocks: 0.02 mm to 45 mm
Edward Garboczi, NIST; Michael Taylor, Granite Rock; Xuefeng Liu, China University of Petroleum (East China)

Application of EAFS as a cement replacement material
Mohammad. Reza. Nilforoushan, Shahrekord University; Sasan Otroj, Shahrekord University

The Performance of Inorganic Adhesive and Its Carbon Fiber Composites for Concrete Strengthening
Zhu Ding, Shenzhen University; Jian-Guo Dai, The Hongkong Polytechnic University Hongkong; Sarfraz Munir, The Hongkong Polytechnic University Hongkong; Bi-Qin Dong, Shenzhen University; Feng Xing, Shenzhen University

Why even difficult to avoid nanostructures in the CaO- SiO2-P2O5-H20 system
Leif Hermansson, Doxa AB

The properties of a chemical-healing microcapsule for cementitious system
Wang Yanshuai, Shenzhen University; Xian Xingping, Shenzhen University; Dong Biqin, Shenzhen University; Ding Zhu, Shenzhen University; Xing Feng, Shenzhen University

A Resistivity-Based Approach to Optimizing Concrete Performance
Elizabeth Nadelman, Georgia Institute of Technology; Kimberly Kurtis, Georgia Institute of Technology

Role of Interatomic Bonding in the Mechanical Anisotropy and Interlayer Cohesion of CSH Crystals
Chamila Dharmawardana, University of Missouri - Kansas City; Anil Misra, University of Kansas; Sitaram Aryal, University of Missouri - Kansas City; Wai-Yim Ching, Curators' Professor in Physics

Freeze-Thaw Performance of Concrete Railroad Ties
Kyle Riding, Kansas State University; Mohammed Albahttiti, Kansas State University; Ahmad Ghadban, Kansas State University

The impact of pretreatments and enzymatic hydrolysis on the pozzolanic reactivity of agricultural residue ash
Feraidon Ataie, Kansas State University; Kyle Riding, Kansas State University

Electrochemical impedance spectroscopy study of ion erosion behavior in cementitious materials
Chen Li, Shenzhen University; Xian Xiangping, Shenzhen University; Dong Biqin, Shenzhen University; Ding Zhu, Shenzhen University; Xing Feng, Shenzhen University

Assessing the Potential of Natural Pozzolans to be a Suitable Replacement for Class F Fly Ash in Concrete
Saamiya Seraj, University of Texas at Austin; Rachel Cano, University of Texas at Austin; Shukui Liu, University of Texas at Austin; Maria Juenger, University of Texas at Austin; Raissa Ferron, University of Texas at Austin; David Fowler, University of Texas at Austin; Jinying Zhu, University of Texas at Austin; David Whitney, University of Texas at Austin

Non-Contact Ultrasonic Method for Evaluation of Reinforced Concrete Elements Subjected to Mechanical Degradation Processe
Hajin Choi and John S. Popovics, The University of Illinois at Urbana-Champaign

Global and nano-scale characterization of heat-induced damage in Portland cement paste
Seungmin Lim, Jeevaka Somaratna, Paramita Mondal and John Popovics, The University of Illinois at Urbana-Champaign

Quality control of steel fiber reinforced cementitious composites using nondestructive evaluation
Stephen Garrett and John Popovics, The University of Illinois at Urbana-Champaign

Alcohol extraction to stop geopolymer formation
Xu Chen, Amr Meawad and Leslie Struble, The University of Illinois at Urbana-Champaign

Effect of temperature control on match-cured cylinder strength
Suyun Ham and John S Popovics, The University of Illinois at Urbana-Champaign

Novel Low Alkali Activated Fly Ash Cement (LAFAC) based Composites
M. Faisal Riyad, Tom Hammann, Ryan Johnson and Surojit Gupta, University of North Dakota

Effect of C/S on Al-uptake by C-S-H
Andrew Bishop, William Hunnicutt and Leslie Struble, University of Illinois at Urbana-Champaign

The effect of calcium hydroxide on gel formation in metakaolin-based geopolymer
Amr Meawad, Xu Chen and Leslie Struble, University of Illinois at Urbana-Champaign

Development of carbonation resistant cement for geologic sequestration of CO2

Chul-Woo Chung, Pukyong National University, Ji-Hyun Kim, Pukyong National University, Hun Bok Jung, Pacific Northwest National Laboratory and Wooyong Um, Pacific Northwest National Laboratory

The effect of Sporosarcina Pasteurii microorganism on the hydration kinetics of cement paste
Jun Cheol Lee, Kyungpook National University, Chang Joon Lee, Kyungpook National University, Woo Young Chun, Kyungpook National University, Wha Jung Kim and Chul-Woo Chung, Pukyong National University

Dispersion of Graphene Nanoplatelets in Polar Fluids
Erik Wotring, Paramita Mondal, University of Illinois at Urbana-Champaign and Charles Marsh, U.S. Army Corps of Engineers ERDC-CERL

Early-Age Volume Change and Hydration Kinetics of Type K Cement: Effect of Chemical and Mineral Admixtures
Piyush Chaunsali and Paramita Mondal, University of Illinois at Urbana-Champaign

The importance of silica additives in carbon nanotube reinforced mortar
Peter Stynoski, Paramita Mondal, University of Illinois at Urbana-Champaign and Charles Marsh, U.S. Army Corps of Engineers ERDC-CERL

Understanding the Fundamental Aspects of ASR-Induced Expansion: A Multidisciplinary Approach
Marc Knapp, Georgia Tech, Alvaro Paul, Georgia Tech, Sarah Hatfield, Kristen Donnell, Reza Zoughi, Missouri University of Science and Technology, Jin-Yeon Kim, Laurence Jacobs and Kimberly Kurtis, Georgia Tech

Multi-method characterization of ASR induced damage in cement composites
Kai Zhang, Alexander Lakocy, David Lange and John Popovics, University of Illinois Urbana-Champaign

Revealing Artifacts Caused by X-ray CT Imaging During Rapid Hydration via Simulation
Jason Mote and David Lange

Rubble to Reconstruction: Closing the Loop on Concrete Recycling
Andrea Vetrone, Hannah Ackermann, Elizabeth Nadelman, Passarin Jongvisuttisun, Soheil Shayegh, Georgia Tech Ismael Flores-Vivian, University of Wisconsin, Milwaukee, Mitchell McKay, Georgia Tech, Konstantin Sobolev, University of Wisconsin, Milwaukee, Reginald Desroches and Kimberly Kurtis, Georgia Tech

Early Age Autogenous Shrinkage in Geopolymers
Ranjani Mosale Vijayakumar and Paramita Mondal, University of Illinois at Urbana-Champaign

THE USE OF NANOPARTICLES TO IMPROVE THE PERFORMANCE OF CONCRETE
Ismael Flores-Vivian, Rani G.K. Pradoto, Mohamadreza Moini and Konstantin Sobolev, University of Wisconsin-Milwaukee

Effects of Microbially Induced Carbonate Precipitation on Cement Paste
Bin Zhang, Paramita Mondal, Pete Stynoski, University of Illinois Urbana-Champaign, Charles Marsh, U.S. Army Engineer Research And Development Center, Construction Engineering Research Laboratory and Wen-Tso Liu, University of Illinois Urbana-Champaign

Graphene Nanoreinforcement for Cement-based Composites
Nima Zohhadi, Nirupam Aich, Fabio Matta, Navid Saleh, Paul Ziehl and Addis Kidane, University of South Carolina

Materials Engineering for Durable and Sustainable Grain storage Structures in Developing Countries for Post-Harvest Loss Prevention
Sravanthi Puligilla, Xinyuan Yang, Paramita Mondal and John S. Popovics, University of Illinois at Urbana-Champaign

High Performance Superhydrophobic Engineered Cementitious Composites (SECC) for use in Highway Applications
Scott Muzenski, Ismael Flores-Vivian and Konstantin Sobolev, University of Wisconsin-Milwaukee

Electrochemical impedance spectroscopy study of chloride ion erosion behavior in cementitious materials
Li Chen , Weipeng Yuan1, Xiangping Xian, Yanshuai Wang, Feng Xing and Biqin Dong, Shenzhen University

7:00 – 8:00 pm ♦Yeh Center
Cements Division Executive Meeting

7:00 – 8:00 pm ♦
Student Networking Dinner

TUESDAY, July 9, 2013

7:30 am – 6:30 pm ♦ Yeh Center Atrium
Registration

8:30 – 8:35 am ♦ Yeh Center
Open Program/Welcome

8:35 – 10:05 am
Technical Session I ♦ Yeh Center 1310
Calcium Silicate Hydrate
Moderator: Jeffrey Chen, Paramita Mondal

8:35 – 8:50 am
Unravelling C-S-H atomic structure via computational and experimental physical chemistry
Mohammad Javad Abdolhosseini Qomi, MIT; Mathieu Bauchy, MIT; Roland Pellenq, MIT, CNRS France

8:50 – 9:05 am
Durability and volume stability of C-S-H/polyaniline nanocomposites
Rahil Khoshnazar, National Research Council of Canada; James Beaudoin, National Research Council of Canada; Laila Raki, National Research Council of Canada; Rouhollah Alizadeh, Giatec Scientific Inc.

9:05 – 9:20 am
Atomistic Study of Inter-particle Forces in C-S-H, and screw dislocations in layered, complex hydrated oxides: case of tobermorite
Soroosh Jalilvand, Rice University; Lu Chen, Rice University; Rouzbeh Shahsavari, Rice University

9:20 – 9:35 am
Vertical Scanning Interferometry (VSI): A Novel Method to Measure the Dissolution Dynamics of Cementitious Minerals
Aditya Kumar, University of California Los Angeles; Gaurav Sant, University of California Los Angeles; Jason Reed, University of California Los Angeles

9:35 – 9:50 am
Effects of elevated temperature on the structure and properties of calcium-silicate-hydrates: The role of confined water
Patrick Bonnaud, Qing Ji and Krystyn Van Vliet, MIT

9:50 – 10:05 am
Carbonation of synthesized C-S-H
William Hunnicutt, University of Illinois Urbana-Champaign; Leslie Struble, University of Illinois Urbana-Champaign

10:05 – 10:30 am ♦ Yeh Center Atrium
Coffee Break

10:30 – 12:00 am
Technical Session II ♦ Yeh Center 1310
Concrete Material Models
Moderator: Rouzbeh Shahsavari, Jeffrey Thomas

10:30 – 10:45 am
Viscoelastic Poisson's Ratio of Porous Cement Paste
Zachary Grasley, VT

10:45 – 11:00 am
A Coupled Chemo-Mechanical Analysis of Ordinary Cement Paste's Microstructure
Daniel Vallée Vallée, Luca Sorelli, Universite Laval and Jeffry Chen, LCR Lafarge

11:00 – 11:15 am
Lattice Discrete Particle Modeling (LDPM) of Alkali Silica Reaction (ASR) deterioration of concrete structures
Mohammed Alnaggar, Northwestern University; Gianluca Cusatis, Northwestern University; Giovanni Di Luzio, Politecnico di Milano

11:15 – 11:30 am
Nano-mechanics of irreversible deformation and failure of the C-S-H gel in cement: polydisperse colloidal model
Enrico Masoero, MIT Emanuela Del Gado, ETH Zurich, Roland J.-M. Pellenq, Sidney Yip and Franz-Josef Ulm, MIT

11:30 – 11:45 am
Modeling chemical compositional changes in concrete pore solution within microenvironments adjacent to steel reinforcement
Burkan Isgor, Oregon State University and Pouria Ghods, Carleton University

11:45 – 12:00 noon
A material model and its application to simulate the composite material structure of mortar and concrete using real-shape particles
Edward Garboczi, NIST; Zhiwei Qian, Delft Technical University; Yang Lu, Boise State University

10:30 – 11:45 am
Technical Session III ♦ Yeh Center 2311
Concrete Durability
Moderator: Tyler Ley, Rouhollah Alizadeh

10:30 – 10:45 am
Material Property Inputs for Chloride Diffusion Prediction: Comparing Fick's Second Law and Nernst – Planck Parameters
Yiwen Bu, Daming Luo and Jason Weiss, Purdue University

10:45 – 11:00 am
Drying of cementitious materials: Influence of liquid properties on the diffusion coefficient
Chiara Villani, Purdue University, Robert Spragg, Purdue University, Mohammad Pou-Ghaz, North Carolina State University and W. Jason Weiss, Purdue University

11:00 – 11:15 am

Influence of Aggregate Properties on Stresses in Freezing Concrete as Determined by Poromechanical Modeling
Syeda Rahman, Texas A&M University; Zachary Grasley, Virginia Tech

11:15 – 11:30 am
Evaluation of Freeze and Thaw Damage in Mortars Containing Deicing Salt Using A Low Temperature Guarded Comparative Longitudinal Calorimeter and Acoustic Emission
Yaghoob Farnam,Purdue University, Dale Bentz, National Institute of Standards and Technology, Aaron Sakulich, Worcester Polytechnic Institute, Daniel Flynn, National Institute of Standards and Technology and Jason Weiss, Purdue University

11:30 – 11:45 am
Alkali-Silica Reaction: Chemical Reaction Sequence, Kinetics and Thermodynamic Modeling
Taehwan Kim, Purdue University; Jan Olek, Purdue University

12:00 – 1:30 pm
LUNCH

1:30 – 2:45 am
Technical Session IV ♦ Yeh Center 1310
Shrinkage, Shrinkage Reducing Admixtures and Other additives
Moderator: Gourav Sant, Narayanan Nathalath

1:30 – 1:45 pm
Development of Shrinkage Limits and Testing Protocols for High Performance Concrete
Tengfei Fu, Oregon State University; Tyler Deboodt, Oregon State University; Jason Ideker, Oregon State University

1:45 – 2:00 pm
Long-term Shrinkage Prediction from Theoretical Considerations and Data Analysis
Mija Hubler, Northwestern University; Roman Wendner, Northwestern University; Zdenek Bazant, Northwestern University

2:00 – 2:15 pm
Computer-Aided Molecular Design using the Signature Molecular Descriptor and the Search for New Admixtures for Concrete – Part 1 Identification of Surface Tension Reducing Agents and the Search for Shrinkage Reducing Admixtures
Hamed Kayello, The University of Akron; Donald Visco Jr., The University of Akron; Joseph Biernacki, Tennessee Technological University

2:15 – 2:30 pm
Computer-Aided Molecular Design using the Signature Molecular Descriptor and the Search for New Admixtures for Concrete – Part 2 Validating Newly Identified Surface Tension Reducing Substances for Potential Use as Shrinkage Reducing Admixtures
Natalia Shlonimskaya, Tennessee Technological University; Joseph Biernacki, Tennessee Technological University; Hamed Kayello, The University of Akron; Donald Visco Jr., The University of Akron

2:30 – 2:45 pm
Effect of Diethanol-Isopropanolamine on the Hydration of Slag Blended Cement
Leslie Jardine, W.R. Grace; Denise Silva, W.R. Grace; Richard Sibbick, W.R. Grace

1:30 – 3:00 am
Technical Session V ♦ Yeh Center 2311
Nano-materials and Bio-materials
Moderator: Zach Grasley, Ardavan Yazdanbakhsh

1:30 – 1:45 pm
Measuring the adhesive properties of nanoclay-modified cement pastes with the tack test
Shiho Kawashima, Columbia University; Mohend Chaouche, CNRS/ENS-Cachan; David Corr, Northwestern University; Surendra Shah, Northwestern University

1:45 – 2:00 pm
Influence of nano materials on the hydration kinetics and rheology of cement paste
Xin Wang, Kejin Wang, Iowa State University and Jussara Tanesi, Turner Fairbank Highway Research Center

2:00 – 2:15 pm
High performance cellulose nanocrystal reinforced cement composites
Yizheng Cao, Purdue University; Jeffrey Youngblood, Purdue University; Jason Weiss, Purdue University; Robert Moon, US Forest Service- Forest Products Laboratory; Pablo Zavattieri, Purdue University

2:15 – 2:30 pm
Utilizing submicron inclusions to enhance the properties of structural concrete made with recycled aggregates
Ardavan Yazdanbakhsh, City College of New York - CUNY; Michel Ghosn, City College of New York - CUNY; Julio Davalos, City College of New York - CUNY; Larry Bank, City College of New York - CUNY

2:30 – 2:45 pm
Effects of incorporating nanosilica on the carbonation of cement paste
Seungmin Lim and Paramita Mondal, The University of Illinois at Urbana-Champaign

2:45 – 3:00 pm
Lightweight Aggregates as Internal Reservoirs of Bioactive Agents
Aaron Sakulich and Hajar Jafferji, Worcester Polytechnic Institute

3:00 – 3:30 pm ♦ Yeh Center Atrium
Coffee Break

3:30 – 4:30 pm ♦Yeh Center
Cements Division Meeting

4:30 – 5:30 pm ♦Yeh Center
Della Roy Lecture and Reception
Sponsored by Elsevier
Moderator: David Lange

Calcium in geopolymers
Leslie Struble, University of Illinois

6:30 – 9:00 pm ♦ Allerton Park
Della Roy Reception and Conference Dinner
Co-Sponsored by Elsevier

WEDNESDAY, July 10, 2013

7:30 am – Noon ♦ Yeh Center Atrium
Registration

8:30 – 10:00 am
Technical Session VI ♦ Yeh Center 1310
Geopolymer
Moderator: Matthew D'Ambrosia, Shiho Kawashima

8:30 – 8:45 am
On the Development of Low Alkali Activated Fly Ash Cement (LAFAC)
Surojit Gupta, M. Faisal Riyad, Ryan Johnson and Tom Hammann, University of North Dakota

8:45 – 9:00 am
Activator, source material, and curing effects on alkali activation reactions
Ussala Chowdhury, Sundararaman Chithiraputhiran, Akash Dakhane and Narayanan Neithalath, Arizona State University

9:00 – 9:15 am
Rheological study on coal, biomass and co-fired fly ash cementitious and geopolymeric pastes
Christopher R. Shearer, Georgia Institute of Technology; Chiara F. Ferraris, National Institute of Standards and Technology and Kimberly E. Kurtis, Georgia Institute of Technology

9:15 – 9:30 am
Geopolymer Densification Using Functional Alkoxysilanes
Brayden Glad and Waltraud Kriven, University of Illinois Urbana-Champaign

9:30 – 9:45 am
Coexistence of C-S-H and K-A-S-H characterized through selective dissolution and FTIR spectral subtraction
Sravanthi Puligilla and Paramita Mondal, University of Illinois at Urbana-Champaign

9:45 – 10:00 am
Mitigation of dehydration cracking and thermal shrinkage in geopolymer systems by the addition of alumina platelet reinforcement.
Gregory Kutyla and Waltraud Kriven, University of Illinois Urbana-Champaign

10:00 – 10:30 am ♦ Yeh Center Atrium
Coffee Break

10:30 – 11:45 am
Technical Session VII ♦ Yeh Center 1310
Alternative Cements
Moderator: Kyle Riding, Paramita Mondal

10:30 – 10:45 am
Studies of PLC Synergies and Their Potential for Enhancement of Concrete Performance
Tim Cost, Holcim (US) Inc; Wayne Wilson, Holcim (US) Inc.

10:45 – 11:00 am
Directions towards High-Volume Limestone Cements: An Overview of Efforts on Enhancing Cement Replacement Levels
Gaurav Sant, University of California, Los Angeles

11:00 – 11:15 am
Evaluating the beneficial effects of lower alkali cementing systems with or without SCMs on ASR
Soley Einarsdottir and R. Doug Hooton, University of Toronto

11:15 – 11:30 am

Mechanisms of Shear Load Transfer in Polymer-cement composites in the Plastic Regime
Navid Sakhavand, Rice University; Rouzbeh Shahsavari, Rice University

11:30 – 11:45 am
Frost Resistance of Geopolymer
Xueying Li, Harbin Institute of Technology; Zhenzhen Jiao, Harbin Institute of Technology; Zheng Wang, Harbin Institute of Technology

10:30 – 11:45 am
Technical Session VIII ♦ Yeh Center 2311
Early Age Properties: Kimberly Kurtis, Benjamin Mohr

10:30 – 10:45 am
Kinetics and activation energy of magnesium oxide (MgO) hydration – Comparison with hydration of cement
Jeffrey Thomas, Schlumberger-Doll Research; Simone Musso, Schlumberger-Doll Research; Ivan Prestini, Schlumberger-Doll Research

10:45 – 11:00 am
A closer look at the experimental and materials related parameters influencing the rheology of cementitious pastes
Kirk Vance, Arizona State University, Aditya Kumar, University of California Los Angeles, Gaurav Sant, University of California Los Angeles and Narayanan Neithalath, Arizona State University

11:00 – 11:15 am
The relationship between the Nurse-Saul Datum Temperature and the FHP Activation Energy for Concrete Maturity and Application of The Bertalanffy Model for Concrete Maturity
Chang-Hoon Lee, Cornell University; Kenneth Hover, Cornell University

11:15 – 11:30 am
Topological constraints : a tool to predict cement aging
Mathieu Bauchy, MIT; Mohammad Javad Abdolhosseini Qomi, MIT; Deater Brommer, MIT; Roland Pellenq, MIT

11:30 – 11:45 am
Robustness of Self-Consolidating Concrete: New Testing Method and Effect of Aggregate Properties
Lin Shen, University of Hawaii at Manoa; Hamed Bahrami Jovein, University of Hawaii at Manoa

11:45 – 1:30 pm
LUNCH

1:30 – 3:00 pm
Technical Session IX ♦ Yeh Center 1310
Analytical Techniques for Characterization, Sensors, Other Smart Materials
Moderator: John Popovics, Aaron Sakulich

1:30 – 1:45 pm
Internal Relative Humidity of Concrete in Railroad Environments
Daniel Castaneda and David Lange, University of Illinois Urbana-Champaign

1:45 – 2:00 pm
Detection of corrosion in steel-reinforced concrete by anti-ferromagnetic resonance
Edward Garboczi, NIST

2:00 – 2:15 pm
Three-Phase Cement Piezoelectric Composites for Use as Sensors for Health Monitoring
Kimberly Cook-Chennault, Rutgers University; Sankh Banerjee, Rutgers University

2:15 – 2:30 pm
Insitu Observations of Hydrating C3S with Synchrotron Nanocomputed Tomography
Tyler Ley, Qinang Hu, Mohammed Aboustait, Jay Hanan, Oklahoma State University and Robert Winarski, Advanced Photon Source - Argonne National Laboratory

2:30 – 2:45 pm
Automated and Manual Characterization of Input Parameters for the VCCTL
Benjamin Watts, Christopher Ferraro, University of Florida, Engineering School of Sustainable Infrastructure and Environment, April Snyder, R J Lee Group and H.D. Deford, Florida Department of Transportation

2:45 – 3:00 pm
Finite Element Modeling of Concrete Based on Quantitative Computed Tomography (QCT)
Arash Razmjoo, Clemson University; Amir Poursaee, Clemson University

MONDAY, July 8, 2013

5:00 – 7:00 pm ♦ Yeh Center Atrium
Poster Session and Opening Reception

Cleavage, Initial Hydration, Agglomeration and Interactions of Organic Molecules in Cement Clinker
Ratan Mishra, ETH Zurich; Robert Flatt, ETH Zurich; Hendrik Heinz, University of Akron

Understanding the surface, structural and chemical properties of cementitious materials have been a challenging problem due to boundaries of experimental technique. We use molecular dynamics simulations to validate force field models of main silicate and aluminate phases of ordinary Portland cement clinker. This study provides excellent agreement with available experimental data, including X-ray structures, cleavage energies, elastic properties, and IR spectra. On the basis of accurate force field parameterizations of atomistic models of tricalcium silicate and tricalcium aluminate, we apply the models to quantify cleavage energies, initial hydration (first step dissolution), mechanisms of mineral surface interactions with organic additives (grinding aids) and approximate agglomeration energies of clinker particle. Selected organic additives include classical grinding aids, which are triisopropanol amine (TIPA), triethanol amine (TEA), glycerine and N-methyl diisopropanolamine (MDIPA). Computed agglomeration energies in the presence of organic molecules correlate directly to the reduction in surface forces and also predict the ranking of grinding aids in connection with measured grinding efficiencies. This work guides in approaches toward energy saving during the grinding process of cement clinker.

The 3-D shape of blasted and crushed rocks: 0.02 mm to 45 mm
Edward Garboczi, NIST; Michael Taylor, Granite Rock; Xuefeng Liu, China University of Petroleum (East China)

Does particle shape depend on particle size? To help answer this question, granodiorite material from a rock quarry in California was prepared by first quarrying large boulders, and then crushing them down to smaller sizes. A range of particle sizes, from 0.02 mm to 45 mm and all from this same material, was scanned using X-ray computed tomography (X-ray CT) and the shape of individual particles obtained from the resulting 3-D images was analyzed using spherical harmonic-based techniques. The size range covered was more than three orders of magnitude in size and more than ten orders of magnitude in volume. For this dataset, comprised of over 58 000 particles, we have computed the distributions of four different and independent shape parameters and found that the shape of the particles was the same, within statistical fluctuation, for three different size classes that covered the complete range considered: 0.0175 mm to 0.24 mm, 0.24 mm to 3.29 mm, and 3.29 mm to 45.1 mm. This implies a degree of similarity between blasting and crushing in terms of the fracture processes involved in fragmenting rocks, since most or all of the rocks were subjected to both. We also compared a simulation of 2-D optical scanning results to the true 3-D X-ray CT results, showing the strengths and weaknesses of a 2-D approach to particle shape and giving empirical fits, with uncertainties, connecting three sets of 2-D and 3-D parameters.

Application of EAFS as a cement replacement material
Mohammad. Reza. Nilforoushan, Shahrekord University; Sasan Otroj, Shahrekord University

Slag is the byproduct of steel companies. Two different types of slag produced during iron ore smelting process. Blast furnace and Electric Arc Furnace slag. The difference between these two slag is mainly due to source of steel production process. The amount of FeO is up to 1% in the former and about 30% in the latter, but both can be used as cement replacement materials if special type of cooling process applies to produce an amorphous structure in slag. A number of works has previously been done on BFS but very little information could be extracted from previous investigation. In this study, the granules of rapidly cooled EAFS have been replaced by part of cement in the concrete mixtures. The results showed that 17% of cement in 350 grade concrete, 20% of 400 grade and 25% of cement in 500 grade concrete may be replaces by granulated EAFS without any reduction on its 28 days compressive strength, and the resulted concrete has better corrosion resistance in chemical environments than plan one./

The Performance of Inorganic Adhesive and Its Carbon Fiber Composites for Concrete Strengthening

Zhu Ding, Shenzhen University; Jian-Guo Dai, The Hongkong Polytechnic University Hongkong; Sarfraz Munir, The Hongkong Polytechnic University Hongkong; Bi-Qin Dong, Shenzhen University; Feng Xing, Shenzhen University

The fiber reinforced polymer (FRP) composites were popular material for strengthening and retrofitting of concrete structures. But there are some problems associated with use of FRP. Inflammability of organic polymer, smoke generation and incompatibility with concrete substrate are some of the typical problems which lead to development of alternate inorganic matrix and bonding adhesive. Inorganic phosphate adhesive, such as magnesium phosphate cement (MPC), has been proved an excellent repair material for deteriorated concrete structures. Due to its high adhesive property, it has high boding strength with old concrete substrate. In this paper, the properties of the improved magnesium phosphate cement, and the properties of the MPC bonded carbon fiber composite were studied. These properties include physical and mechanical of the fresh mixed and the hardened MPC paste, the bond strength of fiber in matrix, tensile strength of the inorganic matrix based impregnated fiber composites. Also, the microstructure of the matrix was investigated. The results show the improved MPC binder is potential to develop a fiber reinforced inorganic polymer (FRiP), as an alternate to externally bonded FRP composites for strengthening of concrete structures. The present study may provide a deep understanding the behavior of MPC bonded fiber composite.

Why even difficult to avoid nanostructures in the CaO- SiO2-P2O5-H20 system

Leif Hermansson, Doxa AB

The chemically bonded bioceramics within the CaO- SiO2-P2O5-H20 system (CBBCs) comprise silicates, aluminates and phosphates with calcium as the main cation. The presentation will give background aspects to the observed microstructures of the CBBC-materials, which all seem to exhibit nanostructures, both nanocrystals and nanoporosity. These cement materials are now establishing their use as injectable biomaterials and as general bone void filler within dentistry and orthopedics, and as carriers for drug delivery. The precipitation of all the nanophases is controlled by very low solubility products of the phases in the systems. The nanostructures of the CBBC systems based on Ca-silicates and Ca-aluminates include in addition to the principle phases of the main systems also a nanosize apatite phase when in contact with body liquid. The alkaline systems transfer hydrogen phosphates in body liquid into pure phosphate, and repeated precipitation of apatite, Ca5(PO4)3(OH) occurs in the contact zone between the biomaterial and the tissue. The chemically bonded bioceramics – especially the materials based on phosphates, aluminates and silicates – exhibit a general nanostructure related to both the crystals (10-50 nm in size) and the pore chanells (1-3 nm in width) between the crystals formed. Due to a low solubility product of the phases formed, nanocrystals are easily formed, and it is even difficult to avoid the nanostructural features.

The properties of a chemical-healing microcapsule for cementitious system

Wang Yanshuai, Shenzhen University; Xian Xingping, Shenzhen University; Dong Biqin, Shenzhen University; Ding Zhu, Shenzhen University; Xing Feng, Shenzhen University

A novel chemical self-healing system based microcapsule technology is designed for cementitious composites, which is accompanied by a chemical trigger mechanism. The fundamental issue of this system is the smart releasing performance in cementitious environment and controlled rebar protection effectiveness against corrosion. The measurements with Ethylene Diamine Tetraacetic Acid (EDTA) titration and electrochemical impedance spectroscopy (EIS) method are applied to achieve above targets. The experimental results show that properties of microcapsule are affected by the time, the wall thickness of microcapsule and the pH value in cementitious environment. An electrochemical model is built up to explain the anti-corrosion pattern of this microcapsule based self-healing system.

A Resistivity-Based Approach to Optimizing Concrete Performance

Elizabeth Nadelman, Georgia Institute of Technology; Kimberly Kurtis, Georgia Institute of Technology

Surface resistivity (SR) testing is increasingly being used to non-destructively assess concrete quality, largely because the test is relatively fast and simple to perform compared to some existing standard tests for diffusion and permeability. Measurements can be made within minutes using an off-the-shelf device available from several commercial producers, and a provisional test standard (AASHTO TP95) provides guidance on performing the test. Currently, SR testing is used as an alternative to the more time-consuming and labor-intensive Rapid Chloride Permeability (RCP) test described in ASTM C1202 and AASHTO T277, but extensions of this test method to other aspects of concrete durability are also possible. This poster will present a novel extension of the SR test for optimizing concrete mix design and performance. The technique will be applied to a variety of conventional concrete mixtures, as well as to mixtures made with green cements. The performance of each mixture will be comparatively assessed, and correlations to RCP test results will also be presented.

Role of Interatomic Bonding in the Mechanical Anisotropy and Interlayer Cohesion of CSH Crystals

Chamila Dharmawardana, University of Missouri - Kansas City; Anil Misra, University of Kansas; Sitaram Aryal, University of Missouri - Kansas City; Wai-Yim Ching, Curators' Professor in Physics

Atomic scale properties of calcium silicate hydrate (CSH), the main binding phase of hardened Portland cement, are not well understood. Over a century of intense research has identified almost 50 different crystalline CSH minerals which are mainly categorized by their Ca/Si ratio. The electronic structure and interatomic bonding in four major CSH crystalline phases with structures close to those found in hardened cement are investigated via ab initio methods. Our result reveals the critical role of hydrogen bonding and importance of specifying precise locations for water molecules. Quantitative analysis of contributions from different bond types to the overall cohesion show that while the Si-O covalent bonds dominate, the hydrogen bonding and Ca-O bonding are also very significant. Calculated results reveal the correlation between bond topology and interlayer cohesion. The overall bond order density (BOD) is found to be a more critical measure than the Ca/Si ratio in classifying different CSH crystals.

Freeze-Thaw Performance of Concrete Railroad Ties

Kyle Riding, Kansas State University; Mohammed Albahttiti, Kansas State University; Ahmad Ghadban, Kansas State University

Literature review shows that freezing and thawing durability testing of pre-stressed concrete ties is currently performed by applying ASTM C-666 on small 3 x 3 x 10 to 16 in. specimens cut out of the shoulders of concrete ties. It is natural to assume that Saw-cutting hardened concrete specimens may result in stress relief and formation of micro-cracks which have unknown consequences and may lead to false interpretations of the results. Testing the entire concrete tie in freezing and thawing, which has been rarely done, would eliminate not only damage from saw-cutting but also sample variability based on the location of sampling. In this research, whole pre-stressed concrete ties supplied by the Illinois Department of Transportation (IDOT) were tested by procedures similar to that of the ASTM C-666, except for how the ties were maintained saturated. They were kept saturated by wrapping them in saturated burlap and vacuum sealed plastic tubes. Testing was performed following the same methods used in the ASTM C-666. The first test is the impact resonance frequency test which was performed on different locations on the ties to get an idea about the cracks that might form inside the ties due to freezing and thawing cycles. The second test is the length change test using a Whittemore gage and small brass points epoxied to the surface of the ties at several locations and directions being placed at 8 in. apart. This test helps in identifying any significant changes in lengths that might arise due to the continuous change in temperature values. Finally, the change in weights of the ties and the weights of the scaled off particles were recorded in order to monitor any significant loss of weights that might result from the damage incurred by the freezing and thawing cycles.

The impact of pretreatments and enzymatic hydrolysis on the pozzolanic reactivity of agricultural residue ash

Feraidon Ataie, Kansas State University; Kyle Riding, Kansas State University

According to Federal Renewable Fuel Standard, lignocellulosic ethanol production is expected to reach 10.5 billion gallons by 2020. Agricultural residues such as corn stover, rice straw, and wheat straw, are potential resources for lignocellulosic ethanol production. Bioethanol production from agricultural residues leaves behind high lignin residues (HLR) that could be potential resources for supplementary cementitious materials (SCMs) production for use in concrete. Utilization of HLR for SCMs production is important for both the concrete and biofuel industries as it will help reduce the environmental impact of concrete and adds value to biofuel waste products. However, because agricultural residues undergo acidic and basic pretreatments techniques to boost ethanol yield, depending on their type, pretreatments could have negative impact on the HLR properties so that it could not be utilized for SCMs production. Therefore, in this study, the impact of sodium hydroxide and dilute sulfuric acid pretreatments along with enzymatic hydrolysis on the pozzolanic properties of the corn stover ash, rice straw ash, and wheat straw ash was investigated. The pozzolanic reactivity of the ashes was quantified based on the heat of hydration and the calcium hydroxide consumption when used as 15% replacement level of portland cement.

Electrochemical impedance spectroscopy study of ion erosion behavior in cementitious materials

Chen Li, Shenzhen University; Xian Xiangping, Shenzhen University; Dong Biqin, Shenzhen University; Ding Zhu, Shenzhen University; Xing Feng, Shenzhen University

In this paper, an electrochemical impedance spectroscopy (EIS) method is applied to characterize the ion erosion behavior in cementitious material, which includes Cl-, SO42-, Mg2+, respectively. The experimental results show that the electrochemical impedance feature is affected by the erosion time, ion concentration and water/cement ratio of the cementitious materials. Moreover, a novel uniform equivalent circuit model is proposed to interpretate the influencing factors on the electrochemical impedance behavior, which takes into account the function of ions diffusion and charge transfer in cementitious materials. The modeling curve gives a good fit both to the resistance and reactance loci depending to the frequency with the experimental data.

Assessing the Potential of Natural Pozzolans to be a Suitable Replacement for Class F Fly Ash in Concrete

Saamiya Seraj, University of Texas at Austin; Rachel Cano, University of Texas at Austin; Shukui Liu, University of Texas at Austin; Maria Juenger, University of Texas at Austin; Raissa Ferron, University of Texas at Austin; David Fowler, University of Texas at Austin; Jinying Zhu, University of Texas at Austin; David Whitney, University of Texas at Austin

Class F Fly ash is extensively used as a supplementary cementitious material (SCM) in concrete because it increases long term strength and durability of concrete to alkali silica reaction and sulfate attack. However, the future availability of Class F Fly Ash has become a source of concern because of impending environmental restrictions that can threaten its supply. Our research focuses on finding alternative SCMs that can provide similar benefits in concrete such as Class F Fly Ash. The materials that are being tested in this research are mostly natural pozzolans such as pumice, vitric ash, clay and shale, that are available in the US.

Non-Contact Ultrasonic Method for Evaluation of Reinforced Concrete Elements Subjected to Mechanical Degradation Processe

Hajin Choi and John S. Popovics, The University of Illinois at Urbana-Champaign

In this paper, a newly developed ultrasonic technology for concrete inspection is evaluated. We use non-contact (air-coupled) ultrasonic scanning measurements to characterize a full-scale concrete columns subjected to simulated earthquake loads. The contactless nature of the measurements enables many data to be collected in a short time, and enables the construction of images built up from those data. Two types of images are considered: stacked time signals and tomographic reconstructions of material ultrasonic velocity and attenuation. The background on the ultrasonic method is described, and the data analysis and image construction processes are demonstrated. Ultrasonic images collected across the plastic hinge zone of the loaded column show that it is possible to monitor the progression of internal damage, and thus provide better understanding of the mechanical degradation process within cement based materials.

Global and nano-scale characterization of heat-induced damage in Portland cement paste

Seungmin Lim, Jeevaka Somaratna, Paramita Mondal and John Popovics, The University of Illinois at Urbana-Champaign

Portland cement concrete degrades when exposed to sustained high temperatures. Although the nature of this degradation has been well studied, some aspects of the behavior remain unknown. In this study we employ a nano-scale characterization tool (static and dynamic nanoindentation) and global mechanical methods (vibration resonance frequency and damping) to better understand the degradation of Portland cement paste subjected to high temperature exposures. Prismatic paste samples are subjected to two different types of temperature exposure: a rapid heating and cooling routine up to a maximum of 350oC, which is expected to promote drying and thermal gradient cracking damage within the paste, and a gradually applied exposure at 700oC sustained for 6 hours, which is expected to produce significant decomposition of main hydration products (C-S-H and CH). Samples without any heat treatment are considered as control. The prismatic samples are subjected to the vibrational tests to obtain the global damage characteristics. Then small samples are drawn of the prisms to run the nanoindentation tests. The 7×7 grid dynamic nanoindentation (49 indents) with a grid spacing of 10 μm will provide storage and loss modulus values across a suite of test locations. Storage modulus values will be compared with static indentation modulus obtained from another set of 49 indents performed on the same sample but at a different location. Storage and loss modulus will also be

compared to global resonant frequency and damping, respectively, for each sample, and conclusions about, and links between, the effect of the two temperature heating regimes on the properties at the global and microstructural scale will be drawn.

Quality control of steel fiber reinforced cementitious composites using nondestructive evaluation
Stephen Garrett and John Popovics, The University of Illinois at Urbana-Champaign

Material developments have paved the way for steel fiber-reinforced concrete (SFRC) to be a viable building material for structural applications. However material variability concerns like the fiber content, dispersion and orientation within an SFRC element, which are inherent with the addition of fibers in the concrete matrix, must be addressed. Nondestructive techniques can be employed to compliment, or replace, the current destructive methods of quality control to address this issue. Electrical- and magnetic-based methods show promise for nondestructive characterization of fiber properties in SFRC, because these techniques utilize the conducting nature of the steel fibers. In this study, we apply several nondestructive tests to SFCR samples with varying fiber content (20, 45, and 70 kg/m3) and orientation, where the fiber orientations in the samples were controlled using flow characteristics of the mixture during casting. Different geometries and the inclusion of additional reinforcing steel elements are considered. Results from tests using surface resistivity and eddy current responses on the samples are reported and compared to results from non-electrical test methods such as resonance vibration and ultrasonic pulse velocity, mechanical wave tests being common quality control measures. The results show that the electrical- and magnetic-based methods are most appropriate for fiber characterization of SFRC, and that reasonable estimation of fiber volume and orientation are obtained when those tests are properly applied and interpreted.

Alcohol extraction to stop geopolymer formation
Xu Chen, Amr Meawad and Leslie Struble, The University of Illinois at Urbana-Champaign

The purpose of this study is to explore whether alcohol, commonly used to stop cement hydration, can be used to stop the geopolymer reaction. A 50/50(vol) methanol/acetone solvent was used. Two aspects were studied: (1) changes caused by the treatment and (2) effectiveness of the treatment at freezing the structure. FTIR and MAS-NMR measurements were conducted. The precursor dissolution was stopped by the treatment but polymerization of the geopolymer gel continued slowly, though no changes in structure were seen until about 50 hours after treatment. The treatment was seen to remove aluminosilicate species with low Q values. Thus the treatment suspends but does not stop the geopolymer reaction.

Effect of temperature control on match-cured cylinder strength
Suyun Ham and John S Popovics, The University of Illinois at Urbana-Champaign

Match curing is a process whereby companion concrete test specimens are cured with the same temperature history as the concrete in a structure that they represent. This technology is commonly used by concrete pre-stressed element manufacturers to determine appropriate stress release and demolding times. Here we investigate the temperature control precision needed to provide accurate match-cured 1- day compressive strength estimates. A novel water bath match curing system was developed for this study. The system allows precise and accurate temperature control of the match-cured companion cylinders. First the water bath system is introduced and compared to air chamber and insulated cylinder mold match cure systems. Then six different temperature profile modifications to the defined adiabatic temperature profile are applied using the water bath system and the strength evaluated. Both transient and continue error profiles are considered. A rigorous statistical analysis is used to evaluate the results from over 200 samples. The test results reveal that transient temperature control disruption (significant loss of temperature control over a short period of time) has much larger influence on 24-hour strength than constant temperature offset error when error area (error maturity) are compared. This suggests that absolute temperature error is the best standard of measurement for match cure temperature control. Limits on temperature control precision are suggested.

Novel Low Alkali Activated Fly Ash Cement (LAFAC) based Composites
M. Faisal Riyad, Tom Hammann, Ryan Johnson and Surojit Gupta, University of North Dakota

The alkali activation of Fly Ash to produce cementitious materials is an important area for fundamental research. From environmental perspective, the use of alkali activators, for example NaOH, is an environmental concern as it is electrochemically generated with the concomitant production of harmful Cl2 or HCl gas as by products. The use of high concentration of alkali solution is also harmful to human health. Most of the current research on activation of fly ash based materials has been done with high concentration of alkali solutions. Recently, we proposed that it is possible to use activate Fly Ash to produce cementitious network by using low concentration of alkaline solutions (<0.05 M). In this poster, we will present some of the recent results on the development of composites of Low Alkali Activated Fly Ash Cement (LAFAC) with different types of additives, for example, sand, calcium carbonate, among others. Detailed mechanical property studies, microstructure analysis, and phase analysis will be presented in this poster.

Effect of C/S on Al-uptake by C-S-H

Andrew Bishop, William Hunnicutt and Leslie Struble, University of Illinois at Urbana-Champaign

As part of ongoing research on the effects of alumina incorporation in calcium silicate hydrate, C-(A)-S-H was synthesized in two steps—the first being synthesis of C-S-H by reaction between fumed silica, CaO, and H2O, and the second being reaction of the C-S-H with an aluminum nitrate solution. Higher C/S is known to produce shorter chains with fewer bridging tetrahedral sites occupied. And AlO4 is known to preferentially occupy the bridging tetrahedral sites. So this study explored whether the amount of aluminum uptake by C-S-H is influenced by its C/S. 27Al and 29Si MAS-NMR, X-Ray diffraction, and X-Ray fluorescence were utilized. The hypothesized relationship between Al uptake and C/S was not supported. However, the C/S was seen to affect the extent of chemical shielding experienced by alumina tetrahedra.

The effect of calcium hydroxide on gel formation in metakaolin-based geopolymer

Amr Meawad, Xu Chen and Leslie Struble, University of Illinois at Urbana-Champaign

The purpose of this study is to investigate the effect of calcium hydroxide addition on the rate of metakaolin dissolution and geopolymer gel formation. The metakaolin is blended with different percentages of calcium hydroxide and an alkaline activator solution containing sodium hydroxide and sodium silicate is used. In situ attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy is performed on all samples for up to 7 days. The results reveal that the rate of dissolution and gel formation is strongly affected by the presence of calcium hydroxide, and that geopolymer gel and calcium silicate hydrate coexists from an early age.

Development of carbonation resistant cement for geologic sequestration of CO2

Chul-Woo Chung, Pukyong National University, Ji-Hyun Kim, Pukyong National University, Hun Bok Jung, Pacific Northwest National Laboratory and Wooyong Um, Pacific Northwest National Laboratory

In order to increase the integrity of the wellbore which is used to prevent the leakage of supercritical CO2 (captured from CO2 capture process), it is necessary to develop a concrete that is strongly resistant to carbonation. In an environment where the concentration of CO2 is exceptionally high (in supercritical CO2 concentration), Ca2+ ion concentration in pore solution of portland cement concrete drops significantly due to the rapid consumption of calcium hydroxide, which decreases the stability of the calcium silicate hydrate. We hypothesize that if fairly large quantity of the hydrated product consists of phases that are more thermodynamically stable than that of calcite, the carbonation process can be minimized. The proposed study aims to modify portland cement concrete system using phosphates, and will show applicability of these materials to enhance carbonation resistance of concrete that will be used for geological sequestration of CO2.

The effect of Sporosarcina Pasteurii microorganism on the hydration kinetics of cement paste

Jun Cheol Lee, Kyungpook National University, Chang Joon Lee, Kyungpook National University, Woo Young Chun, Kyungpook National University, Wha Jung Kim and Chul-Woo Chung, Pukyong National University

From years of research activities, it was shown that the application of microorganism increased the compressive strength of cement based materials when it is cured in culture medium. However, it is economically infeasible to locate the specimens in culture medium because the same curing methodology is unlikely to be applied for the real concrete structure. This research aims to directly incorporate microorganism (Sporosarcina Pasteurii) into cement based material. The role of microorganism on hydration kinetics of cement based materials was investigated without curing the specimens in culture medium. According to the results, it was found that the microorganisms accelerated the early hydration and caused higher strength than that of plain cement paste at 7 days. However, the microorganisms led to the smaller compressive strength after 28 days. There was no clear evidence observed on microbial induced calcite precipitation when the microorganisms were directly mixed with cement paste.

Dispersion of Graphene Nanoplatelets in Polar Fluids

Erik Wotring, Paramita Mondal, University of Illinois at Urbana-Champaign and Charles Marsh, U.S. Army Corps of Engineers ERDC-CERL

This research studied the effects of surfactant on graphene nanoplatelet (GNP) dispersion in water. Several specimens were prepared which contained water, GNPs, and varied amounts of water reducing admixture (WRA). The GNP was added at 0.2% by weight of water. Sedimentation was subjectively characterized by observing the rate at which GNPs settled out of suspension. Particle size and the stability of suspension were objectively characterized with dynamic light scattering (DLS) and by monitoring the evolution of light transmission with ultraviolet-visible spectroscopy (UV/Vis), respectively. In all of these experiments, the amount of WRA was used as the independent variable. Improvement of GNP dispersion in water is expected to lead to the opportunity to exploit the mechanical and electrical properties of graphene in developing new generations of composite materials in the future.

Early-Age Volume Change and Hydration Kinetics of Type K Cement: Effect of Chemical and Mineral Admixtures

Piyush Chaunsali and Paramita Mondal, University of Illinois at Urbana-Champaign

Type K cement has been traditionally used in developing shrinkage-compensating concrete. Ye'elimite (C4A3Ṡ) is one of the main phases present in Type K cement. Hydration of ye'elimite in presence of gypsum results in formation of ettringite, causing early-age expansion. This research presents the early-age behavior of a Type K cement in presence of chemical and mineral admixtures. The Type K cement was prepared by replacing 15% (by mass) of portland cement with a calcium sulfoaluminate additive. Three mineral admixtures: class 'F' fly ash, class 'C' fly ash and silica fume, and a hydration controlling chemical admixture were utilized in this study. Various paste samples were prepared at w/cm ratio of 0.44. The expansion of paste samples was monitored in sealed and saturated lime water curing. The hydration progress of Type K cements was monitored using x-ray diffraction, thermogravimetry and isothermal calorimetry. The importance of various parameters governing the expansion of Type K cement is also highlighted.

The importance of silica additives in carbon nanotube reinforced mortar

Peter Stynoski, Paramita Mondal, University of Illinois at Urbana-Champaign and Charles Marsh, U.S. Army Corps of Engineers ERDC-CERL

Many recent studies have focused on improving the dispersion of carbon nanotubes (CNTs) in cementitious composites using admixtures, functionalization, and high shear mixing techniques. However, little attention is paid to the bond strength and load transfer efficiency between hydrated cement and CNTs. The literature has established that adding silica fume to conventional fiber reinforced concrete and mortar refines the interfacial transition zone near the surface of the fibers. A high concentration of calcium hydroxide at the interface encourages the pozzolanic reaction. The development of C-S-H in this critical region enhances the fracture parameters of the overall composite. In this study, silica fume and silica functionalization are used to apply this concept to CNTs in Portland cement mortar. The silica functionalization is covalently bonded to CNTs, further enhancing the bond between hydration products and CNTs. Additionally, carbon nanotubes and fibers are used together to control cracking at multiple scales. Mixtures included CNTs at a loading of 0.125% by mass of cement, which is equivalent to 0.05% by volume of the mixture, and/or carbon fibers at a loading of 0.25% by volume of the mixture. Workability of the mixtures was controlled using a set neutral high-range water reducing admixture to achieve a target flow measurement. Notched beams were tested according to the Jenq and Shah Two Parameter Fracture Model to determine the critical stress intensity factor and the critical crack tip opening displacement. The effects of silica fume and functionalization were more pronounced at 28 days of age than at 7 days. The CNTs did not improve the fracture parameters of mixtures containing carbon fibers. Mixtures containing carbon fibers and silica fume significantly outperformed all mixtures containing CNTs at 28 days. Future work might attempt to optimize the diameter and aspect ratio of CNTs to approach the critical length of load transfer necessary for improvement of fracture properties. Furthermore, addition of nanosilica powder might improve particle packing and encourage hydration nearer to the surface of CNTs.

Understanding the Fundamental Aspects of ASR-Induced Expansion: A Multidisciplinary Approach

Marc Knapp, Georgia Tech, Alvaro Paul, Georgia Tech, Sarah Hatfield, Kristen Donnell, Reza Zoughi, Missouri University of Science and Technology, Jin-Yeon Kim, Laurence Jacobs and Kimberly Kurtis, Georgia Tech

Long-held technical beliefs surrounding the alkali-silica reaction (ASR) in concrete have been increasingly questioned in recent years, undermining the ability of engineers to assess aggregate reactivity, to design ASR-resistant concrete, and to assess the potential for ASR damage in service. A multi-physics research effort is underway to address the gaps in current understanding of the reaction fundamentals, including understanding of the relationships between location, volume, and composition of ASR gel on potential for expansion and damage to concrete. This comprehensive effort has been developed to take advantage of the sensitivity of microwave methods to moisture content and binding and the sensitivity of nonlinear and linear acoustic methods to microcracking and cracking to overcome some of the challenges associated with the in situ examination of durability reactions in cementititious materials. Correlating these data with temporal changes in multi-scale structure, composition, and mechanical properties will bring new insight to a reaction which is increasingly damaging to concrete infrastructure, allowing for advancements in design, repair/mitigation, and service life modeling.

Multi-method characterization of ASR induced damage in cement composites

Kai Zhang, Alexander Lakocy, David Lange and John Popovics, University of Illinois Urbana-Champaign

Alkali silica reactivity (ASR) can cause significant and widespread damage to portland cement concrete. Standard test methods such as ASTM C227 (mortar bar test), ASTM C1260 (accelerated mortar bar test) and ASTM C1293 (concrete prism test) evaluate potential of an aggregate to expand deleteriously due to ASR by measuring length change of prismatic samples. In this study we employ two new methods in experiments that allow comparison to length change. The two new methods to monitor ASR-induced expansion and degradation are an optical characterization tool (digital image correlation) and a global mechanical method (vibration resonance frequency and damping). Prismatic mortar samples that contain a portion of aggregates replaced with known reactive aggregate (silica glass) are subjected to standard accelerated ASR exposure environment: immersion in 1 N sodium hydroxide solution at 80oC. This environment is expected to promote extensive ASR reaction and material expansion and cracking within days of exposure. In the mechanical methods, samples cured in a standard moist room environment are considered as control. At regular intervals during the exposure, the prismatic samples are removed from the solution and subjected to vibrational tests in order to obtain the global damage characteristics. At the same time, in the digital image correlation test, samples immersed in 1 N sodium hydroxide solution at 80C are considered as control. A sample from the same batch that is housed in a specially built transparent container is digitally photographed at regular intervals, and the images are processed using DIC software (Matlab) to compute the surface strain field in the sample. The axial length extension of each sample is also measured directly. The DIC strain field and the global resonant frequency and damping results will be compared to the length change results for each sample set. Conclusions about, and links between, the two nondestructive characterization techniques with respect to the axial extension and physical appearance of the ASR samples will be drawn.

Revealing Artifacts Caused by X-ray CT Imaging During Rapid Hydration via Simulation

Jason Mote and David Lange

Full volume images of hydrating cement paste collected using X-ray CT techniques can provide a wealth of information regarding the microstructure. Discernment between real features in the sample and artifacts can be challenging. Ongoing research at the University of Illinois at Urbana-Champaign is making use of lab based micro and nano X-ray CT scanners to image cement paste samples at various time intervals. There are several, often competing, factors that must be weighed against one another when setting parameters for collecting X-ray CT data. The image quality of CT scans is often improved by increasing the number of projections collected and increasing the exposure time used for each projection which can lead to lengthy scan durations between collecting the initial and final projections. The use of lab based X-ray sources further increases scan durations for each projection as a result of low photon flux when compared to synchrotron sources. Reconstruction algorithms used to generate the 3D images from the 2D projections assume the microstructure of the specimen is the same throughout the duration of the scan. Software was written to simulate collecting 2D projections from a specimen with a known initial microstructure evolving at a known rate to determine the artifacts that may be generated. Simulating CT imaging can allow the experimentalist to distinguish between actual features present in the specimen and artifacts created by imaging an evolving specimen.

Rubble to Reconstruction: Closing the Loop on Concrete Recycling

Andrea Vetrone, Hannah Ackermann, Elizabeth Nadelman, Passarin Jongvisuttisun, Soheil Shayegh, Georgia Tech Ismael Flores-Vivian, University of Wisconsin, Milwaukee, Mitchell McKay, Georgia Tech, Konstantin Sobolev, University of Wisconsin, Milwaukee, Reginald Desroches and Kimberly Kurtis, Georgia Tech

The reuse of crushed and graded concrete construction debris or waste, often stemming from demolition of existing structures or excess in new construction, is relatively widely practiced throughout the world. Recently, it was proposed that concrete debris resulting from an extreme event could be potentially be used in reconstruction, producing concrete which achieves adequate compressive strengths when the debris appropriately processed and the concrete is suitably proportioned. This research addresses two remaining challenges which partially “close the loop” on assessing the potential for debris recycling in new construction. First, the seismic performance of reinforced concrete containing construction debris as coarse aggregate is reported. Second, the potential use of the fine particles, which derive during the crushing of debris, is examined.

Early Age Autogenous Shrinkage in Geopolymers

Ranjani Mosale Vijayakumar and Paramita Mondal, University of Illinois at Urbana-Champaign

Geopolymers are considered to be a sustainable alternative to cement and offers comparable or enhanced mechanical properties. Depending upon raw materials and curing conditions, geopolymers exhibit a wide variety of properties like high compressive strength, low drying shrinkage etc. Studies have indicated that the geopolymers show much more thermal resistance as compared to Portland cement concrete by showing very little change in volume at high temperatures. Studies have also indicated a smaller drying shrinkage for heat-cured flyash based geopolymer binders compared to Portland cement binders. However, present study has indicated that the early age shrinkage in geopolymer in sealed condition is much higher than those observed in Portland cement pastes made using the same water to solids ratio. The setting time is measured using the proctor test and prisms are demolded once set. The shrinkage measurements are started immediately after demolding. An elaborate study has been undertaken to observe the influence of various factors on the early-age shrinkage of geopolymers in sealed condition made from varying molarities, K2O to SiO2 ratios, and SiO2 to Al2O3 ratios.

THE USE OF NANOPARTICLES TO IMPROVE THE PERFORMANCE OF CONCRETE

Ismael Flores-Vivian, Rani G.K. Pradoto, Mohamadreza Moini and Konstantin Sobolev, University of Wisconsin-Milwaukee

A reduction in size of nanoparticles provides an exceptional surface area-to-volume ratio and changes in the surface energy, surface chemistry, and surface morphology of the particle, altering its basic properties and reactivity. These characteristics significantly enhance the mechanical performance of a variety of materials, including metals, polymers, ceramic, and concrete composites. Concrete can be nano-engineered by incorporating nano-sized building blocks or objects (e.g., nanoparticles and nanotubes) to control material behavior and add novel properties, or by grafting molecules onto cement particles, cement phases, aggregates, and additives (including nano-sized additives) to provide surface functionality, which can be adjusted to promote specific interfacial interactions. Nanosilica (silicon dioxide nanoparticles, nano-SiO2), for example, has been shown to improve workability and strength in high-performance and self-compacting concrete. This article reviews the beneficial effects of the nanoparticles for the improvement of concrete performance.

Effects of Microbially Induced Carbonate Precipitation on Cement Paste

Bin Zhang, Paramita Mondal, Pete Stynoski, University of Illinois Urbana-Champaign, Charles Marsh, U.S. Army Engineer Research And Development Center, Construction Engineering Research Laboratory and Wen-Tso Liu, University of Illinois Urbana-Champaign

Microbially induced carbonate precipitation (MICP) in cement-based construction materials attracted research interest due to its potential for healing cracks. Previous studies showed that different bacterial strains have the capability of producing calcium carbonate to fill up cracks in concrete. However, it is still unclear if the supply of external calcium ions besides calcium silicate hydrate (C-S-H) and calcium hydroxide (CH) present in concrete is necessary for the production of calcium carbonate. Furthermore, effects of consumption of CH and possibly C-S-H during MICP on cement paste and concrete microstructure is unknown. In this study, detailed investigation is performed to compare MICP in cement paste and in liquid nutrient medium when cement paste with and without an additional calcium source (calcium chloride) was used. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and Scanning electron microscopy (SEM) was used to characterize the precipitates. Based on these experiments, vaterite and calcite seemed to form predominantly. Thermal analysis (TGA) is performed for quantitative characterization of the precipitates.

Graphene Nanoreinforcement for Cement-based Composites

Nima Zohhadi, Nirupam Aich, Fabio Matta, Navid Saleh, Paul Ziehl and Addis Kidane, University of South Carolina

Graphene nano-platelets (GNPs) are introduced as reinforcement for ordinary Portland cement-based composites to enhance compressive and tensile strength and toughness. GNPs can be processed at a relatively low cost via chemical exfoliation1. These nano-platelets possess comparable mechanical properties to multi-walled carbon nanotubes (MWCNTs) together with a higher specific surface area, which promises to facilitate bonding with the surrounding cement-based matrices. GNPs in water tend to agglomerate due to their hydrophobicity and strong van der Waals forces. Therefore, suitable functionalization is key to attain uniform aqueous dispersion. In this study, epitaxial GNPs were debundled in water via ultrasonication and stabilized using a commercially available surfactant (SAA). The SAA's amphiphilic molecules are physically bound on the GNPs preventing re-aggregation through electrosteric repulsive interaction, providing better chemical affinity with cement hydrates. A suitable GNP/SAA ratio was determined based on the minimum average hydrodynamic radius measured in aqueous suspensions by dynamic light scattering (DLS). The incorporation of well dispersed graphitic nanoreinforcement results in increased compressive strength of cement paste and mortar by reducing both porosity and meso-pore size, and increasing the amount of high-stiffness calcium silicate hydrate4. In this study, the effectiveness of functionalization of GNPs was first assessed via compression tests of cement mortar cubes with different GNP/SAA weight ratios and GNP concentrations. Five samples per combination were tested. It was found that incorporating a small amount of GNPs (0.05% by weight of cement, wt%) with a specific GNP/SAA ratio selected through DLS leads to an average 40% increase in compressive strength compared to plain mortar within a similar standard deviation. The hypothesis of good dispersion of functionalized GNPs was also supported by evidence from scanning electron microscopy and energy-dispersive X-ray spectroscopy analysis of samples from fracture surfaces. Flexural strength and toughness enhancement were assessed for the selected 0.05 wt% GNP-SAA combination via three point bending tests of 20×20×80 mm single edge notched beam samples made of cement paste. Digital image correlation (DIC) was enlisted for full-field strain measurement near the notch tip. It was found that the flexural strength and Young's modulus increased on average by 33% and 118%, respectively, thus supporting the evidence from the compression tests. The DIC strain maps consistently highlighted a significantly larger fracture process zone with lower maximum strain in GNP reinforced samples, thus supporting the hypothesis of fracture toughening through the incorporation of well dispersed GNPs.

Materials Engineering for Durable and Sustainable Grain storage Structures in Developing Countries for Post-Harvest Loss Prevention

Sravanthi Puligilla, Xinyuan Yang, Paramita Mondal and John S. Popovics, University of Illinois at Urbana-Champaign

Between harvesting and consumption, the quality and quantity of staple crops such as rice is seen to rapidly deteriorate (20-30% loss) due to poor post-harvest management. In this project, construction of an economically viable storage structure on the farm has been proposed to build using locally available materials to reduce post-harvest loss. To avoid deterioration during storage, both moisture ingress into grain storage structure and moisture loss from grains should be prevented. Economic solution to this problem can be provided to the farmers by using a low cost cementitious construction material that incorporates locally available low cost fibers for low shrinkage and better crack resistance. Most common fibrous material available locally in the farm possibly is the burlap (jute) and polyethylene fibers taken out of old sacs used previously for storage and transportation of grains and other agricultural products. In this work, different weight percentages (1%, 3%, 5%) of burlap and polyethylene fibers are used in mortars. Compressive strength, free drying shrinkage and fracture parameters are evaluated for above dosages of fibers. Preliminary results show that mortar with 1 inch and 2 inch burlap fibers show better compressive strength compared to equivalent mortar samples with polyethylene fibers and seems to be promising candidate as construction material for building of grain storage structure.

High Performance Superhydrophobic Engineered Cementitious Composites (SECC) for use in Highway Applications

Scott Muzenski, Ismael Flores-Vivian and Konstantin Sobolev, University of Wisconsin-Milwaukee

The United States infrastructure is in desperate need of repair, especially in regions exposed to harsh environments. Freezing and thawing cycles in northern regions lead to early need for repair or failure of bridges. A more durable concrete is required in order to increase the service life of roadways and to minimize the need for repair. The use of polyvinyl alcohol (PVA) fibers in engineered cementitious composites (ECC) creates a durable concrete capable of withstanding large deformations from temperature variations, freezing and thawing cycles, and cyclic loading; greatly extending the service life of roadways. This is achieved by the increased deformability created by the multi-cracking behavior of the ECC. Combining ECC with superhydrophobic admixtures (SECC) creates a material with water repellant air voids to even further increase the materials resistance to freezing and thawing cycles. This research demonstrates that the durability of the developed material can exceed performance of conventional concrete, since cracks that inevitably form within cementitious materials are held small enough so that minimal amounts of water can penetrate the crack while at the same time the water repellant nature of the crack eliminates water from freezing within the crack. Additionally, the addition of superhydrophobic admixtures creates a well distributed air void system that acts as artificial flaws to promote multi-cracking and strain-hardening behavior.

Electrochemical impedance spectroscopy study of chloride ion erosion behavior in cementitious materials
Li Chen , Weipeng Yuan1, Xiangping Xian, Yanshuai Wang, Feng Xing and Biqin Dong, Shenzhen University

In this paper, an electrochemical impedance spectroscopy (EIS) method is applied to characterize the Cl ion erosion behavior in cementitious material. The experimental results show that the electrochemical impedance feature is affected by the erosion time, ion concentration and water/cement ratio of the cementitious materials. Moreover, a novel uniform equivalent circuit model is proposed to interpretate the influencing factors on the electrochemical impedance behavior, which takes into account the function of ions diffusion and charge transfer in cementitious materials. The modeling curve gives a good fit both to the resistance and reactance loci depending to the frequency with the experimental data.

TUESDAY, July 9, 2013

8:35 – 10:05 am
Technical Session I ♦ Yeh Center 1310
Calcium Silicate Hydrate

8:35 – 8:50 am
Unravelling C-S-H atomic structure via computational and experimental physical chemistry
Mohammad Javad Abdolhosseini Qomi, MIT; Mathieu Bauchy, MIT; Roland Pellenq, MIT, CNRS France

Calcium Silicate Hydrate (CSH) is the main binding phase for the cement paste, which is responsible for its strength and creep behavior. This is a non-stoichiometric hydration phase with calcium to silicon ratio (C/S) ranging from 1 to 2.2. At low C/S ratios, the molecular structure of CSH resembles to that of Tobermorite minerals while in high C/S ratios it mostly looks like disordered glasses. By taking advantage of tools of statistical physics, it is shown that CSH at a given C/S can be associated with degenerate molecular structures called CSH polymorphs. Polymorphs are energetically competitive, i.e. they have the same free energy content, which means they can coexist under equilibrium conditions. To start, SiO2 groups are randomly removed from the layered atomic structure Tobermorite 11A. In this procedure, 150+ CSH structures are created. Grand Canonical Monte Carlo simulation of water adsorption is performed to adsorb water in the interlayer spacing and nano-scale porosities in defected CSH structures. The amount of adsorbed water scales linearly with the number of defects in the calcium-silicate layer. To study the reactivity of ultra-confined water, all samples are relaxed using a reactive potential in canonical and isothermal-isobaric ensembles. We observe that the confined water reacts with the free inter-layer calcium atoms and non-bridging oxygen to form hydroxyl groups. The number of hydroxyl groups scales linearly with the amount of defects. The amount of water in CSH and Ca-OH content match well with Drying and Neutron Scattering experiment in the literature. While the reactive modeling of CSH impacts the water molecules in CSH's nano-confinemnt environment, it does not signifacantly affect the silica chain length. This means that the reactive atomistic modeling does not affect the calico-silicate backbone of CSH structures. The silica mean chain length from atomistic simulation aligns perfectly with experimental Nuclear Magnetic Resonance (NMR) data. The elastic properties and hardness of all CSH polymorphs are measured at a given C/S and are directly compared with nano-chemo-mechanical testing via coupled nano-indentation and X-ray Wavelength Dispersive Spectroscopy (WDS). Atomistic simulation matches with the experimental data in both elastic and plastic regimes. These properties show a range at a given stoichiometry. To unravel the underlying reason behind this variation, the correlation of mechanical properties to structural observables of the molecular structures such as dimer content, mean silicate chain length, density, basal distance, water content, number of hydroxyl groups and topological constraints parameter are calculated. No direct correlations were found at short ranges (bond lengths and angles). The search was extended to the medium range order analysis of the CSH nanostructure and it is found that the polymorphism is a closely related the meadium range order of Si-O bonds. It should be emphasized that since CSH polymorphs are statistically equi-probable in equilibrium conditions, the only way to precipitate a given polymorph during cement setting is through kinetic means of clinker reactions.

8:50 – 9:05 am

Durability and volume stability of C-S-H/polyaniline nanocomposites

Rahil Khoshnazar, National Research Council of Canada; James Beaudoin, National Research Council of Canada; Laila Raki, National Research Council of Canada; Rouhollah Alizadeh, Giatec Scientific Inc.

Concrete materials innovation through the application of nanotechnology has received significant interest in recent years. Most of the investigations have focused on the calcium-silicate-hydrate phase (C-S-H) as it is the primary binding phase in hydrated cement paste. The ultimate goal is to develop a new class of organically-modified C S-H-based nanocomposites with enhanced engineering characteristics. C-S-H/polyaniline nanocomposites are new composite materials which have been recently synthesized using an in-situ polymerization technique. It has been suggested that the polyaniline is formed in two different locations of the C-S-H i.e. grafted on the surface and partially intercalated in the interlayer regions. The current study is intended to investigate the durability and volume stability of C-S-H/polyaniline nanocomposites in various aqueous salt solutions. Samples of phase pure C-S-H and C-S-H/polyaniline nanocomposite were immersed in aqueous solutions of magnesium, sodium and lithium salts, and their time-dependent length-change was determined. The possibility of interaction of these solutions with the C-S-H structure was also investigated using X-ray diffraction and scanning electron microscopy techniques. It is suggested that the C S H/polyaniline nanocomposites have greater volume stability compared to the reference system in all the solutions investigated. Their microstructure is also more stable, and exhibits less degradation during the exposure in the aggressive solutions.

9:05 – 9:20 am

Atomistic Study of Inter-particle Forces in C-S-H, and screw dislocations in layered, complex hydrated oxides: case of tobermorite

Soroosh Jalilvand, Rice University; Lu Chen, Rice University; Rouzbeh Shahsavari, Rice University

Calcium-Silicate hydrate (C-S-H) is the primary binding phase in cement paste that is typically considered as an assemblage of discrete nanoscale particles whose interactions are governed by nano-scale friction and cohesion that occurs at their interfaces. Therefore, a fundamental understanding on the nature of such interfacial forces can provide invaluable insights into overall mechanical properties of such particulate system. In this regards, atomistic simulation provides a powerful tool to decode the complex nanoscale interactions. Here, we are particularly interested in constitutive relations that relate friction and normal forces to the contact area that arise from the interaction of two C-S-H particles. Such description requires the “redefinition” of classical concepts such as friction or contact area to reflect the nanoscale nature of this phenomena; multi-scale picture of nanoscale contact is used for this purpose. The normal force is calculated by relaxation of two C-S-H particles at various distances from each other and with different crystallographic orientations. The effect of watery environment is studied by immersing the particles in water molecules. The friction force, is calculated by sliding the tip over the substrate in various directions. Our study identifies the distinct contribution of van der Waals and electro-static forces to the behavior of C-S-H particles at contact. While the electrostatic forces govern the interaction of particles at short and large distances, the van der Waals forces are responsible for variations in the normal force at intermediate distances. We find that normal force varies sub-linearly with nanoscale contact area between the tip and substrate, while the friction force shows a linear trend. Besides, our calculations identify to what extent atoms of particular type contribute to the total interfacial forces. In turns out due to large electronegativity of Si atoms, they contribute most to the friction and normal forces that occur between the tip and substrate. Our results for the first time provides “atomistic lens” on nanoscale friction and contact phenomena in particulate C-S-H systems. This has a significant impact on fundamental understating of C-S-H and modulation of its behavior, thus impacting the mechanics of cementitious materials.

Dislocations are a common type of defects that significantly influence many mechanical phenomena such as plastic deformation, crystal growth, morphology, or diffusion of materials. While dislocations have been well studied for simple crystalline structures such as pure metals, semi-conductors, ionic materials, and binary oxides, there is very limited knowledge on such defects in complex layered oxides. In this work, we study the mechanisms and the influences of screw dislocations in tobermorite mineral, which is a complex layered oxide material serving as a natural analog of Calcium-Silicate-Hydrate (C-S-H) gel. The latter is the principal source of strength and durability in concrete. We use a cluster-based approach combined with atomistic simulations to investigate the screw dislocation along the interlayer direction of tobermorite. An analytical solution of the sextic theory regarding anisotropic materials was implemented to obtain the elastic displacement field. The nonlinear deformations around the core dislocation were accurately captured by atomistic simulations. The final core has a complex 3D structure involving dramatic spiral displacements as well as formation of defected silicate chains resulting from the screw dislocation. Dislocation displacement map (DDM) indicates an ellipsoid non-planar spreading of the dislocation core extending about in 40 Å the [100] direction and 20 Å in the [010] direction. This analysis illustrates a low mobility of [001] screw dislocation in tobermorite, since any potential movement will inevitably involve silicate chain breakage. After fitting the atomistic data to classical screw dislocation theories, the core radius is found to be 14.3 Å with a core energy of 53.7 eV/Å. This formation energy and the above observation could be used to compare and predict the prevalent defects along different directions in tobermorite, thus providing fundamental insights on deformation mechanisms governing the mechanical responses in C-S-H phases.

9:20 – 9:35 am

Vertical Scanning Interferometry (VSI): A Novel Method to Measure the Dissolution Dynamics of Cementitious Minerals

Aditya Kumar, University of California Los Angeles; Gaurav Sant, University of California Los Angeles; Jason Reed, University of California Los Angeles

The aqueous dissolution rate is a key indicator of a portland cement's reactivity, and is relevant in predicting the progress of reactions and early age property development in cement based systems. Though a valuable material property, dissolution rates for neither the individual cement phases, nor their mixtures have been rigorously determined. This work for the first time applies vertical scanning interferometry (VSI) as a new method, to measure the dissolution dynamics of cement relevant minerals. Special emphasis is placed on measuring the first dissolution rate, i.e., when water initially and for a short duration (i.e., on the order of tens of seconds) contacts the mineral surface. First dissolution rates (DRF, moles/m2/s) are measured for a variety of fast and slow dissolving minerals including: (1a) limestone ($CaCO_3$), (1b) gypsum ($CaSO_4 \cdot 2H_2O$), (2) alite (impure, MIII-Ca_3SiO_5) and (3) an ASTM C150, Type I/II portland cement across a range of solution pH levels. In addition to the VSI, a variety of experimental and computational tools including image acquisition, image-processing, regression analysis and interpretation are utilized to ensure statistical treatment of the results. The outcomes develop quantifications of aqueous dissolution rates- valuable inputs in the simulation of cement hydration, and forward a new means to study correlations between composition, crystallography and the reactivity of cementitious materials.

9:35 – 9:50 am

Effects of elevated temperature on the structure and properties of calcium-silicate-hydrates: The role of confined water

Patrick Bonnaud, Qing Ji and Krystyn Van Vliet, MIT

Water confined within the nano- to microscale pores of cementitious materials plays a crucial role in damage processes affecting the sustainability of cement pastes, especially for the binding material comprising calcium-silicate-hydrates (C-S-H). Here, we employed Grand Canonical Monte-Carlo and molecular dynamics simulations to investigate the effect of temperature on the water content (i.e., number and location of water molecules) within and between C-S-H grains constituting the cement microstructure, and on the associated physical and mechanical properties. We found water content within grains decreased with increasing relative temperature up to $T/T^* = 2$ (T^* being the transition temperature at which the bulk liquid and gas are in equilibrium for a given pressure), and that C-S-H grains densified with attendant increases in heat capacity, stiffness, and hardness. Although intragranular cohesion increased monotonically with increasing relative temperature over this range, intergranular cohesion increased up to a relative temperature of T/T* = 1.1 and then decreased at higher relative temperatures. This finding suggests a rationale for the decreased mechanical performance of cement paste and concrete at high relative temperatures, and supports previous claims of peak hardness in C-S-H at an intermediate relative temperature between 1 and 2.61. Further, these atomistic simulations underscore the important role of confined water in modulating the structure and properties of calcium-silicate-hydrates upon exposure to extreme environments.

9:50 – 10:05 am

Carbonation of synthesized C-S-H

William Hunnicutt, University of Illinois Urbana-Champaign; Leslie Struble, University of Illinois Urbana-Champaign

Carbonation of laboratory synthesized C-S-H is nearly unavoidable and can have significant impact on the molecular structure. Considerable carbonation was observed in C-S-H synthesized from sodium silicate and calcium nitrate solutions but not in C-S-H synthesized from fumed silica and calcium hydroxide solution. Carbonation was induced by stirring synthesized C-S-H in four different water-based solutions containing dissolved CO2. The pH of the solution was seen to strongly influence the degree of carbonation while alkali content had a less significant effect. X-ray diffraction, thermogravimetric analysis, and 29Si nuclear magnetic resonance were used to probe the carbonation and the resulting changes in the molecular structure.

10:30 – 12:00 am
Technical Session II ♦ Yeh Center 1310
Concrete Material Models

10:30 – 10:45 am

Viscoelastic Poisson's Ratio of Porous Cement Paste

Zachary Grasley, VT

In order to effectively analyze the state of stress and strain in concrete structures, it is necessary to incorporate viscoelastic constitutive relations to account for stress relaxation and creep effects. As many structures involve three-dimensional states of stress and strain, at least two viscoelastic constitutive properties (for an isotropic material) are needed for such analysis. While the viscoelastic uniaxial properties of concrete have been widely measured, other viscoelastic properties, such as the viscoelastic Poisson's ratio, are not well characterized. The dearth of data regarding the viscoelastic Poisson's ratio of concrete and cement paste is due in part to the extreme difficulty in measuring the property. Thus, computer simulations were run to evaluate VPR. The simulation results indicate that VPR for porous materials such as cement paste or concrete is highly dependent on the pore structure.

10:45 – 11:00 am

A Coupled Chemo-Mechanical Analysis of Ordinary Cement Paste's Microstructure

Daniel Vallée Vallée, Luca Sorelli, Universite Laval and Jeffry Chen, LCR Lafarge

The mechanical properties of the phases present in the cement paste's microstructure have been widely studied by nano- and micro-indentation techniques in the latest 10 years. However, recent studies based on Focused Ion Beam and Energy Dispersion Spectroscopy found that cement paste is highly heterogeneity at the micrometer scale. Thus, the mechanical result from a nanoindentation test which is actually probing a sample volume of micrometer size is likely a composite behavior. This works aims at disclosing the "pure" mechanical properties of microstructure cement paste by coupling the nanoindentation and SEM-EDS. We considered three systems: hydrated C2S, hydrated C3S and Ordinary Cement Portland (OPC). On each sample, we carried out 400 tests in displacement-control by imposing a maximum penetration depth of 150 nm for 600 seconds. Then, we performed the chemical analysis by tracking the indented points by SEM-EDS. Chemical analysis allowed selecting the indentation tests of the above mentioned phases. The advantage of this one-to-one chemo-mechanical analysis approach is that there is no need of a statistical deconvolution to estimate the property of the phases. The results shows that the mechanical response of is likely due to intermix of hydrated and anhydrate phases in the probed micro-volume. It was possible to identify the value of pure phase by identifying the chemical structure. Finally, we compared the deterministic approach with the statistical one based on the cluster analysis.

11:00 – 11:15 am

Lattice Discrete Particle Modeling (LDPM) of Alkali Silica Reaction (ASR) deterioration of concrete structures

Mohammed Alnaggar, Northwestern University; Gianluca Cusatis, Northwestern University; Giovanni Di Luzio, Politecnico di Milano

A large number of structures especially in high humidity environments are endangered by Alkali-Silica Reaction (ASR). ASR is characterized by two processes: the first is gel formation resulting from the reaction, in presence of water, between alkali and reactive silica in aggregate particles; the second is water imbibition into the formed gel which leads to progressive swelling behavior. This swelling causes deterioration of concrete mechanical behavior in the form of strength and stiffness loss over time. In the recent past, many research efforts were directed towards evaluation, modeling and treatment of ASR effects on structures but a comprehensive computational model is still lacking. In this paper, the ASR effect is implemented within the framework of the Lattice Discrete Particle Model (LDPM). LDPM, in a full 3D setting, simulates the mechanical interaction of coarse aggregate pieces through a system of three-dimensional polyhedral particles, each resembling a spherical coarse aggregate piece with its surrounding mortar, connected through lattice struts [1] and it has the ability of simulating the effect of material heterogeneity of the fracture processes. LDPM is capable of accurately describing concrete macroscopic behavior in elastic, fracturing, softening, and hardening regimes [2]. The proposed formulation, entitled ASR-LDPM, allows precise and unique modeling of volumetric expansion, expansion anisotropy under applied load, non-uniform cracking distribution, temperature effects, effect of relative humidity variation, shrinkage effect and creep effect on concrete subjected to ASR. Simulation of experimental data gathered from the literature demonstrates the ability of ASR-LDPM to predict accurately ASR-induced concrete deterioration.

11:15 – 11:30 am

Nano-mechanics of irreversible deformation and failure of the C-S-H gel in cement: polydisperse colloidal model

Enrico Masoero, MIT Emanuela Del Gado, ETH Zurich, Roland J.-M. Pellenq, Sidney Yip and Franz-Josef Ulm, MIT

The calcium silicate hydrate (C—S—H) gel is the main binding phase of ordinary cements. At scales below the micron it shows a network of meso-pores, several nanometers wide, and a solid skeleton with amorphous molecular structure and abundant presence of nanometer-size regions that are rich in ultra-confined water. Both the meso-pores and the water-rich regions are defects that determine to a large extent the accumulation of irreversible deformation and eventually the strength of the gel. Here we employ a recently developed, discrete colloidal model of the C-S-H gel at the sub-micron scale, which accounts for both the defects in the molecular structure, and for the meso-pores . Model structures are generated using a space filling Monte Carlo algorithm, through which particles of different size (polydispersity) are inserted into an initially empty simulation box. Higher polydispersity leads to more efficient packing, hence controlling the amount and connectivity of the meso-pores. The particles interact via a cohesive potential, parametrized to reproduce the mechanical property of C-S-H at the atomic level. These interactions reproduce the behavior of the solid skeleton of C-S-H, mediated by the presence of weak defect regions. The cohesive strength scales with the particle size, and therefore large particles are "stickier". We sample the response to finite shear strain of model structures with different polydispersity, and therefore different packing density. In our findings and in agreement with the experiments, dense structures have a higher strength and accumulate less irreversible deformations, as simulated via cyclic loading. We show that he triggering or irreversible mechanism is associated with the propagation of non-affine particle displacements, and that a behavior reminiscent of hard inclusions embedded in a soft matrix emerges due to particle size polydispersity. In summary, we provide a systematic modeling of the irreversible shear deformations in the C-S-H gel at the sub-micron scale, which constitutes a basis for future studies on damage accumulation, failure, and creep.

11:30 – 11:45 am

Modeling chemical compositional changes in concrete pore solution within microenvironments adjacent to steel reinforcement

Burkan Isgor, Oregon State University and Pouria Ghods, Carleton University

Solution composition in the pores of concrete facing the steel surface and within other crevice-like features that exist along the concrete-steel interface may be highly different from that of the bulk solution. These microenvironments can become local acidification sites, where the pH of the pore solution might drop below 10 even though the bulk concrete pore solution remains highly alkaline. Similarly, Cl/OH ratio in these microenvironments can be many orders larger than that of the bulk solution. The main driving force behind this local variability in chemical composition is the electrochemical reactions on the steel surface. Anodic and cathodic reactions that take place in active or passive steel electrically polarize micro-scale domains in concrete that are adjacent to steel surface. In the presence of these electrical potential gradients, ions in concrete pore solution move via diffusion, electrical migration and chemical activity. In the case of partially saturated pores, the ion movement has an advective component as well. Accurate modelling of chemical compositional changes in concrete pore solution within microenvironments adjacent to steel reinforcement is critical in the study of a number of phenomena related to corrosion of steel in concrete. These include the studies on the role of (a) binder composition, (b) inhibitors, (c) steel type on the passivity and corrosion of steel in concrete. The presentation will provide a comprehensive framework for modeling chemical compositional changes in concrete pore solution within microenvironments adjacent to steel reinforcement. The framework is based on the nonlinear solutions of coupled Nernst-Plank equations for all critical species of concrete pore solution while the domain is under the electrical potential gradients imposed by polarized steel surfaces. A number of examples using this framework will be presented, and the benefits of such simulations in the absence of reliable experimental procedures will be discussed.

11:45 – 12:00 noon

A material model and its application to simulate the composite material structure of mortar and concrete using real-shape particles

Edward Garboczi, NIST; Zhiwei Qian, Delft Technical University; Yang Lu, Boise State University

At some length scale, the composite structure of mortar can be represented by a model consisting of sand particles embedded in a cement paste matrix and that of concrete by gravel particles embedded in a mortar matrix. Traditionally, spheres have often been used to represent aggregates because of their simplicity, although the accuracy of resulting properties when using this shape can be limited when the property contrast between aggregate and matrix is large. A new material model is proposed and implemented, called the Anm material model, which can simulate the material structures of mortar and concrete with real-shape aggregates without using digital images. The aggregate particle shape is mathematically represented by a spherical harmonic expansion. The take-and-place parking method is employed to put multiple irregular particles together within a pre-defined empty container, which can be interpreted as a representative volume element of the material structure of concrete. To use this structure for mechanical property calculations, one must generate a 3D finite element mesh that is optimized for this kind of material model. The approach used involves the definition of a topological structure suitable for Stereo Lithography file (STL) representation and the development of algorithms for topology and geometry data processing in order to obtain a 3D optimized mesh that incorporates the random material structure. During the mesh generation procedure, we combine both the aggregates and the matrix to ensure perfectly coinciding nodes at their interface, thus bridging the gap between heterogeneous microstructure and computer-aided engineering finite element analysis for this kind of model.

10:30 – 11:45 am
Technical Session III ♦ Yeh Center 2310
Concrete Durability

10:30 – 10:45 am

Material Property Inputs for Chloride Diffusion Prediction: Comparing Fick's Second Law and Nernst – Planck Parameters

Yiwen Bu, Daming Luo and Jason Weiss, Purdue University

Durability of cementitious structures depends greatly upon the time required for chloride ions to build up to a critical concentration at the surface of the reinforcing steels. To predict such initiation time, two methods are more commonly applied: Fick's second law and Nernst-Planck equation. In this study, we demonstrate the influence of various exposure conditions on the chloride penetration profiles. Apparent chloride diffusion coefficients were determined from experimental profiles with Fick's second law and the limitation of such application is discussed. We also provide simulations obtained with a Nernst-Planck approach (standardized by Stadium○R) as to chloride penetration profiles under various exposure conditions. Comparisons between experimental and simulation results shed light on the benefits and disadvantages of both approaches.

10:45 – 11:00 am

Drying of cementitious materials: Influence of liquid properties on the diffusion coefficient
Chiara Villani, Purdue University, Robert Spragg, Purdue University, Mohammad Pou-Ghaz, North Carolina State University and W. Jason Weiss, Purdue University

The drying of cementitious systems is known to be non-linearly related to the moisture content of the sample. While studies are typically conducted to back calculate the diffusion coefficient from measurements on bulk samples, this study will examine the diffusion coefficient measured on small samples over a wide range of humidities. Specifically the work will examine the influence that the properties of the fluid may have on the measured diffusion coefficient (e.g., shrinkage reducing admixtures or deicing salts). The possibility to model the diffusion coefficient of materials containing different pore solution compositions is described using analytical equations. The models reveal good agreement with experimental results showing a realistic possibility to predict drying even in more complex cementitious systems.

11:00 – 11:15 am

Influence of Aggregate Properties on Stresses in Freezing Concrete as Determined by Poromechanical Modeling
Syeda Rahman, Texas A&M University; Zachary Grasley, Virginia Tech

At freezing temperatures, concrete is a complex composite material composed of porous aggregate, porous cement/mortar matrix along with liquid water, water vapor and ice present in the pore network. Aggregates, being the major constituent material of concrete, largely influence the concrete durability at freezing temperatures. In this work, a poromechanical model is developed to model crack initiating internal stresses in concrete under freezing temperatures. Sensitivity analysis to concrete material properties is performed. It is found that large aggregates with high porosity, low permeability, and fine pore structure are the most vulnerable to D-cracking. Such aggregates develop over-pressurization induced by the Mandel-Cryer effect, and generate destructive tensile stress at the aggregate-matrix interface.

11:15 – 11:30 am

Evaluation of Freeze and Thaw Damage in Mortars Containing Deicing Salt Using A Low Temperature Guarded Comparative Longitudinal Calorimeter and Acoustic Emission
Yaghoob Farnam,Purdue University, Dale Bentz, National Institute of Standards and Technology, Aaron Sakulich, Worcester Polytechnic Institute, Daniel Flynn, National Institute of Standards and Technology and Jason Weiss, Purdue University

Deicing salts are often applied to the surface of pavements and bridge decks in the winter to melt ice; thereby improving the safety of the travelling public. The influence of NaCl deicing salt on the freezing and thawing temperatures of pore solution was evaluated and the corresponding damage during freezing and thawing was investigated. A low-temperature guarded comparative longitudinal calorimeter was developed to cool a mortar sample at a rate of 2 °C/h and to then heat the mortar at a rate of 4 °C/h. Heat flux during freezing and thawing cycles was monitored, and the temperatures at which freezing and thawing events occurred were detected. During cooling and heating, acoustic emission activity was measured to quantify the damage due to aggregate/paste thermal mismatch or phase changes. The results show that NaCl solution in a mortar sample freezes at a lower temperature than the value expected from the bulk NaCl phase diagram, while the frozen solution in mortar melts at the same melting temperature as the bulk frozen NaCl solution. As the salt concentration increases, the freezing temperature is reduced. For samples containing more highly concentrated solutions, another exothermic event is observed whose corresponding temperature is greater than the aqueous NaCl liquidus line in the phase diagram. For mortar specimens saturated by solutions with 5 % and 15 % NaCl by mass, greater freeze/thaw damage is observed. The AE calorimeter developed herein is applicable for investigating damage behavior during freezing and thawing of different phases in pore solution (in mortars).

11:30 – 11:45 am

Alkali-Silica Reaction: Chemical Reaction Sequence, Kinetics and Thermodynamic Modeling
Taehwan Kim, Purdue University; Jan Olek, Purdue University

The deterioration induced by alkali silica reaction (ASR) is initiated by complicated heterogeneous chemical reactions. This study describes overall results obtained from the study focused on the kinetics of physical and chemical changes in the reactive aggregate-simulated pore solution system undergoing ASR. Specifically, the study investigated the products formed by exposing reactive silica mineral (α-cristobalite) to the mixture of three alkali solutions and solid calcium hydroxide (Ca(OH)2) The experimental results showed that as long as the solid Ca(OH)2 remains in the system, the dissolution of the silica mineral proceeds at a constant rate and the only reaction product formed is the tobermorite-type C-S-H gel. However, once the solid Ca(OH)2 is removed from the system, the concentration of silica ions increases significantly. At the same time, the previously-formed C-S-H gel becomes more amorphous (most likely due to additional polymerization by incorporation of silica and alkali ions from the solution). Further increase in the concentration of silica ions might lead to formation of the ASR gel as a result of interaction between silica and alkali ions. The experimental results were used to develop thermodynamic model for the chemical sequence and kinetics of the ASR process. The formulation of the kinetic rate law for silica dissolution from the reactive silica minerals used in this model accounts for such factors as pH, temperature, concentration of alkalis in solution and type of the reactive silica mineral. The model was created by using the proposed kinetic rate law as an input to the commercial modeling software (Geochemist's Workbench®). The model generated reasonably accurate predictions of the distribution of species in the reacting system and captured several distinct features of experimental data (i.e. depletion of Ca(OH)2, levels of alkali, silica concentrations, and pH levels).

1:30 – 2:45 am
Technical Session IV ♦ Yeh Center 1310
Shrinkage, Shrinkage Reducing Admixtures and Other additives

1:30 – 1:45 pm

Development of Shrinkage Limits and Testing Protocols for High Performance Concrete

Tengfei Fu, Oregon State University; Tyler Deboodt, Oregon State University; Jason Ideker, Oregon State University

Cracking at an early-age of high performance reinforced concrete structures, in particular bridge decks, results in additional maintenance costs, burden on serviceability and reduced long-term performance and durability. The causes behind cracking in high performance concrete are well known and documented in the existing literatures. However, appropriate shrinkage limits and standard laboratory/field tests which allow proper criteria to ensure crack-free or highly crack-resistant high performance concrete are not clearly established either in the technical literature or in specifications. The purpose of this research is to provide shrinkage threshold limits for specifications and to provide a robust test procedure which allows easy determination on compliance with specified threshold limits. It has been shown that the "ring" tests (ASTM C1581 and AASHTO T334) are the most comprehensive accelerated laboratory tests to accurately identify cracking potentials. In addition, acceptable correlation between the ring test and the field test has been observed and documented. However, a more simple and robust test procedure is in demand from materials suppliers and some Departments of Transportation. A data analysis of current research shows that the free shrinkage to shrinkage capacity (theoretical strain related to tensile strength and modulus of elasticity) ratio, namely "cracking potential indicator", is a promising assessment of cracking resistant performance. In this way, only free shrinkage test (ASTM C157) and basic mechanical properties are required to assess cracking risk of certain concrete mixture design.

1:45 – 2:00 pm

Long-term Shrinkage Prediction from Theoretical Considerations and Data Analysis

Mija Hubler, Northwestern University; Roman Wendner, Northwestern University; Zdenek Bazant, Northwestern University

Upon the release of the data from the tragic collapse in 1996 of the record-span segmental box-girder bridge in Palau, it was found that the 18-year deflection was 200 - 400% larger than the predictions based on the American, European and Japanese design codes or recommendations. This finding triggered further studies that led to a collection of deflection histories of 69 large-span segmental bridges, most of which suffered excessive, logarithmically growing, deflections with no sign of an asymptotic bound. Laboratory data collection led to a new database of concrete creep and shrinkage data. Since the duration of lab tests is <6 years, while

100-year lifetimes are generally desired for prediction, a joint statistical optimization of the fit of the laboratory data and the multi-decade bridge data is performed. The database of laboratory tests is further been extended to include high-strength concretes (up to 167 MPa strength at 28 days), as well as modern concretes with various admixtures, classified into six classes, some of which decrease and others increase the creep and shrinkage. An additional formula for autogeneous shrinkage is introduced to capture the long-term shrinkage behavior of newer cement mixtures. Correlation analyses and published trends are used to provide insights into admixture classifications that would allow the effect of various chemicals on long-term shrinkage models to be captured. This procedure reveals insights for future testing considerations of new cements and admixtures to efficiently predict their effects on time dependent behaviors while making use of existing laboratory and structural data. Within the framework of the new B4 model, a new prediction formula for shrinkage based on concrete strength and/or composition (with admixtures) will be presented.

2:00 – 2:15 pm

Computer-Aided Molecular Design using the Signature Molecular Descriptor and the Search for New Admixtures for Concrete – Part 1 Identification of Surface Tension Reducing Agents and the Search for Shrinkage Reducing Admixtures

Hamed Kayello, The University of Akron; Donald Visco Jr., The University of Akron; Joseph Biernacki, Tennessee Technological University

The development of new admixtures for concrete is normally an experimental endeavor in that the molecular scaffolds of existing admixtures are modified and tested. This approach is time-consuming, incremental and typically expensive. Alternatively, a computer-aided molecular design (CAMD) strategy that uses an inverse quantitative structure property relationship (I-QSPR) is proposed. The CAMD technique is a powerful tool that applies information about how known substances behave in a given application, encodes their molecular structure using what are referred to as “molecular descriptors,” relates the descriptors to its performance, then uses that information to generate new molecules with optimal predicted performance. While this strategy has been used successfully to design drugs and a wide variety of industrial chemicals, it has only recently been demonstrated for the identification of new admixtures for concrete. This contribution outlines the methodology for using the Signature molecular descriptor as a basis for designing molecular structures that aggressively reduce the surface tension of water in an effort to discover new shrinkage reducing admixtures. In particular, this work focuses on two classes of compounds, amines and glycol ethers. By evaluating the initial surface tension reduction of these compounds in solution with water, a number of structure-property conjectures associated with the effect of these compounds were developed. From these conjectures, 14 compounds were identified and utilized as a training set for the CAMD algorithm. After creating and refining a quantitative structure property relationship (QSPR) model for surface tension reduction, a structure enumeration algorithm was employed to generate non-intuitive structures outside of the original training set that have optimally predicted properties. In Part I of this pair of presentations, the CAMD approach is outlined and the previously developed QSPR model is evaluated by experimentally testing the surface tension reduction effect of optimal candidates on water.

2:15 – 2:30 pm

Computer-Aided Molecular Design using the Signature Molecular Descriptor and the Search for New Admixtures for Concrete – Part 2 Validating Newly Identified Surface Tension Reducing Substances for Potential Use as Shrinkage Reducing Admixtures

Natalia Shlonimskaya, Tennessee Technological University; Joseph Biernacki, Tennessee Technological University; Hamed Kayello, The University of Akron; Donald Visco Jr., The University of Akron

In Part II of this pair of presentations, twelve additives were tested for their ability to inhibit both autogenous and drying shrinkage in portland cement. Among these, two were commercial shrinkage reducing admixtures (SRAs) one was an active ingredient in a commercial admixture, five were newly identified compounds predicted by using an inverse quantitative structure property relationship (I-QSPR) and four were original training set compounds. Newly designed compounds were targeted for their ability to reduce the surface tension of water, a primary consideration for shrinkage reducing activity. Results for both drying shrinkage and autogenous shrinkage indicate that designed compounds perform similar to commercial admixtures yet have vastly different chemical functionalities. Accordingly, the selection of potentially new SRAs can be facilitated by the use of the I-QSPR strategy. Hydration data and set measurements were also considered since selection of new SRAs is a multi-parameter problem with many constraints.

2:30 – 2:45 pm

Effect of Diethanol-Isopropanolamine on the Hydration of Slag Blended Cement

Leslie Jardine, W.R. Grace; Denise Silva, W.R. Grace; Richard Sibbick, W.R. Grace

It is not uncommon for the concrete producer to limit the replacement of cement by slag, due to the deterioration of early concrete performance parameters, such as strength and set times. Diethanol-Isopropanolamine (DEIPA) has been found to improve hydration of cements with 50-70% slag. In this research, the impact of DEIPA on the hydration of blast furnace slag blended cements is studied using several analytical techniques, such as semi-quantitative X-ray diffraction, scanning electron microscopy (SEM), optical microscopy, and thermogravimetric analysis (TGA). Isothermal calorimetry was also used to demonstrate the impact of DEIPA on the reactivity of slag in blended cements. Compressive strength tests were performed to assess the impact of the amine in such cements. It is demonstrated that DEIPA modifies the microstructure at early ages by promoting the formation of large, isolated calcium hydroxide plates, and more easily distinguished aluminum hydrates. Later age microstructure is noted to be denser, with a more amorphous appearance, and fewer needle-like hydrates. Optical microscopy has revealed more reacted slag particles at 28 days, in the presence of the amine. The overall impact of the amine on the slag cements tested was of strength enhancement at all ages, which was coincident with the darker color of the specimens, confirming a higher degree of hydration of the slag. Observed in isothermal calorimetry, the amine increases the intensity of the peak associated with the aluminate reactivity. XRD and TGA show formation of carboaluminate and aluminate hydrate phases with the amine. All these changes are likely to be associated with the higher strength brought by the amine to the slag cement systems.

1:30 – 3:00 am
Technical Session V ♦ Yeh Center 2310
Nano-materials and Bio-materials

1:30 – 1:45 pm

Measuring the adhesive properties of nanoclay-modified cement pastes with the tack test

Shiho Kawashima, Columbia University; Mohend Chaouche, CNRS/ENS-Cachan; David Corr, Northwestern University; Surendra Shah, Northwestern University

The pressure exerted on formwork by self-consolidating concrete (SCC) is closely related to its rheological properties, specifically level of thixotropy and cohesion. Previous work has demonstrated that small additions of clays can significantly reduce SCC formwork pressure. To better understand this effect, the present study focuses on the influence of nanoclays on the cohesion of plain cement paste and paste with fly ash replacement. The adhesive properties are evaluated through the tack test, which is commonly used to characterize polymers but novel for granular materials. The influence of plate velocity, preshear condition and resting time (age) is determined. And because cementitious materials evolve due to thixotropic rebuilding and hydration mechanisms, the tack results are supplemented with a measure of the viscoelastic properties of the material over time obtained through low-amplitude oscillatory shear rheometry. The work demonstrates that the nanoclays have a significant influence on cohesion and the tack test is an effective method in evaluating the structural evolution and adhesive properties of cementitious materials.

1:45 – 2:00 pm

Influence of nano materials on the hydration kinetics and rheology of cement paste

Xin Wang, Kejin Wang, Iowa State University and Jussara Tanesi, Turner Fairbank Highway Research Center

Effects of different nano-materials on the hydration kinetics and rheology of ordinary portland cement paste were investigated. Three nano-materials were studied, and they are: nano-limestone, nano-silica, and nano-clay (a highly purified magnesium alumino silicate). These nano-materials were added to a cement paste as an addition at the levels of 0.0, 0.5, 1.0, and 1.5% (by weight) of cement. The heat of the cement hydration of the pastes was measured using isothermal calorimetry. Rheological behavior of the pastes was characterized using a rotational cylinder rheometer. The rheology tests were performed at 10 30, 60, 90, and 120 minutes after cement contacted to water. The experimental results indicate that addition of nano-limestone and nano-silica resulted in an earlier and higher rate of silicate hydration as well as a larger amount of total heat generation during the 24 hours testing period. Addition of the nano-clay shortened the time for the paste to reach sulfate depletion peak, and it also significantly increased the intensity of this peak. The rheology tests suggest that addition of these nano-materials generally increased yield stress and viscosity of the cement paste. Shear thickening behavior were observed from the pastes with nano-silica and nano-clay additions.

2:00 – 2:15 pm

High performance cellulose nanocrystal reinforced cement composites

Yizheng Cao, Purdue University; Jeffrey Youngblood, Purdue University; Jason Weiss, Purdue University; Robert Moon, US Forest Service- Forest Products Laboratory; Pablo Zavattieri, Purdue University

Nanomaterials have been considered for the development of new high-performance multifunctional, renewable and sustainable infrastructure materials. However, there are still concerns due to perceived environmental, cost, health and safety issues. Cellulose nanocrystal (CNC) is a promising nanoscale reinforcing material that is extracted from renewable and sustainable resources. They can potentially be produced at industrial size quantities and at low costs, and have shown low environmental and health issues. CNCs have several unique advantages: High aspect ratio, low density, coefficient of thermal expansion, high elastic modulus and strength. While CNC has great potential to meet a wide range of structural and functionality requirements, a comprehensive understanding of this material is needed. Although research in CNCs has grown rapidly in the last few years, little has been done with incorporating them into cements and other infrastructure materials. In this talk, we will introduce CNC and CNC based cementitious composites, describe several potential opportunities/applications of CNC in cement, and discuss some of our experimental results, including the performance improvement in flexural strength and degree of hydration of CNC reinforced cement composite.

2:15 – 2:30 pm

Utilizing submicron inclusions to enhance the properties of structural concrete made with recycled aggregates

Ardavan Yazdanbakhsh, City College of New York - CUNY; Michel Ghosn, City College of New York - CUNY; Julio Davalos, City College of New York - CUNY; Larry Bank, City College of New York - CUNY

A large amount of concrete waste is produced yearly in the United States. The utilization of recycled concrete aggregates (RCAs) in concrete has been researched for decades. However, despite their considerable potentials, RCAs are not being used in structural concrete. This study investigates the effect of well-dispersed submicron inclusions such as nanosilica on the structural behavior of concrete made with RCAs. The reinforced concrete beams made with natural aggregates and those made with RCAs and submicron inclusions will be compared in terms of flexural strength, failure behavior, and structural reliability.

2:30 – 2:45 pm

Effects of incorporating nanosilica on the carbonation of cement paste

Seungmin Lim and Paramita Mondal, The University of Illinois at Urbana-Champaign

The carbonation of concrete is directly connected to depassivation of steel reinforcement by the neutralization of cement paste, which can result in severe concrete deterioration. The carbonation is a complex physicochemical process that slowly modifies the structure of concrete. Although large number of studies on the carbonation of concrete has been conducted, the mechanism is not fully understood yet. In particular, there are conflicting views on the effects of supplementary cementitious materials (SCM) as cement replacement on the carbonation. In this study, micro and nanosilica are incorporated into cement paste, and exposed to the accelerated carbonation to investigate SCM effect on the carbonation of the system (both carbonation of CH and C-S-H). In order to separate the physical (changes in permeability) and chemical (changes in the nature of hydration products) effects, powdered samples are used for accelerated carbonation experiment. Thermogravimetric analysis (TGA) is employed to estimate the extent of carbonation and differentiate carbonation of CH and C-S-H. Based on experimental results, the effect of nanosilica, which has been reported to increase chemical stability of C-S-H, on the carbonation of C-S-H will be discussed in depth.

2:45 – 3:00 pm

Lightweight Aggregates as Internal Reservoirs of Bioactive Agents

Aaron Sakulich and Hajar Jafferji, Worcester Polytechnic Institute

Steel corrosion is one of the primary deterioration mechanisms that affects the built environment, annually causing at least $58 billion in damage in the United States alone. Bioactive agents, such as cinnamaldehyde and vanillin, have been shown to significantly reduce corrosion on steel and aluminum surfaces, however, they also dramatically interfere with cement hydration when simply added to the fresh mix. A novel system, using lightweight aggregate (LWA) as a delivery method, has therefore been developed. In this system, the bioactive agents are 'locked away' at early ages and only released once the system's mechanical properties have been developed. The agent can then migrate through the matrix to coat the reinforcing steel and mitigate corrosion. Mixture proportioning, the effects of bioactive agent incorporation on early age strength and calorimetric profiles, and the results of a microscopic investigation will be presented.

4:30 – 6:30 pm ♦Yeh Center
Della Roy Lecture and Reception
Sponsored by Elsevier

Calcium in geopolymers
Leslie Struble, University of Illinois

The geopolymer system is being widely studied for many ceramic applications, not the least of which is a binder in structural concrete. Geopolymers form by reaction of a powdered aluminosilicate precursor with an aqueous alkali hydroxide solution. The precursor most widely studied is metakaolin, whose reaction occasionally forms a crystalline zeolite but in our experiments always forms an amorphous gel, whose molecular structure we are probing mainly with nuclear magnetic resonance (MAS-NMR). Calcium is often present in the reaction and is seen to speed up setting and increase strength of the geopolymer. When calcium is present, calcium silicate hydrate is presumed to form in addition to the geopolymer gel, although no direct experimental evidence for this phase is seen in the literature. Identifying calcium silicate hydrate in the presence of geopolymer gel is rather difficult, but we have successfully identified both phases using MAS-NMR. Evidence for this identification will be shown and discussed.

WEDNESDAY, July 10, 2013

8:30 – 10:00 am
Technical Session VI ♦ Yeh Center 1310
Geopolymer

8:30 – 8:45 am
On the Development of Low Alkali Activated Fly Ash Cement (LAFAC)
Surojit Gupta, M. Faisal Riyad, Ryan Johnson and Tom Hammann, University of North Dakota

Fly ash is generated during the combustion of coal for energy production. It is an industrial by-product which is recognized as an environmental pollutant. The alkali activation of Fly Ash has become an important area of research. It is possible to use these materials to synthesize inexpensive cement like construction materials. From environmental perspective, the use of alkali activators, for example NaOH, is a concern as it is electrochemically generated with production of harmful Cl2 or HCl gas as by products. The presence of free alkali can also have deleterious effects on activated fly ash concrete [3]. Most of the research on activation of fly ash has been done with high concentration of alkali solutions. The CO2 emission of geopolymer binder can be further reduced by decreasing the alkali content. The main objective of this presentation is to present a systematic study about development of Low Alkali Content Activated Fly Ash Cement (LAFAC). During this study both class F and class C fly ash were evaluated from different sources. Class C fly ash showed better results as compared to Class F fly ash. Detailed mechanical property studies, microstructure analysis, and phase analysis will be presented.

8:45 – 9:00 am
Activator, source material, and curing effects on alkali activation reactions
Ussala Chowdhury, Sundararaman Chithiraputhiran, Akash Dakhane and Narayanan Neithalath, Arizona State University

Activation of slags and fly ashes using alkali silicate or hydroxide solutions are commonly employed to produce cement-less binder systems. In this presentation, we discuss the following less studied aspects of alkali activation: (i) relative effects of alkali cations (K or Na), (ii) effects of powder activators, (iii) aluminates as activating agents, (iv) soda-lime glass as a major constituent of the source material and special needs for such systems, and (v) microwave assisted thermal processing as a means of alkali activation, in addition to heat curing under dry and moist conditions. The rate and extent of activation reactions and the corresponding reaction product formation are elaborated in detail. The use of advanced spectroscopic techniques to distinguish the influence of studied parameters will be discussed.

9:00 – 9:15 am

Rheological study on coal, biomass and co-fired fly ash cementitious and geopolymeric pastes

Christopher R. Shearer, Georgia Institute of Technology; Chiara F. Ferraris, National Institute of Standards and Technology and Kimberly E. Kurtis, Georgia Institute of Technology

The combustion of biomass and the co-combustion of biomass with coal can reduce carbon dioxide emissions compared with power generation from coal alone when the rate of biomass consumption is less than its rate of growth. However, while the by-product of coal firing—fly ash—is commonly used in concrete, the by-products derived from biomass and co-combustion—biomass ash and co-fired fly ash—are not addressed in U.S. standards for fly ash use in concrete. While recent European standards have permitted co-fired fly ash use in concrete with certain restrictions, research has shown that biomass and co-fired fly ash can have different morphology and composition compared to ordinary coal fly ash. As a result, workability concerns may be one of the main barriers to the widespread and commercial implementation of biomass and co-fired fly ash as a supplementary cementitious material. Research has also been conducted to find alternative uses for these materials. One potential reuse is to form geopolymers, but the rheological properties of geopolymeric materials are not well-understood. In this study, the rheological behavior of binary blends containing co-fired and biomass fly ash as a cement substitution (25% by mass) and fly ash geopolymers were examined. Various techniques were evaluated, such as rheometry, mini-slump and mortar flow. This presentation will discuss the results obtained. Ultimately, this research yields a better understanding of the impacts of these emerging materials on cementitious and geopolymeric pastes at early-ages.

9:15 – 9:30 am

Geopolymer Densification Using Functional Alkoxysilanes

Brayden Glad and Waltraud Kriven, University of Illinois Urbana-Champaign

Geopolymers were synthesized with trialkoxysilane coupling agent additives to improve adhesion to organic polymers and to modify porosity. Uncured geopolymer slurry was found to be miscible with various alkoxysilanes, and the resulting cured geopolymer could adhere strongly to polystyrene foam if the additive possessed an aniline functional group. Geopolymer mesoporosity could be minimized through the use of alkoxysilanes with acrylic acid or similar functional groups, which Fourier transform infrared spectroscopy identified as transforming to sodium acrylates in the high pH of the geopolymer system. Examination with nitrogen adsorption showed an order of magnitude decrease in mesopore volume, while transmission and scanning electron microscopy identified the self-assembly of 100 nm-1µm sheets and tubes of the acrylate-functional alkoxysilane when at least 0.06 mol acrylate/mol geopolymer was used. These phases bound strongly to geopolymer precipitates and inhibited the sequestration of surplus water in mesoporous structures through a waterlocking mechanism. Compressive testing found a 48% increase in Weibull modulus for compressive strength and a probable increase in compressive strength, while mercury intrusion porosimetry measurements showed up to a 24% increase in bulk density.

9:30 – 9:45 am

Coexistence of C-S-H and K-A-S-H characterized through selective dissolution and FTIR spectral subtraction

Sravanthi Puligilla and Paramita Mondal, University of Illinois at Urbana-Champaign

Selective dissolution techniques have been commonly employed in studying clinker phases to separate their response from an overlapped XRD pattern. Salicylic acid in methanol, popularly known as Takashima method dissolves calcium silicates including calcium silicate hydrate and has been used widely to determine the degree of reaction in blended cements. Hydrochloric acid (HCl) dissolution technique is used to dissolve geopolymers and zeolites to determine the reaction degree of fly ash geopolymers. However, there are very few studies which have employed dissolution techniques to study geopolymers made from precursors that contain soluble calcium. EDS studies of such geopolymers indicated the coexistence of C-S-H and geopolymer gel, and interpretation of data can be quite complicated. The present work will discuss the use of dissolution techniques performed successively along with FTIR spectral subtraction on fly ash-slag geopolymers at various ages to confirm the coexistence of C-S-H and geopolymer gel.

9:45 – 10:00 am

Mitigation of dehydration cracking and thermal shrinkage in geopolymer systems by the addition of alumina platelet reinforcement.

Gregory Kutyla and Waltraud Kriven, University of Illinois Urbana-Champaign

Geopolymers have shown potential as both refractory adhesives and composite matrices. The fact that they can be produced inexpensively and do not require any initial firing opens up many niche applications. However, most geopolymeric materials suffer from problems as they are heated. Dehydration typically produces substantial cracking, sometimes to the point of disintegration. Additionally, densification of geopolymer can result in linear shrinkage as high as 18% on first heating. To combat these phenomena, alumina platelets with a mean diameter of 50 microns and an aspect ratio of 5:1 were mixed with metakaolin-based potassium geopolymer in three weight-fractions (30, 50, and 70 wt% aggregate). The resulting composites were heated at varying temperatures up to 1500°C and tested in 4-point flexure at both room and high temperatures. At the highest reinforcement level, samples lost no strength after heat treatment to 1500°C. When tested in-situ, samples retained full strength to 1100°C, and still had failure stresses greater than 5 MPa at 1400°C. Thermal shrinkage was lower than 4% (ΔL/L) even after cooling from 1500°C, more than a factor of 4 less than pure geopolymer. Additionally, samples were highly resistant to thermal shock under several conditions. Thermal evolution of the microstructure was also examined with SEM and XRD. These results indicate that geopolymers can be a basis for versatile refractory concretes given careful selection of reinforcement.

10:30 – 11:45 am
Technical Session VII ♦ Yeh Center 1310
Alternative Cements

10:30 – 10:45 am

Studies of PLC Synergies and Their Potential for Enhancement of Concrete Performance

Tim Cost, Holcim (US) Inc; Wayne Wilson, Holcim (US) Inc.

New provisions for Type IL portland-limestone cements (PLC's) in both ASTM and AASHTO specifications for blended cements are expected to result in greater markets for PLC's in the US, especially in states where transportation agencies use only AASHTO specifications, which did not provide for PLC's prior to 2012. Recent experiences in the US have uncovered interesting performance trends with some PLC's that have not been widely reported in other countries with longer histories of PLC use. This is thought to be influenced primarily by the higher overall fineness of US cements and characteristics of some supplementary cementitious materials (SCM's) commonly available in the US. PLC's (meeting Type IL specs) have in some cases produced systematically improved strength and setting performance in concrete mixtures made with SCM's, as compared with ordinary Type I or II portland cements (OPC's) from the same US plants. Beneficial results of these "synergies" have occasionally been significant. Since these results have not been common to every cement plant or every sample, a better understanding of these influences is needed to help guide production and use of PLC's for optimal performance potential and sustainability impact. The presentation summarizes some recent studies in which performance of PLC's and OPC's were compared and influences of different cement and SCM properties were evaluated. One study compared PLC's produced in laboratory simulations using separately added limestone with actual cement mill-ground samples to investigate limestone fineness and particle size distribution effects on synergies with SCM's. In another study, concrete mixtures representative of transportation structures applications were used to compare the performance of PLC's and OPC's from five different cement plants in combination with different SCM's. A third study compared the influences of certain PLC properties in mixtures with different combinations of multiple SCM's at 50% total cement replacement, in support of a large concrete construction project. Other ongoing work is also cited, and some preliminary conclusions are made based on observed trends. Cement mill-ground PLC's can clearly be produced so as to optimize performance synergies with some of the SCM's that are commonly used in US concrete construction. Resulting benefits may include greater strength efficiency of the cementitious systems used in concrete as well as partial mitigation of the extended setting behaviors commonly associated with high-SCM content mixtures. Research is needed to better understand all of the significant influences and how they can best be optimized.

10:45 – 11:00 am

Directions towards High-Volume Limestone Cements: An Overview of Efforts on Enhancing Cement Replacement Levels

Gaurav Sant, University of California, Los Angeles

Carbon pressures facing the cement industry are driving efforts to decrease clinker and cement factors of binder formulations. While limestone has been identified as a very promising cement replacement vehicle, prevailing limestone replacement levels remain modest. A series of recent studies are providing new guidance on the use of limestone in cement with special emphasis on considering aspects of: (1) mineral acceleration, (2) limestone introduction mode, i.e., blending or intergrinding and (3) exploiting compositional (chemical) compatibilities of materials. Each of these aspects are levers which can be used to substantially reduce cement use, by replacing cement by limestone. This presentation summarizes recent efforts which provide guidance on: (a) the ability of limestone to serve as a preferred mineral filler agent, (b) equivalencies noted in reactions and properties when limestone is introduced by intergrinding or by blending, and (c) the ability to achieve substantial levels of cement replacement (around 45%, mass basis), while maintaining properties when multiple (compatible) material solutions are composed.

11:00 – 11:15 am

Evaluating the beneficial effects of lower alkali cementing systems with or without SCMs on ASR

Soley Einarsdottir and R. Doug Hooton, University of Toronto

The commonly used ASTM C1260, C1567 and C1293 test methods for evaluating the potential for deleterious alkali-silica reactivity (ASR) either require raising the alkali content of the concrete mixture artificially, or immersing the samples in a very alkaline solution. This means that neither of them is useful for evaluating a mix with low alkali cement. By modifying some of the parameters of the test methods it may be possible to adapt them to be used to evaluate the beneficial effects of lower alkali cementing systems with or without SCMs. The effect of sample shape and size as well as cement alkalis and SCMs on expansion and alkali leaching from samples during testing according to the ASTM C1293 concrete prism test have been measured. This may lead to possible test modifications.

11:15 – 11:30 am

Mechanisms of Shear Load Transfer in Polymer-cement composites in the Plastic Regime

Navid Sakhavand, Rice University; Rouzbeh Shahsavari, Rice University

Unlike most man-made materials, in which one quality is sacrificed over the other, stiffness, strength and toughness are almost perfectly balanced in biomaterials such as nacre, bone and spider silk. The unique mechanism of load transfer in these materials is the key to their superior mechanical behavior. This is imparted an increasing interest for synthesizing hybrid polymer-cement composites with analogous mechanical behavior. Hybrid materials of this type are ideally stronger than their constituents while preserving high ductility. While there have been numerous studies on load transfer of layered materials, most of them are focused on specific size and property limitations. Herein, we present a rigorous continuum-based model to study shear load transfer in the plastic regime between layered materials. This model accepts dissimilar layers with varying dimensions, which makes it suitable for studying platelet-matrix composites. Our study shows how changing elastic moduli and the thickness of either tablets and shear modulus of the interface dramatically changes the normal stress and shear distributions. In addition, the efficiency of the load transfer is investigated via finding the optimum length of the composite. We show that for specific combination of tablets there is no optimum length. For such composites, the elastic strain energy density will decrease monotonically with increase in the overlap length. In addition, we show that the contribution of shear and normal deformations to the total elastic strain energy density of a unit composite differs for different combination of tablets. Learning from biological materials, many industries are already benefiting from excellent properties of platelet-matrix composites. Our model is another step toward better understanding of hybrid materials and designing stronger, more durable cementitious composites.

11:30 – 11:45 noon

Frost Resistance of Geopolymer

Xueying Li, Harbin Institute of Technology; Zhenzhen Jiao, Harbin Institute of Technology; Zheng Wang, Harbin Institute of Technology

Properties of fly ash based geopolymer mortar after the freezing and thawing cycle were investigated. Geopolymer were made of Class C fly ash, Class F fly ash and Class F fly ash plus slag separately. The experimental results showed that in the geopolymer made of Class C fly ash and the geopolymer mortar made of Class F fly ash plus slag, the mass and dynamic elastic modulus changed little until under 300 times freezing and thawing cycle. However, after only 100 times freezing and thawing cycle, mass loss of the geopolymer mortar made of Class F fly ash with Calcium Hydroxide reached the restricted value. It indicated that the frost resistance of geopolymer mortar is related intimately to precursors.

10:30 – 11:45 noon
Technical Session VIII ♦ Yeh Center 2310
Early Age Properties

10:30 – 10:45 am

Kinetics and activation energy of magnesium oxide (MgO) hydration – Comparison with hydration of cement

Jeffrey Thomas, Schlumberger-Doll Research; Simone Musso, Schlumberger-Doll Research; Ivan Prestini, Schlumberger-Doll Research

The kinetics of hydration of magnesium oxide to form magnesium hydroxide were measured using isothermal calorimetry at different temperatures. The hydration kinetics of light-burned MgO exhibit a hydration rate peak similar to that of cement and C3S hydration. The hydration kinetics of hard-burned MgO are much slower than that of light-burned MgO at the same temperature, and exhibit a continuously declining hydration rate after the first several minutes of reaction. The hydration kinetics of both light-burned and hard-burned MgO can be fit using a boundary nucleation and growth model that has previously been applied to the hydration of cement and tricalcium silicate. Activation energy values for MgO hydration were determined from the fitted rate constants and were also measured directly using small temperature excursions according to a recently proposed method. For light-burned MgO the activation energy values are all in good agreement and indicate a value of 77 kJ/mol. For the hard-burned MgO the activation energy values vary considerably depending on temperature and how the activation energy is measured.

10:45 – 11:00 am

A closer look at the experimental and materials related parameters influencing the rheology of cementitious pastes

Kirk Vance, Arizona State University, Aditya Kumar, University of California Los Angeles, Gaurav Sant, University of California Los Angeles and Narayanan Neithalath, Arizona State University

This presentation takes a closer look at the influence of a number of materials and experimental parameters on the rheology of plain and modified cementitious systems. The changes in rheological parameters of systems modified with fillers (size classified limestone powders), supplementary cementing materials (fly ash and metakaolin), and combinations are explored. The effects of particle packing, water demand, and the interparticle spacing and contacts (film thickness) either individually or in combination are evaluated using experiments and models. The yield stress and plastic viscosity generally show direct correlations to the particle number density and specific surface area and inverse correlations to the water film thickness. The influence of plate gap on the yield stress and plastic viscosity are explained using the ideas of shear banding (in jammed particulate systems) and confinement effects. Using multiple rheological models at wide shear rates ranges (from 0.1 to 100/s), it is shown that yield stress is an inadequate parameter to describe the rheological response of cementitious systems.

11:00 – 11:15 am

The relationship between the Nurse-Saul Datum Temperature and the FHP Activation Energy for Concrete Maturity and Application of The Bertalanffy Model for Concrete Maturity

Chang-Hoon Lee, Cornell University; Kenneth Hover, Cornell University

"Maturity" methods are used to predict the strength of a given concrete mixture at a given moisture availability as a function of both time and temperature. Temperature sensitivity of a given mixture is characterized by Datum Temperature for the linear Nurse-Saul method and by Activation Energy for the nonlinear Freiesleben Hansen and Pederson (FHP) method. While these methods and their defining parameters were independently developed, those parameters are nevertheless interdependent as a change in a concrete mixture that affects temperature sensitivity as expressed by Datum Temperature will also be reflected in a change of Activation Energy, and vice versa. This paper expands Carino's exploration of the relationship between Datum Temperature and Activation Energy, suggesting alternative approaches by which an appropriate value of one can be calculated from the other for any given range and profile of expected concrete temperatures.

The Bertalanffy growth model is proposed for predicting concrete strength as a function of temperature and time. This model is useful in general, but particularly for accommodating the "cross-over" effect in concrete where high early temperature can lead to a lower later strength. (This same effect is likewise observed in several biological and micro-biological processes.) The mathematical flexibility of the Bertalanffy model allows inclusion of the Arrhenius model, and works well for cement- and concrete-related data sets that produce a non-linear Arrhenius Plot. (A non-linear Arrhenius Plot signals temperature-dependent activation energy. This is a fairly common condition, often ignored by either adopting an average slope as the activation energy over the entire temperature range, or confining the analysis to the range of interest.) The goal is to provide a family of alternative maturity methods for time-temperature regimes over which current approaches may be less suitable.

11:15 – 11:30 am

Topological constraints : a tool to predict cement aging

Mathieu Bauchy, MIT; Mohammad Javad Abdolhosseini Qomi, MIT; Deater Brommer, MIT; Roland Pellenq, MIT

Rigidity theory, initially developed by Lagrange and Maxwell for mechanical trusses, has revealed to offer a practical scheme to study glasses [1, 2] while only relying on their topology. It has led to the recognition of a rigidity transition which separates flexible glasses, showing internal degrees of freedom that allow local deformations, from stressed-rigid glasses. This transition (also called Phillips-Thorpe rigidity transition) occurs when the number of topological bonding constraints (radial bond-stretching BS and angular bond-bending BB) equals the number of degrees of freedom. Recently, the existence of an intermediate phase (IP) characterized by a rigid but unstressed network was reported. Inside the IP, glasses show remarkable properties such as a space-filling tendency and very weak aging effects. Recently, we introduced a new method [3] to enumerate the number of constraints in molecular networks using molecular dynamics trajectories. To count the number of BS constraints, we compute pair distribution functions and divide them into partial distribution function (PDFs) arising from the contribution of each neighbor. A constrained neighbor is then characterized by a low standard deviation of its PDF corresponding to a low radial excursion, its bond length being fixed close to its average value. The number of BB constrained is analyzed in the same fashion by computing angular distributions and the partial bond angle distribution (PBADs) of each angle around a central atom. Each constrained angle is then associated to a low standard deviation of its PBAD which is linked to a low angular excursion. This offers an efficient way to enumerate the number of constraints that manifest inside atomic networks and thus to predict the existence of rigidity transitions. The previous method has been used to study CSH samples produced by molecular dynamics simulations using ReaxFF force-field. Atomic-scale BS and BB constraints enumeration in this material is detailed both inside and between layers. We report the existence of a composition-driven rigidity transition in CSH. We show how the latter shares some analogies with well-known rigidity transitions that are observed in glasses (chalcogenide Ge-Se, alkali silicates). This constraints analysis tool opens new perspective to predict some trends in cement properties like density, hardness or aging.

11:30 – 11:45 am

Robustness of Self-Consolidating Concrete: New Testing Method and Effect of Aggregate Properties

Lin Shen, University of Hawaii at Manoa; Hamed Bahrami Jovein, University of Hawaii at Manoa

The fresh properties of self-consolidating concrete (SCC) is typically sensitive to small changes of material properties such as moisture content of aggregates, dosage of superplasticizer, etc. To consistently maintain the desired performance in mass production of SCC, it is essential to design and select a SCC mix which is robust against small variations in raw materials. A new testing method, modified Segregation Probe, was found to be able to quickly quantify and rank the robustness of various candidate mixes. This test can be performed in a pan or drum mixer and finished in about 15 minutes. It was found that higher paste volume, smaller aggregate size, better gradation, and higher aggregate packing density can improve robustness. Among these factors, smaller aggregate size and better gradation seem to have more significant effects than higher paste volume and higher aggregate packing density.

1:30 – 3:00 pm
Technical Session IX ♦ Yeh Center 1310
Analytical Techniques for Characterization, Sensors, Other Smart Materials

1:30 – 1:45 pm
Internal Relative Humidity of Concrete in Railroad Environments
Daniel Castaneda and David Lange, University of Illinois Urbana-Champaign

Humidity sensors can be used to measure moisture in concrete. Practitioners use sensors to determine favorable conditions for installing floor coverings on concrete slabs. Researchers use humidity sensors to study drying processes, autogenous shrinkage, and cracking potential of concrete. Humidity measurements also offer indirect insight into diffusion and transport properties, moisture gradients, and degree of saturation of hardened concrete. Mathematical models have been developed to describe transport mechanisms and internal stresses created by drying. In this study, the suitability of those models are evaluated for in-situ concrete rail ties that are exposed to Midwest climatic conditions. Sensors were installed into hardened concrete ties and monitored for an extended period of time to measure temperature and humidity. The results are compared against literature to assess the long-term durability potential of the concrete ties.

1:45 – 2:00 pm
Detection of corrosion in steel-reinforced concrete by anti-ferromagnetic resonance
Edward Garboczi, NIST

Steel used in the US infrastructure is usually under a protective layer of some kind, with the prime examples being painted steel and steel-reinforced concrete. Detecting corrosion under another material is a constant driving force for non-destructive evaluation (NDE) techniques to be developed, since detecting early corrosion underneath a protective layer has a large potential for national/international impact. The usual NDE method involves trying to somehow visualize the corrosion that is present or else trying to measure the loss of steel due to corrosion. At NIST, there is a project that is trying to develop a spectroscopic method of detecting iron corrosion products, by exploiting the anti-ferromagnetic properties of hematite and goethite, two common iron corrosion products. The technique actually detects the presence of these compounds, which indicates that corrosion is taking place. The achievements thus far of the project will be outlined, with a prospectus given for potential future success.

2:00 – 2:15 pm
Three-Phase Cement Piezoelectric Composites for Use as Sensors for Health Monitoring
Kimberly Cook-Chennault, Rutgers University; Sankh Banerjee, Rutgers University

Novel three-phase piezoelectric composites with randomly distributed metallic and.or electrically conductive particles and PZT particles in a Portland cement matrix were fabricated at the low poling voltage of 0.6 kV/mm and temperature of 160C. The influence of the electrically conductive inclusions and lead zirconate titanate (PZT) volume fraction, on the dielectric constant, tan δ and piezoelectric properties of the PZT-Cement-aluminum composites was experimentally investigated. The three-phase piezoelectric composites had higher piezoelectric strain coefficients (d33) than the two-phase composites (comprised of PZT and Portland Cement). An analytical model for the prediction of the effective dielectric constant of the three-phase composite was developed and the predicted values compared reasonably well to the measured values of the dielectric constant for various volume fractions of the PZT. Due to their increased dielectric constant and piezoelectric

2:15 – 2:30 pm
Insitu Observations of Hydrating C3S with Synchrotron Nanocomputed Tomography
Tyler Ley, Qinang Hu, Mohammed Aboustait, Jay Hanan, Oklahoma State University and Robert Winarski, Advanced Photon Source - Argonne National Laboratory

This presentation will provide an overview of a large research effort sponsored by the FHWA to investigate the kinetics of cement hydration. This work uses a number of novel experimental techniques in combination with computational models to investigate and model the kinetics of cement hydration. This presentation will contain a subset of the data that focuses on the use of synchrotron nanocomputed tomography completed on synthetic triclinic C3S particles at a 30 nm scale before, during, and after being hydrated in 15 mmol Ca solution at a water-to-cement ratio close to five. Particles are hydrated at different time periods and temperatures. Three dimensional data sets are collected that investigates the structure of the original particle. A novel environmental imaging cell that was created for this research is then used to surround the particle in 15 mmol Ca solution and then radiographs are taken during hydration. After a set period the hydration of the particle is stopped by solvent exchange with isopropanol, and then another three dimensional data set of the hydrated particle is collected. These measurements provide important insights into the mechanisms of the acceleration and deceleration of hydration, the dissolution of the cement particle, the subsequent formation and growth of CSH, and the densification of CSH with time.

2:30 – 2:45 pm

Automated and Manual Characterization of Input Parameters for the VCCTL

Benjamin Watts, Christopher Ferraro, University of Florida, Engineering School of Sustainable Infrastructure and Environment, April Snyder, R J Lee Group and H.D. Deford, Florida Department of Transportation

The Virtual Cement and Concrete Testing Laboratory, developed at NIST has the potential to be a powerful tool for the development and evaluation of cementitious materials and concrete mixtures. One of the primary groups of inputs for this software is derived from the characterization of the cement, specifically the quantification of the volume and surface area fractions of the major constituent phases. The traditional method by which this is accomplished is through the use of Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray Spectroscopy (EDS). Elemental maps for the primary constituents of Portland cement are compared to a Backscattered Electron image of the same field. Using an algorithm developed at NIST, the different phases present in cement can be obtained and converted into the form of a composite image, which can be analyzed to obtain the desired input parameters. A number of fields are collected in order to obtain statistically robust data. The application of automated computer controlled SEM (CCSEM) technology for the collection of images and EDS composition have been investigated with an aim to decrease acquisition time while increasing the statistical data set. The accuracy of the CCSEM techniques was evaluated in comparison to the traditional method, and other potential methods, for the acquisition of the cement constituent data.

2:45 – 3:00 pm

Finite Element Modeling of Concrete Based on Quantitative Computed Tomography (QCT)

Arash Razmjoo, Clemson University; Amir Poursaee, Clemson University

Models have been used in the past to predict the mechanical and transport behavior of concrete. However, almost in all of these studies, aggregates were considered either circle or sphere and the impact of the aggregates geometry and in-homogeneities in concrete structure is ignored. The objective of this study is to develop a novel method for accurate prediction of the mechanical and transport behavior of concrete using the general framework of the quantitative computed tomography (QCT)-based finite element (FE) Analysis. Concrete cylinders were cast and cured for 28 days. The QCT scans were carried out on the samples using a clinical CT scanner. An image processing method was applied to detect aggregates, paste content and the air voids. The distribution of each phase then calculated in each image slice (2D) and in the bulk material (3D). The processed QCT images were directly converted into voxel-based 3D FE models for linear and nonlinear analyses. The FE models were generated by conversion of each voxel into an 8-noded brick element. Air void content of the cylinders (2D and 3D) was determined. In addition, the aggregates content was estimated using the image analysis. In both cases, the results obtained by the image analysis and the actual measurement and ASTM method are in very good agreement. In the next phase, different degrees of damage, failure patterns and the crack tortuosity will be studied.