SUNDAY

12 - 6 pm	**Registration** Woods Common, Civil Engineering
1-4:30	**Tutorial: An Introduction to the Uses of Molecular Dynamics Simulations for Cement-based Materials** RPRH 172, Pharmacy Building
Moderator	Jason Weiss
1-1:05	Welcome
1:05-2:00	Introduction to molecular dynamics simulations of materials Alejandro Strachan, Purdue University
2-2:30	Online MD simulations at nanoHUB.org Alejandro Strachan, Purdue University
2:30-3	**Break/Visit Poster Session**
3-4:00	Computational Molecular Modeling of Cement Systems R. James Kirkpatrick, Michigan State University
4-4:30	Application of MD at Cement Reinforcement Interfaces Florence Sanchez, Vanderbilt University
4:30-6:00	**Poster Session and Opening Reception** Woods Common, Civil Engineering

AFM based indentation of cement paste

Zachary Grasley, Texas A&M University

Christopher Jones, Texas A&M University

Nanoindentation has been successfully utilized to measure the nanometric properties of the phases of hydrating portland cement. Atomic force microscopes (AFM) are capable of nanoindentation on a much smaller length-scale than nanoindenters, but their use in indentation measurements has been limited. The principle issues with AFM based indentation have been the treatment of tip geometry and the surface forces, which are of roughly the same order of magnitude as the force applied to the AFM probe. In this work, an iterative solution is applied to AFM based indentation of cement paste which includes the effect of surface forces, the tip geometry, and the viscoelastic character of the C-S-H phase of cement paste. Measured results are shown and compared to literature values, as well as those obtained from traditional nanoindentation.

Quantitative characterization of fly ash reactivity and geopolymer reaction products

Katherine Gustashaw, University Of Texas At Austin
Ryan Chancey, Nelson Architectural Engineers
Paul Stutzman, National Institute Of Standards And Technology
Maria Juenger, University Of Texas At Austin

This study used a new method for characterizing fly ash and geopolymer reaction products that combines Rietveld quantitative x-ray diffraction (RQXRD) and scanning electron microscopy coupled with multispectral image analysis (SEM-MSIA) to quantitatively characterize both crystalline and glassy phases. The combined information from these methods gives quantitative mass fractions of each independent crystalline and glassy phase inÂ theÂ material analyzed, including unreacted fly ash, partially reacted fly ash, and geopolymer reaction products. The method was used in the present study for characterizing fly ashes prior to alkali-activation with sodium hydroxide and to identify the reaction products formed in geopolymer pastes.Â Â The different phases in fly ash were shown to react differently in the alkaline environment required for geopolymerization, which is useful information for future design of geopolymer mixtures.

Reducing the Energy Demand of Metakaolin Production Using Low Bandgap Energy Fluxes

Sarah Taylor Lange , University Of Texas At Austin
Maria Juenger, University Of Texas At Austin

Metakaolin has been shown to be a good supplementary cementing material (SCM), but the calcinations of kaolinite to form metakaolin has a high energy demand. In this study, activating fluxes were investigated to reduce the duration and activation energy of kaolinite dehydroxylation. Economical and abundant metal oxides with low band gap energies were considered as fluxes, including: ferric oxide [Fe2O3], anatase [TiO2], rutile [TiO2], zinc oxide [ZnO] and tin (IV) oxide [SnO2]. Kaolinite samples with 0.5 wt.% fluxes were pre-fired at temperature intervals of 25oC from 500-600oC for one hour. The resulting metakaolins were examined using x-ray diffraction (XRD), differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA). DSC/TGA results showed an optimum dehydroxylation temperature of 550oC, for samples containing ferric, zinc and tin oxides. Cement pastes with the metakaolins were then tested in an isothermal calorimeter to determine reactivity. The results confirm a reduction in the endothermic energy required (kJ) for kaolinite calcination with use of metal oxide activating agents.

Evaluation of Calcium Aluminate Cement Based Systems Hydration Using Isothermal Calorimetery

Anthony Bentivegna, The University Of Texas At Austin
Kevin Folliard, The University Of Texas At Austin

Calcium aluminate cement (CAC) is a rapid hardening hydraulic cementitious material often used in niche concrete repair applications. The time and temperature history of the concrete affects the hydration products formed by CAC. At certain temperature ranges, CAC forms temporary hydrates; inevitably, these hydrates will convert to stable hydrates resulting in increased porosity and reduced strength. When used in field applications, CAC is used with water reducing admixtures and accelerators to promote workability and rapid strength development. Investigations of the effects of the chemical admixtures on hydration products were completed using an isothermal calorimeter and x-ray diffraction. Four variations of CAC based systems were investigated including: pure CAC, binary and ternary blended CAC systems, and CAC with limestone filler. Characterization of degree of hydration of CAC based mortar mixtures were completed using an isothermal calorimeter at four different temperature (5, 23, 38, and 60Â°C) regimes. Qualitative x-ray diffraction was performed on the samples at distinct time intervals to develop a time-line of the hydration product development and the influence of chemical admixtures. Future research will be conducted on the implications of different dosages of chemical admixtures and the effect on strength development.

Durability of Titanium Dioxide Containing Cement after NOx Abatement

Bo Yeon Lee, Georgia Institute Of Technology

Kimberly Kurtis, Georgia Institute Of Technology

Use of titanium dioxide (TiO_2) in cementitious materials is rapidly being adopted due to its NOx (NOx = NO + NO_2) abatement capabilities. However, loss of mechanical properties is expected in this process. In this study, the durability of TiO_2-cement was investigated when it is subject to NOx abatement. The TiO_2-cement samples were prepared at 5 and 10% TiO_2 weight replacement as well as control samples. The NOx abatement experiment was conducted in an environmentally controlled chamber. The degradation on sample surface was examined mechanically and chemically by microhardness tests and x-ray diffraction analysis respectively. The results were compared to the samples that did not go through NOx abatement process. It was concluded that the TiO_2 containing cement pastes that were active in NOx abatement have lower hardness, which might be due to chemical changes of hydration products or salt formation on the surface of the samples. This result indicate that cement based materials that include TiO_2 are expected to lose its mechanical properties on its surface, which require careful consideration in planning.

Use of bacteria to improve concrete properties

Ashna Chopra, University Of Illinois At Urbana-Champaign
Paramita Mondal, University Of Illinois At Urbana-Champaign
Leslie Struble, University Of Illinois At Urbana-Champaign
Wen-Tso Liu, University Of Illinois At Urbana-Champaign

The use of bacteria in concrete has shown potential in developing self-healing concrete. It is believed that spore-forming bacteria can lie dormant within the high pH of concrete and activate on crack development to deposit minerals, usually calcium carbonate. The process of mineral deposition by bacteria is called biomineralization. The source of carbonate ions for this process is not clear, it may be the atmosphere or it may be biological breakdown of the nutrient medium. Investigations were carried to understand the response of Sporosarcina pasteurii in the high pH environment of concrete with urea as the primary constituent of the nutrient medium and to determine the source of carbonate ions. The bacteria with nutrient medium at pH 9 showed clear growth; and on addition of $CaCl_2$ the bacteria produced vaterite, a form of $CaCO_3$. At pH 11 the bacteria showed no growth, and when pH in these solutions was reduced to about 9 the bacteria still showed no growth, indicating that no spores had formed and cell lysis had taken place. Regarding the source of carbonate ions, it appears that the bacteria use carbonate from either hydrolysis of urea or from the atmosphere, the latter showing promise for carbon dioxide sequestration.

Effects of the high temperature exposure on phase composition and microstructure of cement paste

Seungmin Lim, University Of Illinois At Urbana Champaign
Paramita Mondal, University Of Illinois At Urbana Champaign

The need to better understand the manner in which cement-based materials such as concrete behave at elevated temperatures is clear. Several extreme events in the past have revealed the vulnerability of concrete high rise buildings and tunnels subjected to high temperature exposure. This issue became a major concern with increasing application of high-strength concrete, which shows severe deterioration compared to normal strength concrete. However, the mechanisms that drive the thermal degradation of cement-based composite materials through all stages are still unresolved. So far, most of the research has focused on studying the loss of macroscopic strength and elastic modulus due to high temperature exposure, while very few have studied the complicated interaction of nano- and micro-structural properties and the resulting effect on important macroscopic properties. The objective of this research is to identify the processes that initiate at the micro- and nanoscale and drive the degradation mechanism by the application of advanced materials characterization tools. The investigation performed is aimed at explaining the change of residual compressive strength of cement paste after being exposed to various high temperatures. From compressive strength test of the OPC cement paste exposed to elevated temperature, it is found that residual compressive strength increases above 105 Â°C and higher strength is maintaining until 400 Â°C. The phase distribution and microstructural changes of the cement paste at this range is being studied to explain this phenomenon using scanning electron microscopy. Also, thermogravimetry analysis is employed to determine quantitatively the extent of dehydration of the primary hydration products and non-evaporable water in heated cement paste.

Chemical, Biological, and Physical Deterioration Mechanisms in Coastal Concrete Piling

Robert Holland, Georgia Institute Of Technology
Robert Moser, Georiga Institute Of Technology
Kimberly Kurtis, Georgia Institute Of Technology
Lawrence Kahn, Georgia Institute Of Technology

Biological, chemical, and physical deterioration of concrete piles has caused bridges spanning the coastal and marsh environments of Georgia to be structurally deficient. This poster presents the results of the forensic investigation of four piles showing significant deterioration after only 32 years of service that were recently salvaged from a bridge undergoing replacement near Brunswick, GA and delivered to the Georgia Tech Structural Engineering and Materials Laboratory. The bridge originally serviced I-95 over the Turtle River but required replacement due to deterioration of the concrete piling and corrosion. A visual inspection of the piles was performed and showed evidence of surface abrasion and corrosion induced cracking in the splash and tidal zones, as well as significant damage in the submerged regions, where limestone aggregates present at the surface of the concrete were severely deteriorated. The corrosion potentials were measured to determine the depth of active corrosion in the piles. Profile grinding was performed to determine the chloride profile and for qualitative x-ray diffraction to characterize changes in the cement paste microstructure. The results of the forensic investigation are being used to develop materials and design methods to lengthen the service lives of coastal bridge structures to over 100 years.

Characterization of Cement Paste Hydration and Setting Using Ultrasonic Wave Reflection

Prannoy Suraneni, University Of Illinois At Urbana-Champaign
Chul-Woo Chung, University Of Illinois At Urbana-Champaign
Leslie J.Struble, University Of Illinois At Urbana-Champaign
John S. Popovics , University Of Illinois At Urbana-Champaign

Simultaneous longitudinal and shear ultrasonic wave reflection (P-wave and S-wave UWR) measurements are conducted on cementitious materials to characterize their early hydration and setting behavior. The reflection coefficient, R, at the interface of the hydrating cementitious materials and a high-impact polystyrene buffer is monitored as a function of time. It is observed that the time of inflection of S-wave R and the time of debonding of P-wave R occur at roughly the same time for all materials tested. It is proposed that this time corresponds to the onset of autogenous shrinkage. This time also correlates well with the time of final set as measured from penetration resistance. Pastes with chemical and mineral admixtures show interesting UWR responses and these are presented here to showcase the applicability and versatility of the method in characterizing hydrating cementitious materials.

Early Age Properties of Fly ash- Slag Based Geopolymer System

Sravanthi Puligilla, University Of Illinois At Urbana-Champaign
Paramita Mondal, University Of Illinois At Urbana-Champaign

This research focuses on study of fly ash and slag based geopolymer. This particular system is chosen because a geopolymer system with only fly ash needs highly concentrated base, 8M and 10M for the activation, which is considered to be corrosive to work with on the site. Furthermore, general practice of high temperature curing is not feasible for field application. A fly ash- slag based geopolymer with potassium silicate as an activator and room temperature curing provides the possibility to develop a system that is more field friendly. However, there are many challenges that must be overcome before this technology can be implemented in the field. It has been observed that the setting time of alkali activated fly ash decreases considerably when slag (~15%) is added to the system. The mix is not workable beyond five minutes after mixing; it is thixotropic till it gets unworkable. Few attempts have been made to understand the setting behavior of the metakoalin- slag system. It has been proposed that when calcium is added in any soluble form, even at relatively small amounts, setting and hardening of geopolymerisation slurries are significantly accelerated. This may be due to the precipitation of $Ca(OH)2$ or calcium silicate hydrate from the solution, providing nucleation sites which then trigger rapid geopolymer gel formation. In this research, the influence of ground granulated blast furnace slag and potassium silicate on setting times is being studied by monitoring the amount of portlandite content using XRD. The

extent of dissolution of the alkali activated fly ash, alkali activated slag and that of the mixture are being studied that will give an idea of influence of dissolution of silicon and aluminum from fly ash in the presence of slag.

Drying shrinkage of concrete with using recycled concrete aggregate by new approach of mixing procedure

Atsushi Teramoto, University Of Illinois At Urbana-Champaign
Hyungu Jeong, University Of Illinois At Urbana-Champaign
Andres Salas, University Of Illinois At Urbana-Champaign
David Lange, University Of Illinois At Urbana-Champaign

With an increasing in the interest of recycled concrete aggregate(RCA), the effort to understand properties of RCA in the construction field has been required. For responding to this effort, our research group has performed a new mixing procedure that would help to reduce drying shrinkage. Some previous studies showed that RCA can absorb larger amount of water than natural aggregates because RCA has a higher porosity which leads concrete to increase shrinkage. However, our test showed that drying shrinkage was able to reduce by new mixture rocedure. The main point of the new mixing procedure is that RCA was around 80% saturated when it was mixed with other materials. Firstly, to make 80% saturated RCA, it was treated with fully saturated and dried for 1day. In this study, drying shrinkage was compared by using 80% and 100% saturated RCA to clarify the influence of water content in RCA at the beginning of concrete mixing. In addition, ring test and dog bone tests are conducted to confirm the drying shrinkage when it is restrained and is affected by internal tensile stress.

Effect of decalcification on the microstructure and performance of CNF cement composites

Florence Sanchez, Vanderbilt University
Lesa Heintzman, Vanderbilt University

Carbon nanofibers (CNFs) possess a high strength-to-weight ratio and chemical resistance, indicating their potential as reinforcements for cement composites. Studies to date have focused on the physical, mechanical, and electrical properties provided by the CNFs, and little attention has been given to the durability of CNF cement composites and the effect of environmental weathering forces. These forces can cause internal chemical changes and micromechanical stresses, resulting in material damage and a decrease in the mechanical properties of the composite. One type of internal chemical change that causes deterioration of cement composites is decalcification caused by exposure to neutral or acidic waters. Portland cement pastes with and without 0.2% CNFs per weight of cement were subjected to accelerated decalcification by exposure to ammonium nitrate (NH_4NO_3) solutions. The microstructural and morphological changes within the composite and at the CNF-cement interface will be presented. In addition, the flexural strengths as a function of the extent of decalcification will be discussed.

Measuring the coefficient of thermal expansion of hardening cementitious materials

Carmelo Di Bella, Empa, Swiss Federal Laboratories For Materials Testing And Research
Roman Loser, Empa, Swiss Federal Laboratories For Materials Testing And Research
Beat Muench, Empa, Swiss Federal Laboratories For Materials Testing And Research
Pietro Lura, Empa, Swiss Federal Laboratories For Materials Testing And Research

In this poster, a novel technique for measuring with high accuracy the coefficient of thermal expansion (CTE) of hardening materials is presented. The main application of the technique is the measurement of the CTE of cement pastes or mortars at early age. Knowledge of CTE is of paramount importance for the determination of the cracking risk of concrete structures. The technique consists of casting a small amount of cement paste or mortar into flexible membranes. The specimens are then immersed in an oil bath, whose temperature can be precisely regulated and rapidly altered in cycles. By suspending the sample from a high-precision balance and reading the change of mass after each temperature step, the CTE can be calculated from the measured temperature and strain. Results on cement pastes and mortars showed a good repeatability. In particular, a sudden decrease in the CTE at setting time, as well as a gradual increase due to self-desiccation were measured.

Suppression of internal RH in nanoporous media due to the formation of interfaces during drying

Zachary Grasley, Texas A&M University
Kumbakonam Rajagopal, Texas A&M University

As nanoporous materials such as concrete dry, new interfaces are generated within the pore network. In this poster, we show that the generation of new interfaces during drying suppresses the internal RH within a nanoporous material such that it is lower than the surrounding open boundary RH, even at equilibrium. The results of this analysis have great implications on accurately modeling drying shrinkage, thermal expansion, and moisture transport in concrete.

The development and implementation of nano-engineered cementitious composites for infrastructure and construction industries

Suvankar Sengupta, Metamateria Technologies Llc
Mahir Dham, Metamateria Technologies Llc
Richard Schorr, Metamateria Technologies Llc
Ramachandra Rao Revur, Metamateria Technologies Llc
Richard Helferich, Metamateria Technologies Llc

MetaMateria Technologies has developed a process to produce nanoscale cementitious materials. When added in small quantities to conventional cement, significant improvements in properties were observed. Addition of this nanoscale material to Type I, Type I/II, Class H, Ultra High Performance, and Rapid setting cements was investigated.   Significant improvement in compressive and tensile strengths with minimal change in modulus was observed. Depending on the formulation of the nanoscale cementitious material utilized, improvement was observed in early, intermediate as well as long term or ultimate strength of the composite. Integration of nano-cements may also lead to a denser product microstructure with higher ultimate compressive and tensile strengths. Potential also exists to reduce the permeability of the structures involved and to strengthen the interfacial transition zones within the material. With such improvements, nano-cement can serve as a tool to further optimize various construction systems for enhanced properties and may further enhance the durability of the concrete.

A mixing procedure to mitigate drying shrinkage of concrete with recycled concrete aggregate

Hyungu Jeong, University Of Illinois Urbana-Champaign
Atsushi Teramoto, Nagoya Unibersity
Andres Salas, University Of Illinois Urbana-Champaign
David Lange, University Of Illinois Urbana-Champaign

Interest in recycled concrete aggregates (RCA) is increasing with the broadening interest in sustainability through the construction industry. An increased effort to understand properties of RCA in the construction field is required. Our research group has explored a mixing procedure that would help to reduce drying shrinkage. RCA absorbs more water than natural aggregates because RCA has a higher porosity associated with the hardened cement paste portion of the RCA, and this makes the concrete produced with the RCA to exhibit higher drying shrinkage. Our trials suggest that a special mixing procedure will mitigate this behavior. The essential point of the new mixing procedure is that RCA is preconditioned at a moisture content that is 80% of the water content required for saturation. We accomplish this by first fully saturating the RCA and then letting air dry for 1d. In this study, the drying shrinkage of concretes using 80% and 100% saturated RCA was contrasted to clarify the influence of water content in RCA at the beginning of concrete mixing. In addition, ring test and dog bone tests will be conducted to confirm the drying shrinkage when it is restrained and is affected by internal tensile stress.

Experimental investigation of the effect of internal curing on high w/c systems

Javier Castro, Purdue University

Jason Weiss, Purdue University

The increased propensity for shrinkage cracking in low w/c concrete has resulted in the development of new methods that can reduce the risk of early-age cracking such as internal curing. Internal curing can use saturated lightweight aggregate to supply â€˜curing waterâ€™. Normally this has been used in concretes with low w/c intending to reduce shrinkage and stress development. While, information about the contributions of internal curing on transport properties of low w/c systems exists (e.g. water absorption or diffusivity), no information on its effect in higher w/c systems is reported. This study focuses on testing the water absorption, relative humidities, degree of hydration and the electrical conductivity in mortar specimens made using internal curing with wider range of w/c (i.e. 0.30~0.45). The results indicate that the inclusion of saturated lightweight aggregate can increase the degree of hydration of the cement and reduce both the total porosity and the interconnection of the pore structure of mortar specimens.

Developing a Robust Transferable Empirical Force Fields for Cement Hydrates

Rouzbeh Shahsavari, Mit

Roland J.-M. Pellenq, Centre Interdisciplinaire Des Nanosciences De Marseille (Cnrs)

The use of empirical force fields is now becoming a standard approach in predicting the properties of complex hydrate oxides, which are omnipresent in both natural and engineering applications. Transferability of force fields to analogous hydrated oxides without rigorous investigations may result in misleading property predictions. Herein, we focus on two common empirical force fields, the single point charge ClayFF potential and the core-shell potential to study tobermorite minerals, the most prominent models for Calcium-Silicate-Hydrate family that are the main product of cement hydration. We benchmark the predictive capabilities of these force fields against first principles results. While the structural information seem to be in close agreement with DFT results, we find that for higher order properties such as elastic constants, the core-shell potential quantitatively improves upon the single point charge model, and shows a larger degree of transferability to complex materials. In return, to remedy the deficiencies of the single point charge potential for hydrated calcio-silicates, we suggest using both structural data and elasticity data for potential calibration, and propose a new force field potential, CSH-FF. This re-parameterized version of ClayFF is then applied to simulating an atomistic model of cement hydrates (Pellenq et al PNAS, 2009). We demonstrate that this force field improves the predictive capabilities of ClayFF, being considerably less computational intensive than the core-shell model.

Statistical Mechanics of Cement Setting: Molecular Dynamics of a Colloidal Model

Paul Monasterio, Massachusetts Institute Of Technology

Sidney Yip, Massachusetts Institute Of Technology

Cement hardening is studied by modeling the microstructural evolution of a slurry as a colloidal system of binder C-S-H in a C-H solution. We aim to demonstrate the extent to which the dynamical behavior of such a binary mixture, probed by atomistic simulations extended with activated state dynamics, can describe the classic three-stage kinetic behavior of cement hydration â€“ coagulation, incubation, and setting. This coupling of chemical reactions with mechanical behavior poses new challenges not yet addressed by multiscale materials modeling. In this context the present work is a first attempt to develop a mechanistic model of cement hydration from the chemo-mechanics perspective, where chemistry and mechanics are treated on equal footing.

Our colloidal model makes use of potential functions describing the effective interactions among the C-H particles (species A) and the C-S-H particles (species B). The A-A, B-B, and A-B interactions have isotropic (central) repulsive and attractive components characterized by depth and range. In addition the B-B interactions have a directional component to describe preferential bonding which is realized by considering the particles as soft spheres with sticky points on their surfaces. The parameters of the model are adjusted from those in previous models of colloidal gelation to achieve incubation, but can also be informed from chemical studies of cement microtextures. We also implement a metadynamics formulation developed in our study of shear relaxation of supercooled liquids. This extension is necessary because normal MD simulations cannot reach the time scales of seconds to hours which are relevant in the chemical kinetics of cement setting.

Our preliminary results show that the colloidal model is able to capture qualitatively the three-stage kinetic behavior, with stage I corresponding to the gel formation of species A, stage II to the diffusion of species B for the nucleation and growth of B clusters, and stage III to the percolation of B clusters. With the establishment of the reference colloidal model a systematic study of size, mass, and concentration of the particles is underway, along with the effects of temperature and strain rates (in determining an effective shear modulus). Additional model refinements which will be studied include spatial effects (dissolution and nucleation at the clinker surface). Once the model becomes sufficiently chemically realistic, it will be used to map out reaction pathways and activation barriers that can feed into more realistic chemical kinetics models of cement hydration.

Development of Testing Method for Measuring Residual Stresses in Concrete Pavements

Daniel Castaneda, University Of Illinois At Urbana-Champaign
David Marks, University Of Illinois At Urbana-Champaign
David Lange, University Of Illinois At Urbana-Champaign

The development of residual stresses in rigid pavements introduces additional forces that diminish a pavement's ability to sustain its designed load. As a result of its loss in capacity, a pavement will suffer premature damage necessitating costly repairs or replacement. Testing to quantify residual stresses has already been developed for steel wherein a small hole is drilled adjacent to an affixed strain gage (ASTM E837). The change in strain reading is correlated to a residual stress in the steel material. While rigid pavements are as detrimentally affected by the formation of residual stresses as steel, no similar testing method exists for concrete. Recent research conducted by the Federal Aviation Administration's National Airport Pavement Test Facility investigated the strain relaxation of cantilevered concrete beams when a blind-depth hole using core drilling is made in the vicinity of a strain gage. Initial findings indicated that the testing procedure partially quantified the residual stresses. Later testing conducted by the University of Illinois at Urbana-Champaign modified the testing procedure by instead sawing a linear notch near one end of the strain gage and sawing two linear notches near both ends of the strain gage. Results for the doubly notched concrete beam seemingly fully quantify the residual stresses in comparison to the core-drilled concrete beams. In order to determine the viability of this modified testing procedure, recent field work on in-situ plain concrete pavements has been performed. Preliminary results indicate that the residual stresses can be reliably measured.

Microstructural properties of recycled concrete aggregates

Yogini Deshpande, Michigan Technological University
Jacob Hiller, Michigan Technological University

The recent push for sustainable development of infrastructure systems has increased the demand for recycled materials such as recycled concrete aggregates (RCA) for production of new concrete. RCA consists of the natural aggregate used in the original concrete as well as some portions of old mortar adhering to it. The mortar adhered to the RCA plays an important role in the durability characteristics of the new concrete.

In this study, three generations of crushed gravel aggregate were used: 1) virgin crushed gravel aggregate , 2) recycled concrete aggregate containing crushed gravel as the virgin aggregate, and 3) twice recycled concrete aggregate containing crushed gravel as the virgin aggregate or third generation (3G) RCA. Concrete specimens manufactured from these aggregates were studied using optical microscope and SEM micrographs. Significant microscopical observations were made at the following interfaces in the specimens-

1. Interface between new mortar and mortar adhering the RCA
2. Interface between original coarse aggregate and adhered mortar
3. Interface between new mortar and original coarse aggregate

It was observed that the mortar on the RCA can be either the weakest link or the strongest depending upon the quality of the adhered mortar. A distinctive transition zone between the mortar on RCA and the new mortar was observed in SEM micrographs. Concrete containing 3G aggregates exhibited lower porosity and higher compressive strengths compared to concrete manufactured using RCA. Lower porosity was related to the well-defined and compact interface observed in the 3G RCA mortar. Higher amount of calcium hydroxide and calcium silicate hydrate was observed in specimens of RCA and 3G concretes.

Characterization and Chemical Admixture Interaction of Biomass Co-fired Fly Ash

Christopher Shearer, Georgia Institute Of Technology
Nortey Yeboah, Georgia Institute Of Technology
Kimberly Kurtis, Georgia Institute Of Technology
Susan Burns, Georgia Institute Of Technology

The co-combustion of biomass (e.g., trees, switchgrass) with coal can be a sustainable energy source and reduce carbon dioxide emissions. The product of this process, biomass-derived fly ash, is not addressed in U.S. standards for fly ash use in concrete; however, recent European standards have permitted its use with certain restrictions. The engineering properties of co-fired fly ash are relatively unknown compared to coal fly ash. This study characterizes the composition, structure, and performance of co-fired fly ash. Results indicate that the co-fired fly ash morphology can be different than coal fly ash. The coal and co-fired fly ash samples exhibit similar size and carbon distributions; however, co-combustion may result in finer carbon particles. Foam index tests show that fly ash replacement of cement increases air-entraining admixture (AEA) demand, likely a result of increased carbon surface area. A mitigation technique to lower the unburned carbon content of high loss-on-ignition (LOI) samples through dry sieving reduced LOI to within standard limits. However, foam index testing revealed that processing coal or co-fired fly ash through removing large carbon particles may not be a productive technique in reducing AEA demand. Ultimately, the results indicate that the exclusion of co-fired fly ash from the standards may be inappropriate with respect to chemical, physical, and durability requirements.

Specimens for Testing Concrete Pipe Formulations

Andres Salas, University Of Illinois
Leslie J. Struble, University Of Illinois

A method has been developed to produce specimens of stiff, highly consolidated mixtures for laboratory testing using a vibration method designed to mimic the production of concrete pipes. The specimen molds were fastened to a high frequency vibrating table and a modest downward force was applied during vibration. With vibration of 15 sec, specimens using typical concrete pipe formulations (w/cementitious material ratio of 0.22) were well consolidated. After consolidation, specimens were cured at 45Â°C for 20 hours to further simulate pipe manufacture. The method was used to produce cement pastes and concretes to determine the effect on strength of replacing high proportions of portland cement with fly ash (up to 100%). Compressive strengths were measured at 1 day and 7 days. Mixtures met the compressive strength value of 27.5 MPa required by the ASTM standards for reinforced concrete pipe with cement replacements up to 60% for the Class C fly ash and 40% for the Class F Fly ash. Although the strength values for paste were somewhat higher than the values for concrete, paste and concrete strengths showed the same relationship with fly ash replacement level, decreasing as fly ash content increased.

Designing Liquid Stone: Modulating Cement Mechanics via Computation and Physical Chemistry

Karen Stewart, Massachusetts Institute Of Technology
Meng Qu, Massachusetts Institute Of Technology
Sandra Lebreiro, Cimpor Tec
Sid Yip, Massachusetts Institute Of Technology
Franz-Josef Ulm, Massachusetts Institute Of Technology

Although cement is a ubiquitous material formed from hydration of calcium silicates, until recently the molecular structure of the calcium-silica-hydrate (CSH) granular phases that comprise cement pastes was uncertain. We have recently reported a structure for CSH that is consistent with the density and C/S ratio of CSH indicated from experiments [Pellenq et al., PNAS 106: 2009]. Here, we leveraged atomistic modeling to consider whether the mechanical properties of the CSH phase itself can be modulated by altering the ratio between calcium and silica in the CSH phase. Our new atomistic simulations predict a peak elastic modulus of CSH at a calcium/silicon (C/S) ratio of of ~1.5, representing a 60% increase in stiffness from C/S = 1.85. In an effort to achieve this ratio experimentally, we systematically varied both clinker phase chemistry and dissolution conditions, and characterized the composition chemistry through x-ray spectrometry. We found that the composition of the nanoscale CSH phase within actual cement pastes can be altered with existing materials and processes. Further, through nanoindentation maps and semi-analytical relations of packing density within each phase, we observed that the indentation elastic moduli ms of fully dense CSH can increase as much as 20-26% when the C/S ratio is decreased from 1.88 to 1.52. The hardness hs or resistance to permanent deformation of the CSH can also be varied experimentally, as a function of C/S ratios. Such chemomechanical characterization of these cements, motivated by computational predictions, allows clear identification of the processing variables that most directly alter the distribution of calcium-rich phases and CSH C/S ratios in hardened cement pastes, and also facilitates correlation with mechanical performance of macroscopic volumes. These computational predictions and experimental findings enable the potential design of this so-called â€œliquid stoneâ€□ to improve salient physical and mechanical properties while reducing environmental impact.

Preliminary findings from research to extend internal curing concepts to mixtures with higher volumes of fly ash

Igor De La Varga, Purdue University
Javier Castro, Purdue University
Jason Weiss, Purdue University

Fly ash has historically been used in concrete transportation structures. Recent interest has developed in the US to reduce the clinker content (ordinary portland cement) in concrete as a method to improve sustainability. This paper reports preliminary results from an ongoing research project that is investigating the use of higher volumes of fly ash (higher than what is currently permitted) in transportation structures. The paper focuses on testing performed on three mortar mixtures: a water to cement ratio (w/c) of 0.42, a w/c of 0.30, and water to cementitious ratio (w/cm) of 0.30 with 40% fly ash by volume. Compressive strength, elastic modulus, autogenous shrinkage and restrained shrinkage testing were performed. Chemical shrinkage, internal relative humidity, and moisture desorption measurements are presented to better understand how self-desiccation results in autogenous shrinkage and residual stress. In addition, this research lays the groundwork for extending internal curing concepts to these mixtures.

Vapor Diffusion in Mortars Containing Shrinkage Reducing Admixtures

Mohammad Pour-Ghaz, Purdue University
Robert Spragg, Purdue University

Jason Weiss, Purdue University

Properties of pore solution, such as surface tension and viscosity, affect the rate of vapor diffusion in cementitious materials. Shrinkage reducing admixtures (SRA) can alter the properties of the pore solution. This presentation, discusses the effect of SRAs on the rate of vapor diffusion in cementitious materials. Desorption spectra are measured to obtain the moisture diffusivity of plain mortar and mortar containing different loadings of SRA. Using a non-linear diffusion theory the relative humidity profile and mass loss in slab and cylindrical geometry is calculated. The results of diffusion theory are compared with physical measurement. Relative humidity and temperature sensors embedded in slabs to directly measure the relative humidity profiles.

Cement Seal Integrity: Microstructural Characterization of CO_2 Alteration Zones in Class H Portland Cement

Circe Verba, Department Of Energy

Thirty Class H Portland cement core samples were subjected to a headspace of supercritical CO_2 and CO_2-saturated brine for durations of 28, 56, and 84 days. The test conditions were intended to simulate down hole CO_2 sequestration in saline aquifers at 50ºC and 4200 psi (28.9 MPa) within 1.2 L static SS autoclave vessels containing 600 mL of brine. These samples were exposed to several CO_2-saturated brines, including a surrogate brine composed of three major salts (1 M: 0.82 M NaCl, 0.02 M $MgCl_2$, and 0.16 M $CaCl_2$), and 3 synthetic brines derived from basin-specific data found at 3 of the 7 NETL Phase III Regional Partnership sites: the Illinois Basin (MGSC), southwest Mississippi (SECARB), and southwest Wyoming (Big Sky). Petrographic analysis by polarized light microscopy (PLM) and scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS) identified an oxidized, reddish rim ranging from diffuse intrusions to discrete alteration zones including: (1) a high-silica porous region, (2) $CaCO_3$ precipitated from $Ca(OH)_2$ and C_2S/ C_3S, (3) Ca-depleted, and (4) Cl-enriched zones. The observed general trend was that the alteration depth increases and zones became more distinct with time; although the penetration depth was sample specific on brine chemistry. Higher salinity brines exhibited less alteration penetration depth, likely due to their reduced CO_2 solubility. The presence of portlandite crystals that remained on the outer rim also plays a role in inhibiting penetration.

Characterization of alkali-reactivity of aggregates by measurements of nonlinear elastic response of mortars in vibrations

Jun Chen, Georgia Institute Of Technology

A R Jayapalan, Georiga Institute Of Technology

J-Y Kim, Georgia Institute Of Technology

Laurence Jacobs, Georgia Institute Of Technology

Ke Kurtis, Georgia Institute Of Technology

A novel nondestructive evaluation (NDE) technique is developed to measure the nonlinear elastic response of mortars undergone alkali-silica reaction (ASR) in the bending vibrations. The rate of resonance frequency shift of mortar samples with respect to the excitation magnitude of vibrations is defined as a new damage index for the progressive ASR damage occurring in mortars during a standard ASTM C 1260 test. Four representative aggregates having different alkali-reactivity are examined. The new NDE results show a better distinction among four aggregates tested in a shorter time than the ASTM C 1260 expansion measurements. The enhanced sensitivity of the new NDE technique in ASR tests indicates its great potential for a more general application for the detection of material degradation in cement-based materials.

8:00-9:00 **Cements Division Executive Meeting**

G212, Civil Engineering Building

MONDAY
7:30 am - 6:30 pm **Registration**
Woods Common, Civil Engineering

8:30-10 **Hydration: Modeling and Experiments**
RPRH 172, Pharmacy Building
Moderator Zachary Grasley

8:30-8:35 Open Program/Welcome

8:35-8:50 **Modeling Cement Hydration as a Nucleation and Growth Process**
George Scherer, Princeton University
Jie Zhang, Princeton University
Jeffrey Thomas, Northwestern University

The hydration and setting of cement has been successfully modeled by assuming that it involves a process of nucleation and growth. Several types of model have been applied, including the original Johnson-Mehl-Avrami-Kolmogorov theory that assumes random nucleation in the bulk, and the Cahn theory that assumes that nucleation begins on particle boundaries. The latter model assumes that the new phase can cross boundaries as it grows, but this is not realistic for hydration, as it would imply that inner product could grow into the interparticle space, and outer product could cross the interparticle space and invade another cement particle. Alternative models have been developed in which the growing phase does not cross boundaries. We will explore the application of such models to hydration, and quantify the consequences for the rates of nucleation and growth that are inferred by fitting the theory to hydration data.

8:50-9:05 **A Mass Continuity-Based Continuum Mechanical Single Particle Model for Alite/C3S Hydration**
Joseph Biernacki, Tennessee Technological University
Tiantian Xie, Tennessee Technological University

The hydration behavior of portland cement phases continues to be debated with new insights fueling the controversy. What causes the induction period? What initiates acceleration? What causes the onset and rapid decrease in reaction rate post peak? Does diffusion play a role and what causes low, but sustained reaction rates for long periods of time. Recent modeling efforts suggest that boundary nucleation and growth can explain at least some of the observations and that such a mechanism occurs in a â€œlimited reaction volumeâ€□ that represents about 30% of the initial cement mass. Yet, other efforts offer an alternative theory that would suggest that densification occurs in two steps. In an effort to resolve these and other questions, a single particle model for alite/C3S hydration has been developed using a mass continuity-based continuum approach as an alternative to the Avramian basis used in most recent studies. Such single particle models are relevant starting points for fast model-based experimentation, more elaborate single particle models and simulation platforms that incorporate ensembles of particles. The present model includes transport effects, solution phase chemistry, and incorporates intra-particle nucleation.

9:05-9:20 **Early Stage Hydration: Direct Evidence For Production of Loosely-Packed C-S-H Filling Most of the Pore Space**
Sidney Diamond, Purdue University
Ko Kjellsen, Norcem As

Results of backscatter SEM examinations of early-age mortars carried out several yeas ago have been previously reported with emphasis on (a) local variations in the initial distributions of cement grains that lead to subsequent development of a patchy structure, and (b) the presence of narrow well-defined water-filled layers adjacent to aggregate surfaces. In the present communication we illustrate findings on the nature and development of early C-S-H hydration products in these mortars. It is commonly assumed that the deposition of a dense layer of inner product around the cement grains induces the onset of â€œdiffusion controlâ€□, which results in the slowing down of the hydration process after the main heat evolution peak. In contrast to this supposition, we have found that little or no inner product is produced during the first 12 hours of hydration; rather, during this period hydration produces a loose, porous obviously low density form of C-S-H that quickly spreads to fill most of the originally water-filled space. This was found to be the case regardless of the water/cement ratio. Recently Bishnoi and Scrivener hypothesized that such a pattern might occur on the basis of the results of their modeling of alite hydration in an alite-water paste

9:20-9:35 **Micro-CT study on micro structure evolution of cement paste**

David Lange, Uiversity Of Illinois At Urbana-Champaign

Yongjia He, Uiversity Of Illinois At Urbana-Champaign

Jason Mote, Uiversity Of Illinois At Urbana-Champaign

Shuguang Hu, Wuhan University Of Technology

Micro computed tomography (Micro-CT) was applied to obtain three dimensional images of the microstructure of cement paste (water to cement ratio of 0.5) at different ages. By using the Amira software, component phases of the cement paste such as pores, hydration products, and unhydrated clinker particles were segmented from each other based on their 3D image grey levels; their relative content percentages were also calculated with the software. The calculated pore ratio and hydration degree at different ages were compared with the published experimental data acquired by mercury intrusion porosimetry (MIP) tests and non-evaporable water tests. Results show that the calculated and measured data reasonably agree with each other, which indicate that micro-CT is a useful and reliable approach to characterize the micro structure evolution of hydrating cement paste.

9:35-9:50 **Effects of Curing on Hydration Kinetics**

Kyle Riding, Kansas State University

Md. Sarwar Siddiqui, Kansas State University

Water curing is common and widely used technique to achieve higher degree of hydration (DOH) in concrete structures. Water curing allows adequate supply of water to the unhydrated cement grains to allow for continued hydration. The rate of water supply from the cured surface that is available for continued hydration is controlled by the network of micro pores present. The curing temperature has an effect on the transport of water through the porous hydrated structure, including the water diffusion rate and the rate of densification of the microstructure. The effect of different depths of water curing at different temperatures has been studied using isothermal calorimetry to investigate the effective depth of curing for construction and the effects of external curing solutions on hydration. The effects of fine lightweight aggregates as internal reservoirs (FLAIR) on early age hydration has also been examined using isothermal calorimetry. The experimental results of curing conditions on hydration give insight into the ability to compare isothermal calorimetry results to that of other commonly used experiments such as chemical shrinkage experiments.

9:50-10 Discussion

10-10:30 Coffee Break

Woods Common, Civil Engineering

10:30-12 **C-S-H: Structure and Properties**
RPRH 172, Pharmacy Building
Moderator Maria Juenger

10:30-10:45 **Effect of synthesis method and C/S ratio on morphology and structure of calcium silicate hydrate**
Linnu Lu, Wuhan University Of Technology And University Of Illinois
Yongjia He, Wuhan University Of Technology And University Of Illinois
Leslie.J Struble, University Of Illinois At Urbana-Champaign

Â Several series C-S-H samples with different C/S ratios were prepared by different methods - reaction of CaO and SiO2 at room temperature, hydrothermal reaction of CaO and SiO2, aqueous reaction of Ca(NO3)2.4H2O and Na2SiO3, hydration of C3S and C2S. Phase composition and structural and morphology characteristics of C-S-H samples were analyzed by XRD, IR, SEM and NMR, etc. Both the degree of polymerization of silica tetrahedra and the C-S-H morphology were seen to vary systematically with C/S and to vary with the synthesis method.

10:45-11 **A comparison of the atomic packing density of C-S-H with that of related minerals, and implications for chemical shrinkage**
Jeffrey Thomas, Northwestern University
Hamlin Jennings, Northwestern University
Andrew Allen, National Institute Of Standards And Technology

Relationships between composition, mass density, and atomic packing density for C-S-H, the main hydration product of cement, and its mineral analogues tobermorite and jennite, are examined, and new experimental measurements for the composition and mass density of C-S-H in cement paste cured at elevated temperatures, dried and resaturated, and hydrated with silica fume are presented. A graphical approach, similar to a phase diagram, is used to display the variation in density as a function of water content. To provide insight into atomic packing density differences between these phases, hypothetical phase transitions are performed by adding the stoichiometrically correct amount of CaO and H{sub}2{\sub}O to convert one phase into another, and then the molar volumes before and after the transformation are compared. These calculations indicate that C-S-H formed from cement hydrated under normal conditions has a considerably higher atomic packing density than both tobermorite and jennite. The solid density values for C-S-H are used to predict the amount of chemical shrinkage that should occur in a pure tricalcium silicate or dicalcium silicate paste, and these calculations are in good qualitative agreement with published experimental measurements for cement paste. and interpreted using the same approach. An important finding is that curing at 80ËšC leads to a C-S-H phase with a lower atomic packing density, providing an explanation for experimental observations of less chemical shrinkage at elevated temperatures.

11-11:15 **Dynamic Thermo-Mechanical Response of Calcium Silicate Hydrates**
Rouhollah Alizadeh, Institute For Research In Construction, National Research Council Canada
James Beaudoin, Institute For Research In Construction, National Research Council Canada
Laila Raki, Institute For Research In Construction, National Research Council Canada

The relation between the chemistry and mechanical properties of calcium silicate hydrate (C-S-H, the principal component of hydrated Portland cement) has not been fully resolved. This is partly due to the experimental limitations in the engineering investigation of phase pure C-S-H preparations that are in the form of powder. The compaction technique was utilized in the current study in order to prepare solid rectangular specimens from synthetic C-S-H of variable stoichiometry (C/S ratio). The dynamic mechanical properties of compacted samples of C-S-H were investigated at various temperatures. The stiffness and damping behavior of the C-S-H systems were monitored at various drying stages from 11%RH following the removal of the adsorbed and interlayer water as the temperature increased. A unique oscillatory response was identified in the storage modulus (Eâ€™) and internal friction (tan Î´) experiments for C-S-H. The results are discussed in terms of the state of water present in the nanostructure of C-S-H, the evolution of the silicate structure and the interaction of calcium ions in the interlayer region. Hydrated Portland cement paste and porous glass specimens were also examined for comparison. It was shown that the C-S-H in the hydration products of Portland cement has a complex yet analogous dynamic mechanical behavior to that of synthetic C-S-H. The response of these systems upon the removal of water was explained by a layered model for the C-S-H. A mechanistic model was proposed to describe the changes occurring at various stages in the dynamic mechanical performance of C-S-H.

11:15-11:30 **Bridging chemistry and mechanics of concrete at the nanoscale**

Jeffrey Chen, Lafarge Centre De Recherche
Luca Sorelli, Universite Laval
Matthieu Vandamme, Ecole Des Ponts - Ur Navier
Franz Ulm, Mit
Gilles Chanvillard, Lafarge Centre De Recherche

The mechanical properties of concrete are generally interpreted through variations in microscale capillary porosity. A recent study on highly concentrated cement paste (water/cement = 0.20) reveals an added layer of complexity at the nanoscale. We exploited a novel coupling of nanoindentation and ex-situ SEM X-ray microanalysis over a grid of indentation points. Since simulations showed that the microvolumes solicited in each method were of similar size (~ 1.5 Âµm in linear dimension), we could directly compare the local mechanical and chemical information provided by each method. Results showed the first direct evidence for a mechanically robust nanocomposite structure comprised of a calcium silicate hydrate gel (Câ€“Sâ€“H) and Ca(OH)2. Micromechanical calculations furthermore indicate that the elevated modulus values are due to filling of Câ€“Sâ€“H pores with nanoscale Ca(OH)2 crystals. It is hypothesized that the formation of this nanocomposite structure occurs in the confined aqueous films separating individual cement grains, where liquid supersaturations are highest and atomic transport is limited. On a general level, this study illustrates the great potential in coupling microanalysis, nanoindentation, and micromechanics to advance our understanding of highly heterogeneous composite materials.

11:30-11:45 **Elastic Properties of CSH systems determined by Atomistic Simulation methods**

Hegoi Manzano, Massachusetts Institute Of Technology
Jorge Sanchez, Labein-Tecnalia
Andres Ayuela, Csic-Upv
Roland Pellenq, Massachusetts Intitute Of Technology
Franz-Joseph Ulm, Massachusetts Institute Of Technology

Cement paste is a complex multi-component material where many crystalline phases are surrounded by an amorphous hydration product called C-S-H gel. It represents up to the 70% in weight of the cement paste and, therefore, is the main responsible for the properties of the materials. The C-S-H gel, acronym of Calcium-Silicate-Hydrated, has a variable stoichiometry usually characterized by its calcium to silicon ratio (C/S) which ranges from 1.2 to 2.1. However, the C/S ratio is not the only variable that plays a key role in the C-S-H gel nanoparticles. To study those other variables, such as the density or water content, 21 compounds of the crystalline hydrated calcium silicates family. We calculate the elastic properties of the crystals by force field methods. The structure and elastic properties of these compounds were analyzed as a function of their composition, their density and their water content, and were compared with the experimental values available for the C-S-H gel. Tobermorite and jennite, the most employed structural models for the C-S-H gel, are two members of the crystalline CSH family and have been intensively studied. However, the analysis of other CSH family members is very useful for the comprehension of the C-S-H gel properties.

11:45-12 **Water, water everywhere: Effects of computational water models on the structure and dynamics of confined water in C-S-H**

Krystyn J. Van Vliet, Massachusetts Institute Of Technology
Qing Ji, Massachusetts Institute Of Technology
Roland J.M Pellenq, Massachusetts Institute Of Technology

Although water molecules help to define the properties of the calcium-silica-hydrate (CSH) gel phase in cement and concrete, very little is known about the structure and dynamics of this water under the extreme confinement and soluble ion content of the CSH phase itself. Two chief challenges in understanding the role of water and aqueous electrolytes in the nanoscale pores of the CSH electrolytic gel are (1) incomplete knowledge of the CSH structure; and (2) the longstanding challenge of computationally modeling water itself. Indeed, the molecular structure of the CSH phase in hardened cement pastes has only been recently proposed [Pellenq et al., PNAS 106: 2009], and the complex behavior of water has resulted in nearly 50 computational models of this universal solvent! An empirical interatomic model for CSH has been developed by assuming one particular and simple model of H2O termed ""single point charge"" or SPC, but this choice has not been validated by comparison with other computational models of water that confer additional bond flexibility or charge distribution. Here, we consider five distinct, classical atomistic water models (SPC, TIP3P, TIP4P, TIP4P05, and TIP5P) to determine the effects of these computational simplifications on CSH properties. We rigorously compare the structure & elastic constants of CSH, as well as the dynamics of both interlayer water (between silicate-rich chains) and intralayer water (within the calcium oxide-silica layers that define the oxide-rich phase of the CSH molecular structure). We find that all five of these classical water models stabilize the same structure of CSH over 100s of nanoseconds of molecular dynamics simulation, with minimal densification of the initial structure. We further observe that the elastic properties are essentially independent of the water model details. In contrast, our movies & quantification of the dynamics of aqueous diffusion along and through the CSH layers show strong dependence on the mechanical flexibility assumed in each water model. These simulations provide the first systematic optimization of computational simulation time required to capture key structural, mechanical, and dynamic properties of CSH at the molecular dynamic scale. Further, these results represent the first predictions of interlayer and intralayer water structure and dynamics within the nm-scale CSH molecular structure. Ongoing work on these optimized models enables rapid comparison of water dynamics as a function of mesoscale CSH gel porosity, electrolyte concentration, pH, and mechanical pressure.

12-2:00 Lunch

2-3:30 Cement Production, Processing and Microparticle Additions
RPRH 172, Pharmacy Building
Moderator Joseph Biernacki

2-2:15 **Production of High-Performance Cement Using Mechano-Chemical Activation**

Konstantin Sobolev, UW-Milwaukee

Chemical admixtures can be used to modify the cement grinding process and induce changes in the structure of cement minerals due to mechano-chemical activation. A reactive silica-based complex admixture was developed for modification of cement grinding. This paper examines the effect of grinding on the strength of modified cement containing granulated blast furnace slag in high volumes. According to the test results, mortars based on the modified cement possess a compressive strength of up to 91.7 MPa, a 62% increase over the reference. It is proposed that developed cements can find their application in high-performance concrete.

2:15-2:30 **Hydration and admixture interaction characteristics of the cement made with high sulfur petcoke fuel**

Chengqing Qi, Cemex Technical Center
Hugh Wang, Cemex Technical Center

Hamid Farzam, Cemex Technical Center

Petroleum coke (petcoke), a residual by-product from crude oil refining process, is often used as an alternate fuel in the production of portland cement clinker. The sulfur in the petcoke easily transfers from the petcoke into the clinker during the burning process, and incorporates in the clinker matrix as various sulfur-containing compounds such as sodium sulfate, potassium sulfate, calcium sulfate and potassium calcium sulfate etc. However, not all the sulfur-containing compounds in the clinker are fully available during the cement hydration process due to the solubility limitation. This is particularly true for clinker with low alkali content.

The high amount of unavailable sulfur in the clinker produced using high-sulfur petcoke will have a domino effect on the subsequent cement production regarding the gypsum addition to control cement setting characteristics. For example, cement made with petcoke may contain high sulfur on its own sometimes reaching or exceeding the specification limits and thus preventing or limiting additional gypsum to be added during the final cement grinding process. Because of this, the cement produced without adequate amount of gypsum addition may not possess a controllable setting behavior. When such a cement is used in a concrete mixture containing chemical dispersing admixtures and/or supplementary cementitious material (SCM), uncontrolled setting behavior can significantly be aggravated due to the increased demand for soluble sulfate. Often, this type of problem is referred to cement-admixture incompatibility.

This study will investigate the hydration behavior of the cement made with high- sulfur petcoke; the paper will also discuss the sulfur optimization method through the calorimetric technique. Most importantly, this study will discuss the interaction and incompatibility of the high-sulfur clinker cement with high calcium fly ash and low calcium fly ash, and the incompatibility with some typical water-reducing chemical admixtures.

2:30-2:45 **Development of simulated whole fly ash as a model system for investigating fly ash reactivity**

Walairat Bumrongjaroen, The Catholic University Of America
Richard A. Livingston, University Of Maryland At College Park
Isabelle S. Muller, The Catholic University Of America

The major properties that influence fly ash reactivity include the chemical composition of its glassy phases, its particle size distribution (PSD) and inert fraction. However, it is not possible to investigate these factors individually using actual fly ash itself. Therefore, there is much interest in using synthetic fly ash as a model system of for studying reactivity. Current research has focused on the development of a simulated whole fly ash that would all match the major properties. This involves making synthetic fly ash glass. However, it has been found from the analysis of thousands of individual glassy particles from real fly ashes by the Computer Controlled SEM (CCSEM) technique that the glassy phase cannot be represented by a single chemical composition. Instead a fly ash is composed of a mixture of several types of glassy particles with characteristic chemical compositions. Therefore, 5-7 batches of synthetic fly ash glasses have to be prepared to match these compositions. They are then combined together in proportion to their weight percentages in the real fly ash. To match the PSD the synthetic fly ashes are crushed and sorted by size by sieving or air separation. To simulate the spherical morphology of glassy particles in real fly ash, the synthetic glass particles are spheroidized by passing them through a propane torch flame. Finally, the inert fraction is simulated by adding proportionate amounts of quartz and mullite particles. The reactivity of these simulated whole fly ashes can then be evaluated by various tests. One involves reacting a sample in a closed vessel with a specified solution for a fixed period of time. The amount of silicate species in the solution can then be used to calculate the etch rate. A mechanical test method is based on measuring the crushing strengths of simulate fly ash mortar cubes. The results can be compared to those for the raw fly ashes to determine the feasibility of using the simulated fly ash as a model system for real fly ash.

2:45-3 **Early age properties of cement in the presence of nano and micro particle additions**

Amal Jayapalan, Georgia Institute Of Technology
Sarah Fredrich, Georgia Institute Of Technology
Kimberly Kurtis, Georgia Institute Of Technology

The early age behavior of cement hydration reaction in the presence of fine filler addition was studied as a part of this research. Titanium dioxide nanoparticles and limestone microparticles were added to cement at varying percentage addition rates and the variations in the early age properties were researched. The effect of the particles on rate of hydration was studied using an isothermal calorimetry, chemical shrinkage tests were conducted according to ASTM standard test 1608 and degree of hydration was studied using thermal analysis. Scanning electron microscopy was used to characterize the microstructure of the hydration products. Nanoparticle addition resulted in an increase of the rate of hydration and an increase in the chemical shrinkage, whereas â€œcoarserâ€ microparticle additions resulted in a lower rate of hydration and decreased chemical shrinkage. The nanoparticle additions resulted in an increase the rate of reaction due to nucleation effect, whereas â€œcoarserâ€ microparticles decreased the rate of reaction by dilution effect. Thus the size of the particles was observed to be the dominant factor in the effect of particles on the hydration reaction. The chemical shrinkage data and the degree of hydration obtained from TGA results were compared and correlated. SEM image analysis indicated a denser microstructure formed around the TiO2 particles compared to a porous microstructure away from the particles. The results from this research suggest that below 3 microns the inert particles would accelerate cement hydration and increase chemical shrinkage. The particle size of the inert additive could thus be selected and the mix tailored to increase the rate of reaction, possibly prevent damage due to chemical shrinkage and increase the density of the hydration product formed.

3-3:15 **Workability Problems In Plain And Fly Ash Mixtures Arising From Binder and Admixture Incompatibilities**

Chaitanya Paleti, Purdue University
Jan Olek, Purdue University

Growing demand for creating more sustainable and superior performing concretes lead to the increased usage of various cementitious materials and chemical admixtures in the mixes. However, the increased usage of these components resulted in more complex mixtures that sometimes cause unexpected incompatibility problems.

This paper studies the parameters that may lead to workability problems in both plain and fly ash paste and mortar mixtures. Based on literature review and preliminary tests, four cements and three fly ashes (two class C and one class F) with varying chemical compositions were selected for inclusion in the test matrix. The selected cements cover the range of tricalcium aluminate (C3A) content (7.7 - 10%), alkali content (0.2 - 1%) and sulfate content (2.6 - 3.5%). Two types of water reducers (WR) â€“ Type A lignin based WR and Type F poly carboxylate(PC) type high range WR; and two types of air entraining agents(AEA) - vinsol resin based and synthetic type AEAs were used in the study. Pastes with water - cementitious materials ratio of 0.42 were used to perform the mini slump and the isothermal calorimetry tests. Setting time experiments were performed on standard normal consistency pastes according to ASTM C 191. The early age stiffening tests were performed on mortars following the ASTM C 359. In total, more than 100 different specimens were evaluated. Preliminary tests identified certain cements and admixtures which when combined together were prone to incompatibility. It was observed that cements with high C3A content were more prone to incompatibility problems for a given sulfate (3.6%) and alkali (~1%) contents. It was also observed that mixes with Type A WR had higher tendency for rapid stiffening than mixes with Type F PC type high range WR. The observed incompatibility problems manifested themselves as abnormal slump losses, as well as, abnormal setting and early age stiffening responses. Results from the mini slump tests correlated well with the setting time and early age stiffening test results. It was found that these test methods were effective in identifying early age workability properties.

3:30-4:30 Cements Division Meeting

RPRH 172, Pharmacy Building

4:30-6:30 Della Roy Lecture and Reception

Lecture in RPRH 172, Pharmacy Building, Reception to follow in Woods Common, Civil Engineering
Moderator Florence Sanchez
NMR Spectroscopy in Cement Science
R. James Kirkpatrick, Michigan State University

TUESDAY

7:30 am - 12 pm **Registration**

Woods Common, Civil Engineering

8:30-10am **Alternative Binder Systems: Part I**

RPRH 172, Pharmacy Building

Moderator Jason Ideker

8:30-9 **Invited: Microstructure and Properties of Metakaolin-based Geopolymers**

Trudy Kriven, University Of Illinois At Urbana Champaign

9-9:15 **Tailoring geopolymer structure to improve performance**

John Provis, University Of Melbourne

Jannie Van Deventer, University Of Melbourne/Zeobond Pty Ltd

We present an overview of the current progress towards the tailored design of geopolymer nanostructure and microstructure, with a view towards optimising performance, in terms of mechanical strength and (possibly more importantly) durability. Nanostructural design is achieved in large part by specifying activator composition according to the physicochemical properties of the solid precursor (fly ash and/or slag) used. Pre-processing of precursors, blending of different raw materials, seeding of reaction mixes and control of curing conditions are also potential avenues by which nanostructures can be tailored and controlled.

In addition to modification techniques, it is necessary also to develop and/or adapt novel methods of analysis for the study of geopolymer binders, as these materials (as is the case in most cements and concretes) consist of a complex multiscale hierarchy of solid reaction products, unreacted precursors, pores and aggregates. Geopolymer formation kinetics and reaction mechanisms play a key role in determining the morphology and structure of the final products, and both laboratory and beamline-based (synchrotron and neutron) techniques have been applied to this problem. X-ray microtomography, electron microscopy, elemental and chemical mapping and other spectroscopic techniques can all aid in understanding geopolymer structures. However, it is only by combining data from each of these methods that is will be possible to obtain a detailed understanding of geopolymer structure from the nanoscale up to the macroscale.

Commercialisation of geopolymer technology in Australia and elsewhere has been linked closely with these scientific developments, in particular through the analysis and prediction of durability, and in understanding and controlling reaction mechanisms. We will also highlight the importance of leading-edge scientific research in the commercialization of geopolymer concretes, and some of the remaining technical and non-technical hurdles which must be overcome will be identified.

9:15-9:30 **Hydration kinetics and microstructure developments in cement kiln dust activated slag concrete.**

Sulapha Peethamparan, Clarkson University

Piyush Chaunsali, Clarkson University

Concern over the green house gas emission during the manufacturing process of cement has urged the cement and concrete industry to use increased amount of pozzolanic materials in concrete. Radical efforts are also underway to develop clinker/cement free alternative binding materials, in order to make more environmentally friendly and energy efficient sustainable concrete. In this study, a detailed investigation on the properties of cement kiln dust (CKD) activated granulated blast furnace slag (GGBFS) is presented. GGBFS was activated using cement kiln dust at a constant waterâ€“to-binder ratio. The early age properties such as the workability, setting time and chemical shrinkage were determined. The compressive strength of the CKD-activated GGBFS slag paste was determined at 7, 28 and 90 days of normal moist curing. The mineralogical and morphological changes were monitored using XRD, TGA, SEM and TEM techniques. The results show that the CKD activated slag could produce a hardened paste with a compressive strength of 30 MPa after 28 days curing. Extensive formation of ettringite and Al/Mg incorporated C-S-H phases were found in the system and the strength development in the CKD-activated GGBFS can be attributed to these products.

9:30-9:45 **Using Class C-fly ash to Study Effect of Si/Al Ratio on Microstructure and Compressive strength of Geopolymer Cured at Room Temperature**

Kiatsuda Somna, King Mongkut'S University Of Technology Thonburi
Chai Jaturapitakkul, King Mongkut'S University Of Technology Thonburi
Puangrat Kajitvichyanukul, Naresuan University

High calcium fly ash from Mae Moh Electricity Generating Authority in Thailand was used as a starting material for geopolymer matrices to investigate the effect of Si/Al ratio on microstructure and compressive strength. The fly ash was ground and mixed with 14 molar of NaOH. The percentage of amorphous in fly ash was determined for calculate atomic ratio of Si/Al. Lab grade SiO2 was added for various atomic ratios of Si/Al from 1.4:1 to 3.0:1. The products were characterized by FTIR and XRD techniques. The compressive strength of geopolymer was also investigated. From the results, it was found that by increasing atomic ratio of Si/Al in the mix, the compressive strength of geopolymer increases. The FTIR spectra of geopolymer show the change in intensity of Infrared band (R) near 1000 cm-1which is associated with asymmetric Si-O-Si or Si-O-Al stretching vibrations and the IR band near 620 cm-1 and 561 cm-1 which is associated with symmetric stretching (Si-O-Si or Si-O-Al) and to symmetric stretching (Al-O-Si), respectively This change suggests the more polymerization of the geopolymer gel which can be due to the combination of the increase in atomic ratio of Si/Al of geopolymer gel and the addition of C-S-H gel to the structure. The C-S-H gel is doable as the calcium leaching out from fly ash can react with available silica to form C-S-H gel. This gel can contribute the strength to structure as well the geopolymer gel. However, it is beyond the scope of this study to identify the presence of C-S-H gel in the mix.

9:45-10 **Discussion**

10-10:30 **Coffee Break**

Woods Common, Civil Engineering

10:30-12 **Alternative Binder Systems: Part 2**

RPRH 172, Pharmacy Building

Moderator Kim Kurtis

10:30-11:00 **Invited: Lessons learned from biomineralized marine organisms applied to the design of biomimetic materials**

Pablo Zavattieri, Purdue University

The attractive mechanical properties of some hard biological materials, in particular the combination of strength and toughness, have inspired a large class of biomimetic organic/inorganic composites. In fact, this is part of an ongoing quest to develop a new generation of high-performance multifunctional materials for a wide range of applications. The first steps in this biomimetic approach comprise the characterization of the mechanical performance of these natural materials, examination of their intricate hierarchical microstructures and the fundamental investigation of the key energy dissipation mechanisms. Although biomimetics opens the door to a whole set of new materials with various structural and functionality requirements, appropriate computational models and optimization strategies should be devised to address the lack of quantitative and comprehensive analysis of the design parameters that allow the mechanisms to operate.

In this presentation I will talk about some of my recent work on biomimetic material design including a combined computational/experimental analysis of the mechanical performance of hard biological materials, and the development of design strategies based on novel numerical modeling methods together with rapid prototyping techniques to guide the design and processing efforts. The talk will be focused on two biomineralized systems: (1) Nacre, the iridescent material found in some mollusks shells, as a good example of a toughness optimization, and (2) the radular teeth of chitons, a group of elongated mollusks that are able to erode hard substrates, with remarkable damage tolerance and abrasion resistance properties.

11-11:15 **Ca-aluminate based biomaterials**

Leif Hermansson, Doxa Ab
Adam Faris, Doxa Ab
Gunilla Gomez-Ortega, Doxa Ab
Jesper Loof, Doxa Ab

The presentation will describe some features of the Ca-aluminate (CA) system when used within life science as biomaterials. These deal with both the technology and the chemistry involved, and specifically 1) the cement phase, 2) the particle size of the cement, 3) the hydration temperature, 4) the environment (complementary ions), 5) processing agents, and 6) the volume involved. Other aspects deal with influence of inert additives and compact density including the w/c ratio. The following product areas have been identified; namely dental cement, endodontic products, sealants, restoratives, and pastes for augmentation and implant coatings.

The CA-cements exhibit some inherent properties not so often taken into account. These deal with the huge water up take capacity of the cement. Another aspect is the fact that the hydrates, katoite and gibbsite, after precipitation appear as nano-crystals in the size interval 20-50 nm. This can be optimally utilized if the reaction is allowed to continue to completion. Another aspect seldom used is the fact that the cement yields open porosity, even if the porosity level is low. The pore channel size is estimated to be 1-2 nm. The nano-size pore system can favorably be used when the cement functions as a carrier for controlled drug delivery. Filler particles are included to contribute to some additional aspects, mainly of the microstructure (homogeneity aspects) and mechanical properties (especially hardness, YoungÂ´s modulus and strength). Additives for dental applications are preferably glass particles for transparency reasons, and for orthopedic applications high density oxides are selected for radio-opacity reasons. The surface and bulk composition was analysed using thin-film XRD and SEM combined with EDX. The microstructure was studied with (S)TEM. TEM samples were prepared using focused ion beam microscopy (FIB) for high position site accuracy.

11:15-11:30 **Use of Chemical Shrinkage Measurements to Predict Conversion in Calcium Aluminate Cement Systems**

Jason Ideker, Oregon State University

Calcium aluminate cement (CACs) is a class of cement containing primarily monocalcium aluminate (CA) and is recognized for its rapid hardening properties and increased durability over portland cements in aggressive environments. Despite the fact that CAC was developed over 100 years ago and has many advantageous characteristics, it has not seen widespread use due to a lack of fundamental understanding behind the properties of this unique material. In particular, issues surrounding conversion, where initially formed metastable hydrates convert to stable hydrates commensurate with loss of strength, have hindered its use. This presentation will highlight a new approach to monitoring and predicting hydration reactions, specifically time to conversion using chemical shrinkage measurements. Chemical shrinkage was monitored using an automated image acquisition system that allowed for continuous measurements over a two week time frame. It was found that mixtures cured at and below 30 C isothermally had lower chemical shrinkage values than mixtures cured above 30 C, where accelerated conversion was favored due to the increased temperature. Furthermore, the time to complete conversion was significantly reduced as the temperature was increased to 55 C. Implications of conversion and use of this method to better characterize field applications of CAC systems will be discussed.

11:30-11:45 **Understanding expansion in calcium sulfoaluminate cements**
Maria Juenger, University Of Texas At Austin
Irvin Chen, Calera Corporation
Calcium sulfoaluminate (CSA) cements are attracting increasing attention because of their lower energy and CO2 emissions during clinkering compared to portland cement. The primary phase in CSA cements is C4A3Åœ, a phase employed in expansive cements for its rapid production of expansive ettringite. It has been observed that some CSA cements are more expansive than others, a behavior that can be linked to the cement composition. However, the degree of expansion is not simply and directly related to the amount of ettringite formed. In this study, expansion of laboratory-synthesized CSA cements was examined and compared to hydration product development determined using Rietveld quantitative x-ray diffraction. It was observed that the amount of expansion is related the rate of development of both ettringite and AH3, an amorphous phase. This knowledge has helped develop a CSA cement that is non-expansive and gains strength at a rate identical to a Type I portland cement.

11:45-12 **Discussion**

12-2:00 **Lunch**

2-3:30 **Moisture in Cement-based Materials: Transport and Impacts on Performance**
RPRH 172, Pharmacy Building
Moderator Jeff Thomas

2-2:15 **Effect of hydration temperature and C-S-H seeding on the properties of cement paste**
John Valenza, Schlumberger-Doll Research
Jeffrey Thomas, Northwestern University
The properties of cement paste govern the durability of cementitious materials in aggressive environments. For example, the permeability controls the ingress of water and ionic species, which may result in freeze/thaw damage and corrosion of reinforcing steel. In this study we employ the beam bending technique (G. W. Scherer, J. Am. Ceram. Soc., 83 [9] (2000) 2231-39) to determine the properties of cement paste exposed to various handling protocols. Beam bending consists of measuring the load necessary to sustain a small deflection on a simply supported beam of saturated paste. When the permeability is low, the pore fluid supports a portion of the initial load. In response, as suggested by Darcyâ€™s law, the pore fluid flows to alleviate the pressure, and the initial load relaxes to a smaller value. The permeability is determined by analyzing the kinetics of this load relaxation, the elastic modulus of the porous skeleton is determined from the load corresponding to the end of hydrodynamic relaxation, and the

viscoelastic properties are derived from analyzing the load relaxation observed thereafter. In this study, beam bending is applied to cement paste cured at different temperatures (10-60 ËšC), and pastes made with C-S-H seed. Curing at elevated temperature causes the C-S-H gel to form with less internal porosity yielding a coarser capillary pore system. Alternatively, C-S-H seed encourages C-S-H gel to form away from the cement grain, producing a finer capillary pore system. In this presentation we quantify the effect of these variables on the properties of hardened cement.

2:15-2:30 Early Prediction of Concrete Durability by Monitoring Moisture Diffusivity with Broadband Dielectric Spectroscopy

Benjamin Mohr, Tennessee Technological University
Nan Guo, Tennessee Technological University
Joshua Ojo, Tennessee Technological University

Water plays a very important role in concrete production and service life. The ability of concrete to maintaining its desired engineering properties has been linked to the observation and monitoring of water movement in concrete. Unfortunately, the lack of capable systems for monitoring moisture movement in concrete has remained a challenge. In order to improve the present state of knowledge concerning the water transport kinetics in concrete, broadband dielectric spectroscopy has been adopted. Dielectric spectroscopy, which is an inexpensive situ revealing approach, is a relevant method for quality characterization of moisture movement in the concrete, provided that the permittivity spectra are measured with high precision over a broad frequency range. The dielectric constant (permittivity) of moisture in the concrete was monitored with high precision using coaxial transmission/reflection sensor in the broad frequency range of 1 MHz to 8 GHz. The dielectric analysis of the results provides both the dielectric and rheological data for early ages of the tested concrete materials. The high sensitivity of the system was confirmed by using two permittivity calculation methods of standard fluids measurements.

2:30-2:45 Ca ion leaching from cementitious systems under slow and accelerated transport regimes

Narayanan Neithalath, Purdue University
Jitendra Jain, Purdue University

Leaching of calcium ions from cementitious matrices is a combined diffusion-dissolution process that results in long term durability issues. The concentration gradients between the pore solution and the pure water cause diffusion of calcium ions from the pore solution to the surrounding ion free water. The reduction in concentration of calcium ions in the pore solution forces the dissolution of calcium hydroxide (CH) and calcium-silicate-hydrate (C-S-H) gel, leading increased porosity and permeability, and loss of mechanical properties. This paper deals with an analysis of Ca ion leaching behavior from cementitious matrices modified with fly ash or silica fume, subjected to slow (in deionized water) and accelerated (in 6 M ammonium nitrate) leaching regimes. The physico-chemical effects of modification of cementitious matrices through the use of pozzolanic cement replacement materials on Ca ion transport rates are brought out for the different exposure regimes. It is noticed that the presence of CH in the paste systems act as a buffer for the C-S-H gel under exposure to accelerated leaching. The influence of nano-particle modification on improving the leaching resistance of cementitious matrices is also brought out. Finally, equilibrium concentration diagrams are used to quantify the amount of Ca ions lost from the CH and C-S-H phases of different pastes so as to facilitate the modeling of leaching kinetics.

2:45-3 Experimental and Numerical Investigation of the Effect of Cracking on Moisture Transport in Concrete Materials

Farshad Rajabipour, Penn State University
Alireza Akhavan, Penn State University

It is well known that cracks accelerate the degradation of concrete materials by providing pathways for rapid penetration of moisture and salts into concrete. As such, for service-life prediction purposes, in addition to the material properties of un-cracked concrete, the transport properties of cracks must be considered. The objective of this paper is to characterize moisture transport through cracks as a function of crack geometry (i.e., crack width, roughness, and tortuosity). Cement paste, mortar, and concrete disk specimens were prepared and cracked using closed-loop splitting tensile test to achieve average crack widths in the range 10 to 300Î¼m. A digital image acquisition and analysis procedure was used to examine crack profiles along the diameter and through the thickness of each specimen. The results are used to determine the average and effective crack widths which are then related to the permeability coefficient of the crack measured using a Darcian flow-thru pressure cell. In addition, the roughness and tortuosity of cracks are obtained from the image analysis and electrical conductivity measurements. This information is used to establish a characteristic parabolic function (suggested by theory) between crack width and permeability and to examine whether this function is unique for different materials (i.e., paste, mortar, or concrete). Knowledge of the relationship between permeability and crack geometry is vital in predicting moisture transport in cracked concrete. As an example application, a simple sharp from model is introduced to predict moisture and solute penetration into concrete with dry surface cracks.

3-3:15 **Cracking and fluid transport in textile fabric reinforced cement-based elements**
Amir Poursaee, Purdue University
Alva Peled, Ben Gurion University

Cracks in concrete influence the fluid permeability and dramatically reduce its service life. The crack pattern, crack length, and crack width all substantially influence the fluid transport. Smaller cracks and less connected cracks result in less fluid transport in the concrete, improving concrete permeability and durability. Fiber reinforcement has been suggested as an effective method to reduce crack width in concrete. The influence of fibers depends on the fiber content, fibers cross section, circular or non-circular and the modulus of elasticity of the fiber, either it is higher than the matrix or lower. In recent years, innovative textile fabrics reinforced cement-based elements (TRC) have been intensively investigated as reinforcement for cement-based elements. Modern textile technology offers a wide variety of fabrics made by different production methods which allow great flexibility in fabric design. This flexibility enables the accurate control and design of fabric geometry, yarn geometry, yarn orientation, and yarn material combinations. Research findings show the benefits of these high performance fabric reinforced cement composites. Superior tensile strength, toughness, ductility and energy absorption were reported with TRC. It was also reported that fabric reinforcements control cracking behavior, providing relatively fine cracks. The overall behavior of the composite including crack pattern and crack width depend on fabric geometry, fabric materials (low or high modulus), and the nature of yarns made the fabric, either monofilament or multifilament. Up to this point the majority of research on textile fabric reinforcements for cement-based products was studied to improve mechanical behavior under tensile, bending, shear and impact loadings. Not much work has been reported on the effects of these textile reinforcements on the related fluid transport properties. In this work the crack pattern caused by cement paste shrinkage at early age was studied for cement-based composites reinforced with different fabrics. The results were compared to plain cement matrices. Coated and non coated carbon fabrics made from multifilament yarns were used for this work. The crack pattern and crack width were studied by x-ray radiography and florescent optical microscopy. The fluid transport of the different fabric-cement systems and plain matrix were studied under x-ray radiography. This paper will present the main results obtained in this work. The basic mechanisms involved with these systems will be discussed.

3:15-3:30 **Discussion**

3:30-4:00 **Coffee Break**
Woods Common, Civil Engineering

4-4:45 **Novel Sensing Applications in Cement-based Materials**
RPRH 172, Pharmacy Building
Moderator Ben Mohr

4-4:15 **Interpretation of Early Ultrasonic Wave Reflection (UWR) Response of Cement Paste**

Chul-Woo Chung, University Of Illinois At Urbana Champaign
John Popovics, University Of Illinois At Urbana Champaign
Leslie Struble, University Of Illinois At Urbana Champaign

This work describes research undertaken to interpret the ultrasonic wave reflection (UWR) response of early-age portland cement paste. The buffer is high impact polystyrene, which provides high sensitivity necessary for measuring early stiffening. A non-hydrating alumina suspension was utilized for most experiments, chosen because it is easy to manipulate the microstructure from dispersed to flocculated or vice versa by adjusting the pH. The UWR response of dispersed suspensions of coarse silica particles was also measured to understand the effect of segregation. Based on these experiments, the P- and S-wave UWR responses from hydrating portland cement paste are interpreted as follows: the early change in P-wave reflection is caused by segregation of cement particles and the initial reduction in S-wave reflection is caused by by flocculation of cement particles.

4:15-4:30 **Monitoring early age mechanical properties of cement paste using bender elements**

Jinying Zhu, University Of Texas At Austin
Yi-Te Tsai, University Of Texas At Austin
Raissa Ferron, University Of Texas At Austin

Ultrasonic waves have been used to monitor early age microstructure development in cementitious materials. The conventional ultrasonic setups typically measure longitudinal (P) waves in fresh cement pastes and need access two sides of the specimen. This type of setup is not suitable for in-situ field testing. In this study, embedded piezoelectric bender elements were used to generate and measure both P and shear (S) waves in fresh cement pastes. Shear waves were observed immediately after cement hydration starts. The velocities of P and S waves were obtained from B-scan images of a collection of recorded signals over time. Experimental results indicate that the shear wave velocity better represents the setting time of cement pastes and less affected by air contents than the P wave velocity. Shear modulus and Poissonâ€™s ratios of the cement pates are derived from the measured P and S wave velocities. Measurements from the bender elements setup were compared and related to the Vicat and rheometer test results.

4:30-4:45 **Passive and Wireless RFID Based Corrosion Sensors for Concrete**

Tyler Ley, Oklahoma State University
Nicholas Materer, Oklahoma State University
Allen Apblett, Oklahoma State University

Concrete infrastructure commonly relies on internal steel reinforcing for its safety and reliability. Corrosion of this reinforcing steel can impact the serviceability of the structure, and lead to significant maintenance costs. Owners would benefit if methods existed to monitor the potential for corrosion in reinforced concrete structures in an economical manner that required little maintenance. An inexpensive wireless corrosion sensor that does not require any external power is presented. These sensors are based on novel uses of passive radio-frequency identification (RFID) tags that are commonly used to track consumer goods at extremely low-costs. These small (25mm x 7 mm) unobtrusive sensors can be directly imbedded into the cover of a concrete structure to monitor the chloride penetration. These sensors are monitored with a hand held wand or an antenna mounted to the back of a vehicle. The use of these sensors will allow the potential of corrosion of the reinforcing steel to be monitored. This will allow early detection of the penetration of chlorides into concrete before corrosion has initiated. This sensor can help the owner make informed maintenance decisions that will ultimately extend the service life of concrete structures.

4:45-5:45 **Cement-based Nanocomposites**
RPRH 172, Pharmacy Building
Moderator Paramita Mondal

4:45-5 **Microstructure and macroscopic properties of CNF/cement composites**
Florence Sanchez, Vanderbilt University
Catherine Gay, Vanderbilt University

The unique properties of carbon nanofibers (CNFs) such as high aspect ratios, strength to density ratios, thermal and electrical conductivities, and corrosion resistivity give them potential to act as cement composite reinforcement. Two issues with using CNFs in cement composites that need to be addressed in order that the full potential of CNFs can be obtained include the dispersion of the CNFs in the cement paste and creating an adequate bond between the CNFs and the cement matrix. Surface functionalization of the CNFs has potential to improve both the dispersion of the CNFs in the cement paste and the bond between the CNFs and the cement matrix. The use of surfactants and dispersing agents can also improve the dispersion of the CNFs in the cement matrix. Surface treatment of CNFs with nitric acid was investigated, as well as the use of two dispersive agents and a surfactant. Cement pastes with and without silica fume and CNF loadings up to 1% by weight of cement were investigated. The issue of dispersion, evidence of CNF-cement phase interaction, and the effects of CNFs and dispersion method on the microstructure and macroscopic properties of the cementitious composite will be presented.

5-5:15 **Distribution uniformity of nano inclusion in cementitious nanocomposites**
Zachary Grasley, Texas A&M University
Ardavan Yazdanbaksh, Texas A&M University
Bryan Tyson, Texas A&M University
Rashid Abu Al-Rub, Texas A&M University

In the past decade, carbon nanotubes (CNTs) and nanofibers (CNFs) have been widely used in materials such as polymers and metals as inclusions to enhance their mechanical, electrical or thermal properties. Nano inclusions tend to greatly attract each other and agglomerate mainly due to van der Waals forces. Methods such as ultrasonic processing, using surfactants, and functionalization are being used to partially disentangle the agglomerates and keep the inclusions apart before the solidification and final formation of nanocomposites. However, in most of the cases achieving a fully uniform distribution of nano inclusions within a composite is impossible. The quantitative characterization of the distribution uniformity of inclusions in nanocomposites is very useful. In this presentation, some of the dispersion quantification methods developed in the past are reviewed and their shortcomings are discussed. Finally, a novel method is presented, which measures the distribution uniformity based on the amount of work required to move the inclusions to the locations in which they form a fully uniform distribution.

5:15-5:30 **Novel processing techniques for improving the dispersion and bonding of carbon nanotubes in cement-based composites**
Peter Stynoski, University Of Illinois At Urbana-Champaign
Paramita Mondal, University Of Illinois At Urbana-Champaign
Charles Marsh, Us Army Construction Engineering Research Laboratory
Leslie Struble, University Of Illinois At Urbana-Champaign

Carbon nanotubes (CNTs) are attractive materials due to their high strength-to-weight ratio, valuable electrical responses that vary with chirality, and unique geometric properties. Possible applications of CNTs in cement composites include improvement of mechanical properties or incorporation of embedded sensors. Two challenges exist in the production of successful cement composites: obtaining effective dispersion of the constituents and strong bonds between them. CNTs tend to flocculate in water since they are hydrophobic, and it is difficult to bond to CNTs without harming their structure or providing precise reaction conditions. Two processes have been explored to address these concerns. In the first, multiple-walled CNTs (MWCNTs) are grown directly on ground Portland cement clinker via a catalytic chemical vapor deposition (CCVD) method. In the second method, MWCNTs are functionalized with silica using tetraethyl orthosilicate. Samples were characterized using scanning electron microscopy, energy dispersive x-ray spectroscopy, transmission electron microscopy, and Raman spectroscopy. Preliminary investigations of cement-based composites containing the particles and CNT discussed here are in progress.

5:30-5:45 **Effect of Nano-SiO2 on Microstructure, Interface and Mechanical Properties of Whisker-reinforced Cement Composites**

Jianqiang Wei, Dalian University Of Technology

Mingli Cao, Dalian University Of Technology

CaCO3 whisker-reinforced cement-based composite is composed of cement paste as matrix, and whisker as reinforcement, which can remarkably improve the mechanical properties and microstructure of composite. However, the weak interfacial bond and dispersity of whiskers in cement matrix severely restrained the further improvement of properties. Interfacial optimization between whiskers and cement matrix are now becoming essential to ensure the reinforcement of whiskers be given full play. Adding silica fume may be an effective way to improve the interfacial composing, fabric and performance according to its effects in common fiber composites. Compared with common silica fume, nanometer silica has more excellent pozzolanic activityï¼Œ which is propitious to interfacial modification. Crystal structures, microcosmic appearances and characterizations of nano-silica, CaCO3 whisker and the composite were analysed by X-ray diffraction (XRD), scan electron microscope (SEM/EDAX), and transmission electron microscope (TEM), etc. Effect of different silica content on the microstructure, interface and mechanical properties of whisker-reinforced cement was investigated. The results show that the incorporation of nano-SiO2 resulted in an increase in interfacial properties between whisker and cement matrix. The mechanical properties of whisker/cement composite and the microstructure of matrix were all improved. Furthermore, by microscopic analysis, mechanism of whisker/cement's interface optimized by nano-SiO2 was also discussed.