CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: 16th ACBM/NIST Computer Modeling Workshop (AI 20.06002.01.011.024)

DATE/PLACE: June 27–30, 2005
National Institute of Standards and Technology (NIST)
Gaithersburg, Maryland

AUTHOR: Roberto T. Pabalan

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PERSONS PRESENT: Roberto T. Pabalan

BACKGROUND AND PURPOSE OF TRIP:

The purpose of this trip was to attend a workshop on computer modeling of cement-based materials organized by the Center for Advanced Cement-Based Materials (ACBM, Northwestern University) and the National Institute of Standards and Technology (NIST). The objective was to gain state-of-the-art knowledge on computer modeling of cement-based materials that may be useful in evaluating the performance of concrete vaults and cement-based wasteforms that may be used for disposal of radioactive wastes at DOE sites.

SUMMARY OF PERTINENT POINTS AND ACTIVITIES:

The workshop was held at the National Institute of Standards and Technology in Gaithersburg, Maryland. It consisted of four days of lectures that covered the computational materials science of concrete, including simulation of microstructural development and prediction of physical properties. In the context of cement-based materials, microstructure ranges from nanometer to meter length scales, while physical properties include ionic diffusion, electrical conductivity, percolation, pressure-driven fluid flow, rheology, mechanical properties, neutron scattering, SEM microscopy, and various x-radiation probes like diffraction and tomography. Computer modeling encompasses computational materials science, direct simulation and computer representation of microstructure, and direct computation of experimentally measurable properties.

The lecture topics included

- Microstructure in portland cement pastes and concretes,
- Cement hydration, Virtual Cement and Concrete Testing Laboratory, and applications,
- Hydration and x-ray transmission microscopy,
- X-ray computed tomography,
- Analyzing aggregate and cement particle shape in three-dimensional,
- Neutron scattering and the materials science of concrete,
- Modeling ionic transport in cement paste pore solution,
- Computing the linear elastic properties of random materials,
- Characterizing materials,

- Experimental concrete rheology,
- Computational rheology,
- Multi-scale models of porous sedimentary rocks,
- Multi-scale mechanical models for concrete, and
- Statistical learning methods applied to multi-scale microstructure.

The workshop was attended by about 30 participants from industry, academia, and government (see attached attendance list). Several workshop participants also made presentations on their own work. In addition, a tour of several National Institute of Standards and Technology facilities was conducted. One of these facilities was Building 202, where structural steel, which was recovered from the World Trade Center site and used in the National Institute of Standards and Technology investigation of the World Trade Center collapse, is stored. Other facilities toured were the National Institute of Standards and Technology Center for Neutron Research and the National Institute of Standards and Technology Inorganic and Polymeric Materials Laboratory.

P. Stutzman (National Institute of Standards and Technology) presented work conducted at National Institute of Standards and Technology regarding the microstructure of portland cement pastes and concrete. The main tools used in this study are x-ray diffraction (powder and Laue) analysis and scanning electron microscopy (backscattered electron and x-ray images). These tools were used to study the kinetics of cement hydration by tracking cement phase consumption as hydration proceeds. The tools also were used to study concrete failure mechanisms such as alkali-silica reaction in carbonate aggregates and sulfate attack. These studies help improve understanding of the potential for reactivity and pore solution and mineral interactions.

J. Bullard (National Institute of Standards and Technology) presented studies on cement hydration, the National Institute of Standards and Technology Virtual Cement and Concrete Testing Laboratory, and applications of virtual testing. Physical tests on concrete require large amounts of material and long time (~28 days). One approach is to use computer models with a virtual representation of the material and to simulate physical tests to get virtual results for comparison with measured values. Such virtual testing could be used in designing new materials, to supplant QA testing, and provide an understanding of cement hydration processes and the effects of various parameters. Virtual testing is done by creating a three-dimensional virtual cement paste, simulating hydration reactions to evolve a microstructure, then calculating hydration properties, such as heats of hydration, chemical shrinkage, and setting time; mechanical properties (e.g., elastic moduli, compressive strength), and degradation behavior such as leaching and sulfate attack; and transport properties such as formation factor and transport factor. Virtual Cement and Concrete Testing Laboratory is designed to integrate and enhance the National Institute of Standards and Technology state-of-the-art computational materials science models into a tool that is relevant and useful to industry. It uses an integrated modeling approach that is based on a three-dimensional microstructure with spatial resolution at the sub-particle level. Virtual Cement and Concrete Testing Laboratory has modules for cement hydration that calculates degree of hydration, setting time, and chemical shrinkage; a module for mechanical properties of concrete (elastic moduli), transport properties of concrete (transport factor). Applications include calculating elastic properties and compressive strength of mortars; determining the effect of cement composition on mortar strength; and the influence of cement fineness on mortar strength. Virtual Cement and Concrete Testing Laboratory is supported by a consortium. A public domain version of Virtual Cement and Concrete Testing Laboratory Version 1.1 can be accessed via the website http://ciks.cbt.nist.gov/vcctl/, but some features are disabled in Virtual Cement and Concrete Testing Laboratory Version 1.1 in accordance with the consortium agreement.

M. Juenger (University of Texas at Austin) described her studies examining cement hydration and admixture interactions using soft x-ray microscopy. In a sense, soft x-ray microscopy is just like optical microscopy, which is commonly used to characterize cementitious materials, but uses smaller wavelengths, allowing structures on the scale of 0.0001 to 0.1 micrometer to be studied. The study described by M. Juenger used Beamline 6.1.2 at the Advanced Light Source of the Lawrence Berkeley National Laboratory. Specimens that have been studied in her work include tricalcium silicate (C3S), tricalcium aluminate (C3A), portland cement, ground granulated blast furnace slag, and hemihydrate. Her studies show that transmission soft x-ray microscopy is a versatile tool for *in-situ* imaging of hydration for a variety of cementitious materials, and for documenting the effects of admixtures on morphology and hydration rates (kinetics).

P. Halleck (Penn State University) presented x-ray computed tomography studies using the computed tomography facilities at the Center for Quantitative Imaging of Penn State University. The presentation included a discussion of the nature of x-ray computed tomography, a description of the facility at Penn State, what can be measured, an overview of potential applications, and several illustrative case studies. These case studies included determination of concrete aggregate structure, structure of fire retardants, pore structure of carbonate and volcanic rock, and deformation studies in rocks and soils.

E. Garboczi (National Institute of Standards and Technology) presented a lecture on models of aggregate and cement particle shape in three-dimensional. Analysis of aggregate shape are needed because composites are affected by the shape and topology of their phases and the property contrast between phases. Concrete is a composite, comprising cement paste + aggregate or mortar + coarse aggregate. Elasticity is affected by aggregate shape, especially at early ages of cement hydration, where elastic property contrast is high (~50 percent or more). Rheology potentially can be greatly affected by aggregate shape, since there is a large property contrast (~100 percent). Thus, aggregate shape characterization is needed to be able to successfully model concrete properties. It is possible to mathematically characterize three-dimensional shapes using spherical harmonic expansion which can then be used to classify particles, to incorporate arbitrary shapes into computational/mathematical models, and to understand aggregate shape dependence of concrete properties. Examples were given using spherical harmonic analysis, x-ray computed tomography, and laser detection and ranging to characterize different particle shapes and sizes.

Ken Snyder (National Institute of Standards and Technology) presented a lecture on modeling ionic transport in cement paste pore solutions. The lecture included discussions of modes of transport, definitions of flux, governing equations, volume averaged quantities, definitions of material coefficients, real electrolytes, and validation of transport codes.

D. Neumann (National Institute of Standards and Technology) presented neutron scattering studies of cement conducted at the National Institute of Standards and Technology Center for Neutron Research. Quasielastic neutron scattering is used to determine the state of water in cement, particularly in the diffusion limited regime and as functions of the particle size distribution and of the C3S/C2S ratio.

C. Ferraris (National Institute of Standards and Technology) described different methods for characterizing and different models for describing the rheological properties (e.g., viscosity, yield stress, fluidity, flow) of cement and concrete. Measurement of rheological properties are important for predicting the flow of concrete. For concrete rheological properties, these methods include confined flow methods, free flow methods, vibration methods, and rheometers. Methods for comparing the results of different types of measurements were described and practical recommendations in the use of several measurement methods were provided. Results of computer simulations methods were compared with experimental data and showed good agreement. The models are being developed in order to predict rheological properties and workability of concrete based on the composition of individual components.

F. Ulmer (Massachusetts Institute of Technology) described his work on developing multiscale models for predicting the rheological properties of natural and man-made materials, including concrete. The work uses nanoindentation measurements to determine the hardness and stiffness of cement pastes at the nanoscale (0.1 nm resolution) and using these to predict the macroscopic behavior of cement pastes. The predictive model is based on the observation that macroscopic behavior depends on the packing density, and not on the chemistry, of system components. The model, termed GeoGenome Approach, has potential applications for nanoengineering of new high performance cements and other materials.

The presentation materials are available in CD format from the author of this trip report.

CONCLUSIONS:

The workshop provided state-of-the-art information on computer modeling and characterization methods applied to cement-based materials. The methods discussed in the workshop appear useful to industry, which is interested in the rheology, workability, and short-term performance of cements and concrete. However, the ability to predict the long-term performance (i.e., mechanical and chemical durability during hundreds to thousands of years) of cement-based materials, which is of interest in nuclear waste management, is still not practicable, but is a goal of researchers active in the field of cement-based materials.

PROBLEMS ENCOUNTERED:

None.

PENDING ACTIONS:

None.

RECOMMENDATIONS:

None.

SIGNATURES:

Roberto T. Pabalan
Institute Scientist

7/12/05
Date

CONCURRENCE:

Budhi Sagar
President, CNWRA

7/12/2005
Date

Paul Maldonado for Patrick C. Mackin
Patrick C. Mackin
Director of Administration

7/12/2005
Date

16th ACBM/NIST Computer Modeling Workshop

DATE and LOCATION

Monday June 27, 2005 to Thursday June 30, 2005
Lecture Room E, Administration Building
Building and Fire Research Laboratory
National Institute of Standards and Technology
Gaithersburg, Maryland 20899 USA

INSTRUCTORS

Edward Garboczi (coordinator), Jeff Bullard, Nicos Martys, Paul Stutzman, Chiara Ferraris, and Kenneth Snyder, NIST Materials and Construction Research Division
Dan Neumann, NIST Center for Neutron Research
Joseph Biernacki, Tennessee Tech, Chemical Engineering
Maria Juenger, University of Texas, Civil Engineering
Franz-Josef Ulm, Massachusetts Institute of Technology, Civil Engineering
Phillip Halleck, Penn State University, Energy Institute and Center for Quantitative Imaging
Mark Knackstedt, Australian National University, Applied Mathematics
Veera Sundararaghavan, Cornell University, Mechanical Engineering

GENERAL DESCRIPTION

The workshop lectures will cover the computational materials science of concrete, including simulation of microstructural development and prediction of physical properties. "Microstructure" ranges from nanometer to meter length scales, while physical properties include ionic diffusion, dc and ac electrical conductivity, percolation, pressure-driven fluid flow, rheology, mechanical properties, neutron scattering, SEM microscopy, and various x-radiation probes like diffraction and tomography. Close cooperation between computations and experiments is crucial for making progress in the materials science of concrete and so is an emphasis of the workshop, along with the multi-scale aspects of concrete. There will also be some coverage of the Virtual Cement and Concrete Testing Laboratory, as well as aspects of other random porous materials and the common scientific issues between them and cement-based materials. The workshop will have a mix of tutorial lectures and short 15-minute talks by the participants describing their technical work.

WORKSHOP SCHEDULE

MONDAY June 27, 2005 Lecture Room E, Administration Building

8:30 Welcome...............James St. Pierre, Acting Chief, Materials and Construction Research Division

8:45-9:05 Lecture No. 1...............Ed Garboczi
Introduction to Workshop: Materials and Concepts and Problems

9:05-10:15 Lecture No. 2.............Paul Stutzman
Microstructure in Portland Cement Pastes and Concretes

10:15-10:45 Break

10:45-12:00 Lecture No. 3...........Jeff Bullard
Cement Hydration, VCCTL, and Applications

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:30 Lecture No. 4...............Maria Juenger
Hydration and X-ray Transmission Microscopy

2:30-3:00 Break

3:00-4:15 Workshop Participants Presentations (5)

5-5:15
4:30 Reception in Employee's Lounge (refreshments served)
5:30 Bus leaves for Holiday Inn
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TUESDAY June 28, 2005 Lecture Room E, Administration Building

8:30-9:45 Lecture No. 5...........Phil Halleck
X-ray Computed Tomography

9:45-10:15 Workshop Participants Presentations (2)

10:15-10:45 Break

10:45-12:00 Lecture No. 6...........Ed Garboczi
Analyzing Aggregate and Cement Particle Shape in 3-D

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:15 Lecture No. 7....................Dan Neumann
Neutron Scattering and the Materials Science of Concrete

2:15-3:15 Workshop Participant Presentations (4)

3:15–3:30 Break

3:30 Bus to Building 202
3:40 25 MN testing machine, WTC steel
4:20 Bus to Neutron Reactor
4:25-5:00 Tour of Neutron Reactor
5:00 Bus back to Holiday Inn (from Neutron Reactor)

WEDNESDAY June 29, 2005 Lecture Room E, Administration Building

8:30-9:30 Lecture No. 8 ....Ken Snyder
Modeling Ionic Transport in Cement Paste Pore Solution

9:30-10:30 Lecture No. 9.............Ed Garboczi
Computing the Linear Elastic Properties of Random Materials

10:30-11:00 Break

11:00-12:00 Workshop Participant Presentations (4)

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:15 Lecture No. 10.................Joe Biernacki
Characterizing Materials

2:15-3:15 Workshop Participant Presentations (4)

3:15-3:30 Break

3:30 Walk to Building 226
3:40-4:45 Inorganic and Polymeric Materials Group Lab Tours
Rheology/Particle Size Analysis (Clarissa Ferraris)
SEM/XRD (Paul Stutzman)
NIST SPHERE (Joannie Chin)
4:50 Walk back to Administration Building
5:00 Bus leaves for Holiday Inn

THURSDAY June 30, 2005 Lecture Room E, Administration Building

8:30-9:20 Lecture No. 11.........Clarissa Ferraris
Experimental Concrete Rheology

9:20-10:15 Lecture No. 12.........Nick Martys
Computational Rheology

10:15-10:45 Break

10:45-12:00 Lecture No. 13.................Mark Knackstedt
Multi-scale models of porous sedimentary rocks

12:00-1:15 Lunch, NIST Cafeteria

1:15-2:30 Lecture No. 14...........Franz Ulm
Multi-scale mechanical models for concrete

2:30-3:00 Break

3:00-4:15 Lecture No. 15.........Veera Sundararaghavan
Statistical learning methods applied to multi-scale microstructure

4:15 Summary and Wrap-Up of Workshop

4:30 Bus leaves for Holiday Inn

16th ACBM/NIST Computer Modeling Workshop
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