Development of Next Generation Simulation Tools for Evaluating Cementitious Barriers

August 1, 2007

8:00am	Introductions	
8:10am	Opening Remarks NRC NIST DOE	 Andy Campbell Ken Snyder Linda Suttora
8:40	Example Application Scenarios: NRC examples DOE examples	 David Esh and Jake Phillip (NRC) Christine Langton (SRNL)
8:45	STADIUM	Eric Samson (SIMCO)
10:10	LeachXS with Orchestra	Hans van der Sloot (ECN)
10:50	GoldSIM	David Esh and Glen Taylor (SRNL)
11:30	CEMHYD 3D	Ed Garboczi (NIST)
12:10pm 12:30	Discussion/Other Models Lunch	
2:00	Lessons Learned in Model Development	Richard Dimenna (SRNL)
2:30	Model Development – systematic approach to development	David Kosson (CRESP/VU)
4:00	Approaches to Probabilistic Uncertainty Analysis	Sankaran Mahadevan (CRESP/VU) and David Esh
5:15	Day in Review and Adjourn	David Kosson

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August 2, 2007

8:00am	Summarize results of Day 1	David Kosson
8:10	CNWRA Analyses to Support NRC Non-High-Level Waste Determination Reviews	David Pickett (SWRI)
8:45	Existing Data and Data Needs Discussion	Christine Langton facilitate
9:00	Simulation Toolbox Development and Structure: 1. System goals and priorities 2. Multi-disciplinary structures 3. Model components, structures and linkages 4. Input and output formats and structures 5. Data needs 6. Methods development or standardization needs	David Esh and Ken Snyder facilitate
11:00am	Funding Approaches	Linda Suttora
11:30	Lunch	
1:00pm	Developing a Path Forward: 1. Technical scope outline 2. Management structure 3. Schedule 4. Resource requirements 5. Proposal development 6. Peer Review 7. Next steps	David Esh, Ken Snyder and Linda Suttora facilitate
3:00pm	Adjourn	

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Organizations represented

U.S. Department of Energy – Office of Environmental Management

U.S. Department of Energy – Savannah River Site

U.S. Nuclear Regulatory Commission - Office of Reactor Research

U.S. Nuclear Regulatory Commission - Office of Federal and State Materials and Environmental Management Programs

Consortium for Risk Evaluation with Stakeholder Participation

Materials Service Life & SIMCO Technologies

ECN Netherlands

Center for Nuclear Waste Regulatory Analyses

Minutes of the Cement Meeting

August 1-2, 2007

Welcomes were extended from Andy Campbell (NRC) and Linda Suttora (DOE). Andy also discussed precedents set by previous DOE-NRC partnerships (e.g., RESRAD). Ken Synder (NIST) presented an overview of cement simulation computer tools developed at NIST and the technical developments initiated through collaboration with Laval University and SIMCO.

Scoping Presentations

David Esh (NRC) presented an overview of how NRC uses performance simulation tools to formulate questions in support of judgment reviews. He cautioned that, although the goal of the partnership may be to describe the properties of cementitious/admixture materials with time, different applications of cement barriers (e.g., low-level waste disposal, various nuclear power plant uses) may require different evaluation tools. David mentioned that NRC would benefit from a validated and flexible simulation tool, or set of tools, tracking long-term properties (e.g., physical, chemical, structural) of cement barriers and chemical composition of any effluents with consideration for degradation mechanism, different application scenarios, and parameter and model uncertainty. Discussion included the use of Richard's equation to describe unsaturated flow through cracks, applicable degradation mechanisms, importance of modeling in NRC decision-making processes and use of monitoring for compliance vs. monitoring for failure.

Christine Langton (SRNL) described use of cement materials simulation for support of DOE performance assessments. Previously, focus has been placed on cementitious barriers for low-level waste disposal in typically unsaturated shallow land environments. SRNL performance assessment process uses several simulation codes including the HELP code for infiltration and cap failure, MINTEQ/Geochemist's Workbench for chemical interactions and leachate properties, PORFLOW for flow and transport, and ANSYS-based structural failure models for concrete degradation. Some SRNL personnel have experience with GOLDSIM for sensitivity analyses. Cement barriers applications include LAW vaults walls, LLW "components in grout" disposal, waste tank closure materials, and wasteforms and vaults of the Saltstone Disposal

Facility. Further opportunities to improve performance assessments would come from descriptions of mechanistic long-term physical/chemical properties, the evolution of cracks and transport of contaminants/corrodents through fractures, and model/material/scenario uncertainties. The discussion of SRNL viewpoint addressed the status of DOE complex-wide standardization in approaches, methodologies and models, the sophistication of MINTEQ to describe complex chemistries, manual input/output switching between current simulation tools at SRNL and monitoring for performance indicators (National Academy report).

Technical Presentations on Current Simulation Approaches

Eric Samson (SIMCO Technologies) provided an overview of the technical aspects of the STADIUM model for estimating service life of structural cement materials. STADIUM describes the 1-D the dissolution and transport of eight ionic species from seven solid phase minerals using a Nernst-Planck equation modified to include advection following the Richard's equation. Input parameters to the model are easily determined from simple characterizations or standardized tests. The materials database includes 24 different concrete mixtures (e.g., combinations of water/binder ratios, cement types, admixtures, corrosion inhibitors) with transport properties evaluated as a function of time and, in some cases, exposure to chloride solution for up to 2 years. Development of the STADIUM software is not commercial, but is conducted through the SUMMA consortium of companies supporting the development of STADIUM. Discussion topics included technical parameterization (e.g., chemical activity models, verification by comparison to model by E. Reardon at University of Waterloo), application issues (e.g., structural concrete life spans vs. waste assessment intervals, handling of cracks/microcracks, capabilities to describe oxygen transport and interaction) and collaborations with other entities (e.g., CEA in France).

Hans van der Sloot (ECN) presented an overview of LeachXS, a leaching/geochemistry/data management expert system developed between ECN in the Netherlands, Vanderbilt University and DHI Water Environment Health in Denmark. The need for LeachXS came as a result of regulatory issues surrounding use of alternative materials in construction applications and harmonization of leaching/assessment procedures within European standardization group (CEN). The software package includes tools for geochemical speciation (ORCHESTRA code), mass transfer modeling including gas interaction, database management of leaching characteristics for materials/lysimeters/field data, quality control programs, and guidance on selection of leaching procedures and information specific to different management scenarios. Geochemical capabilities include (i) chemical speciation on full multi-element spectrum, (ii) adsorption to organic matter, mineral oxides and clays, (iii) partitioning between solid and particulate phases, and (iv) redox under unsaturated conditions (e.g., oxidation of wasteforms). The system allows for comparison of leaching test data between different materials, comparison with user-defined or regulatory criteria, and statistical parameter evaluations. LeachXS is the graphical user interface and manager for system with export functions with spreadsheets, figures, forms, and output files for other models. The current materials database includes inorganic and organic species representing 8-9 M € in database information. Inclusion of radionuclides into the materials database is in process. Discussions of LeachXS focused on integration into assessment methodology by looking at transport from or interaction between waste material and surrounding environments, geochemical speciation of species at different ionization states (e.g., Pu), and how transport coefficients in LeachXS are describe via tortuosity values from tank leach data.

David Esh (NRC) discussed NRC experience with the dynamic simulation platform, GOLDSIM, which originally developed for radioactive waste for DOE HLW repository and current used by NRC to help develop questions for reviews. GOLDSIM can handle stochastic modeling, balances (e.g., mass, heat), user-defined functions, and iteration/looping. The platform has good capabilities for integrating processes for linking models and other external links; however, it is not very good as a process model and does not handle transport well. The group discussed the use of probabilistic modeling (e.g., Monte Carlo sampling, Latin hypercube) in GOLDSIM and the possibility of using GOLDSIM as wrapping model or main program for a potential set of simulation tools.

Ed Garboczi (NIST) presented the evolution of NIST cement microstructure models for predicting properties starting in the 1990's through CEMHYD3D. These models have been developed to capture physical properties (e.g., diffusion/dissolution/nucleation growth of hydration chemistry, changes material sets, degradation) using real material thermodynamic and kinetic parameters and known rate laws. Capabilities of CEMHYD3D include hydration, temperature evolution, curing, setting time, mineralogy, and phase distribution with time. The principle limitations of CEMHYD3D are the absence of real kinetics and difficulty in introducing new materials. Group discussion focused on how microstuctural models would benefit the current needs by describing long-term reactions in the microstructure and generating effective parameters to feed into continuum models (structural, transport, leaching models).

Uncertainty Approaches

Sankaran Mahadevan (Vanderbilt University) compared methods to account for inherent randomness, uncertainty in data, and model uncertainty. Monte Carlo simulation is the most general and easy to implement approach; however, a lot of high quality data and a large number of simulations are required for a good analysis. Optimum symmetric Latin Hypercube sampling is an analytical approximation to limit uncertainty which is extremely powerful in concrete, steel, bridge, aerospace applications using only a limited number of simulations. As opposed to these classical uncertainty methods, Bayesian approaches work with little data and provide likelihood ratios (Bayes factor), quantitative measure of confidence, and extrapolation using Bayesian networks. One limitation is that some uncertainties may not be amenable to the Bayesian framework.

Glen Taylor (SRNL) provided a list of thoughts on uncertainty as it pertains to SRNL applications of cement barriers in light of sparse data sets and extended assessment intervals. Uncertainty issues include the assumptions that barriers are not intact in the long-term, cement barriers maintain chemistry although porosity increase with degradation, and use of pore flushes to represent flow through concrete in the field. Computational capabilities are limited due to scaling effects and sparseness of data. The competing rates of transport and radioactive decay mean that conservative estimates are not arrived at intuitively.

Ongoing NRC-funded Research

David Pickett (Center for Nuclear Waste Regulatory Analyses) reviewed ongoing research funded through NRC on cementitious materials in nuclear applications. CNWRA acts as a consultant to NRC for technical assistance, primarily conducting literature reviews of topics for

support of NRC reviews. Current topics include chemical and physical stability of cement-based material (e.g., degradation mechanisms and models), chemical performance (e.g., pH, redox, effects of degradation), use of coupled reactive transport models, effects of fast pathways like cracking on contaminant transport, and radionuclide release mechanisms from cementitious wasteforms.

Next Generation Simulation Tools

Rich Dimmena (SRNL) described some lessons learned from previous modeling projects (e.g., SRS tank program and GNEP modeling). He stressed that for a large development project to be successful, it is imperative to define the objective, define the approach, identify the deliverables, and keep the customer informed. Rich also suggested that the project, both organization and products, be based on an object-oriented paradigm making it easier to facilitate multi-development fronts and integrate models components, respectively.

David Kosson (CRESP/Vanderbilt University) led an initial discussion on the generic structure and properties of a next generation simulation approach for cement barriers. Discussion topics included outputs of interest (e.g., physical, structural, and leaching or chemical properties), test bed scenarios (e.g., spent fuel pool, saltstone vaults, saltstone wasteforms), pertinent release and degradation mechanisms, model and scenario interfaces, up-scaling paste hydration to structural elements, structured uncertainty analysis. It was agreed that some form of object oriented or compartmentalized software architecture linking current stand alone models or developed model subcomponents would provide timely improvements to current approaches while mechanistic refinement progresses. Also recognized was the need for a defined suite of standardized characterization tests to support performance simulations. Release and degradation mechanisms should include ion diffusion, mineral dissolution, advective transport through cracks, moisture transport, long-term matrix evolution, external stresses due to exposure to gas- and liquid-phase corrodents (e.g., decreased reducing capacity due to oxidation, boundary layer formation through carbonation, depassivation of reinforcing steel through chloride ingress), and physical loads (e.g, seismic events).

Organizational and Programmatic Issues

David Kosson (Vanderbilt University) facilitated a discussion on how the partnership should be organized and issues to address in the next month. Lead personnel representing each partner organization were identified as a management board to include Linda Suttora (DOE-EM), David Esh (NRC-DWMEP), Jake Philip (NRC-RES), Ed Garboczi (NIST), Christine Langton (SRNL), Rich Dimmena (SRNL), and David Kosson (CRESP/Vanderbilt University). The management board would take lead roles on the development of a proposal outline for the DOE. David Kosson suggested that CRESP organize an External Advisory Board of experts from a broad-range of pertinent fields to act as an independent review panel. This approach has been used previously with transparency and confidence with other DOE-EM projects. Issues identified for future discussion included expertise identification and nominations for the External Advisory Board, organization of weekly conference calls, and development of an intellectual property policy.