U.S. Nuclear Regulatory Commission

NRC Technical Review of the Quality Assurance Documentation for the CBP Toolbox

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Introduction

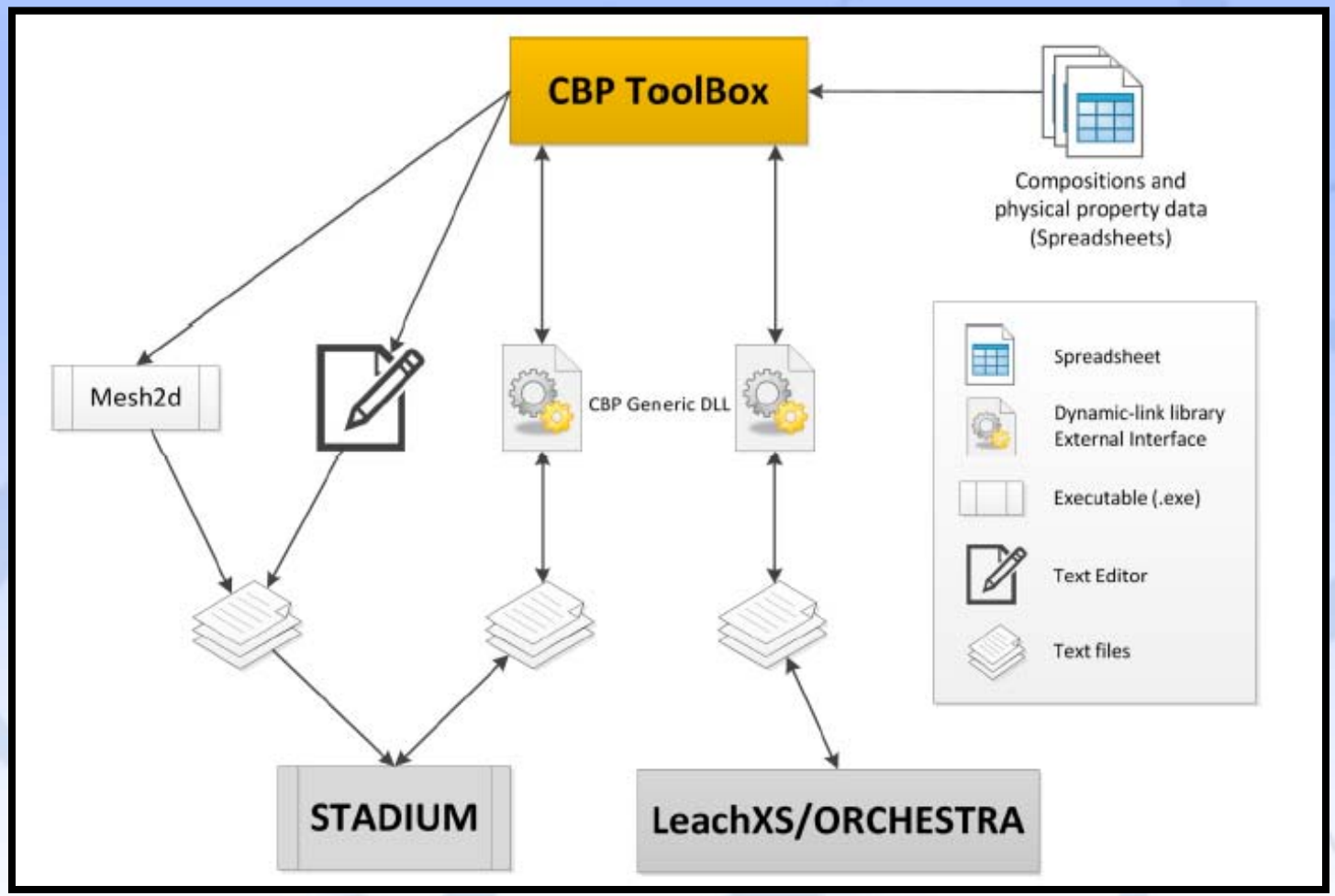
CBP Objective

Develop a set of reasonable and credible tools to predict the long-term structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames (http://cementbarriers.org/)

CBP Partners

- **U.S. Department of Energy (DOE) Office of Environmental Management**
- **Savannah River National Laboratory (SRNL)**
- **Vanderbilt University Department of Civil and Environmental Engineering**
- **Consortium for Risk Evaluation with Stakeholder Participation (CRESP)**
- **Energy Research Centre of the Netherlands (ECN)**
- **SIMCO Technologies Inc. (SIMCO)**
- **U.S. Nuclear Regulatory Commission (NRC)**

CBP Toolbox Framework



Brown, et al., 2013

Capabilities of the CBP Toolbox Software

LeachXS/ORCHESTRA

- **Combined database and modeling system for simulating transport and degradation phenomena in cementitious materials**
- **LeachXS database includes:**
  - **Equilibrium leach test results from pH-dependence leach tests (e.g., EPA 1313)**
  - **Dynamic leach test results from percolation tests (e.g., EPA 1314)**
  - **Monolith leach tests (e.g., EPA 1315)**
  - **Lysimeter tests**
  - **Field measurements**
- **LeachXS test results coupled with equilibrium geochemical modeling using ORCHESTRA**
- **Currently, LeachXS/ORCHESTRA designed to model sulfate attack, carbonation, oxidation, and leaching**

Seignette, 2015

Capabilities of the CBP Toolbox Software

STADIUM

- **Reactive transport model for cementitious materials exposed to aggressive environmental conditions**
- **Simulates the ingress of deleterious species into the concrete matrix, as well as leaching of species as a consequence of the following cementitious degradation processes: chloride ingress, sulfate attack, and carbonation.**
- **Tested under a range of conditions and variety of applications as it has been used on more than 150 projects**
- **Model specified by the U.S. Department of Defense to evaluate the service-life of concrete waterfront structures**

Samson, 2015

CBP Toolbox Quality Assurance (QA)

Motivation for CBP Toolbox QA

- Laboratory investigation (SIMCO) of cement paste mixes based on formulations for Saltstone Disposal Structure (SDS) 1 & 4 and cylindrical SDSs
- Pastes exposed to different aggressive contact solutions (carbonate, nitrate, sulfate, sodium, pH)
- Unexpected observations of severe degradation, apparently from alkali-silica reactivity of silica fume agglomerates
- Not clear to what extent differences between laboratory and field conditions were responsible for degradation (e.g., no sand or aggregate, limited curing time, contact versus immersion)

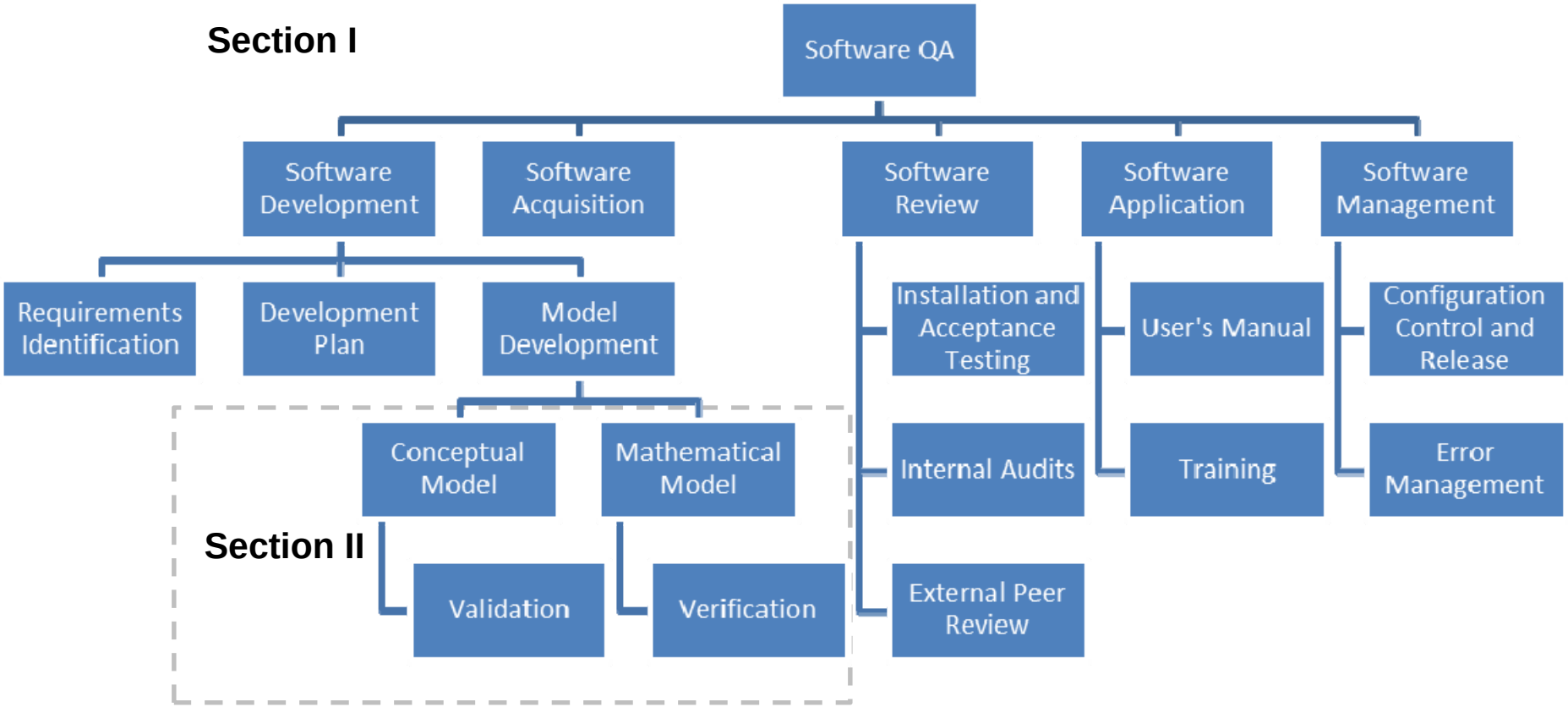
Protiere and Samson, 2015; Langton, 2016

CBP Toolbox Quality Assurance (QA)

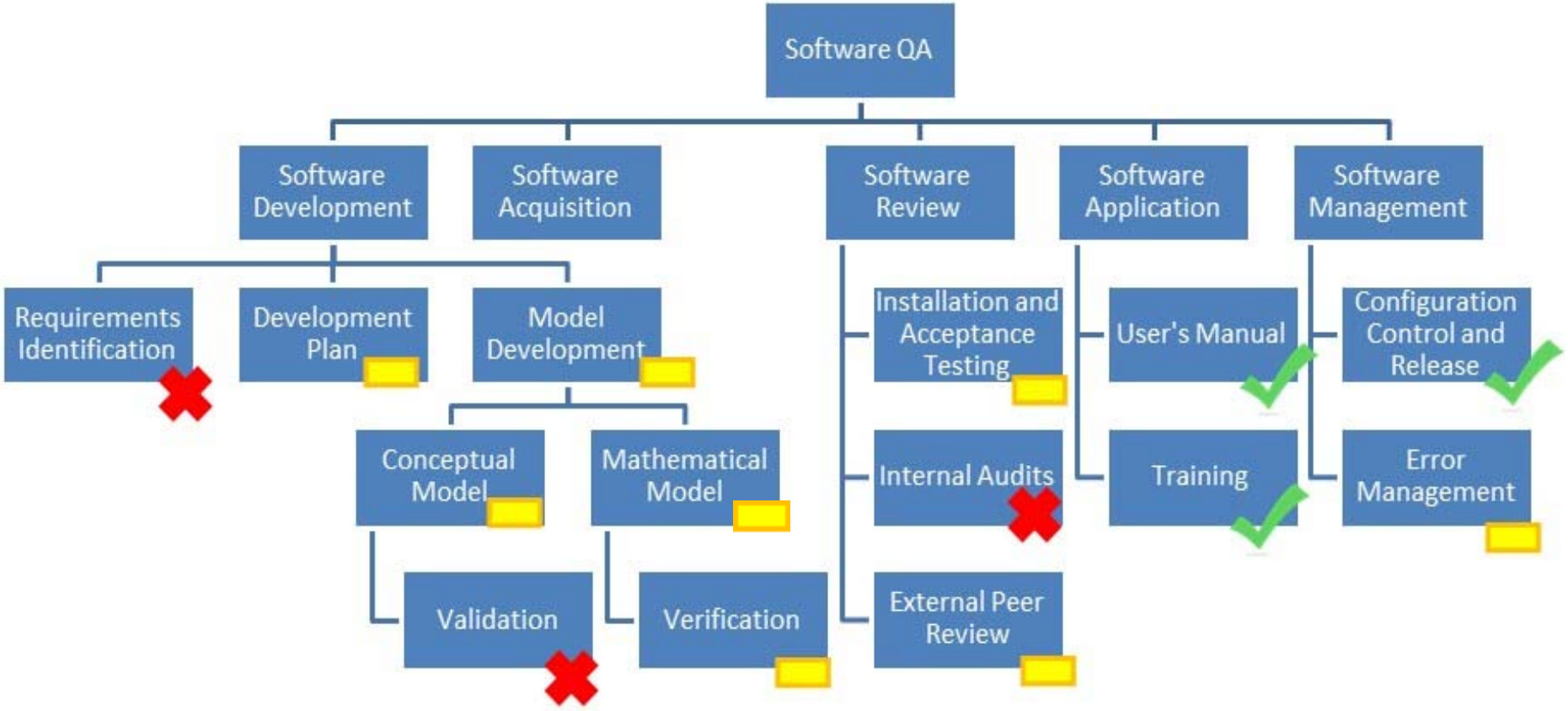
Motivation for CBP Toolbox QA (continued)

- DOE continuing to investigate cause of cracking and discrepancy between observations of cracking and CBP Toolbox predictions of long-term performance
- DOE requested CBP Toolbox QA information
- CBP compiled QA documentation
- NRC conducted a technical review of the CBP Toolbox QA documentation (ML16196A179)

Software QA Process



Software QA Process



Verification and Validation General Limitations of the CBP Software

Incomplete set of degradation mechanisms and limited coupling of mechanisms

- **Toolbox includes the following chemical degradation mechanisms: chloride ingress, sulfate attack, carbonation, and leaching.**
- **Additional chemical degradation mechanisms may also be relevant to the long-term performance of cementitious materials.**
- **Feedback between degradation mechanisms could result in a synergistic effect on the rate and extent of degradation relative to degradation mechanisms acting in isolation.**
- **Coupling of chemical degradation mechanisms with the mechanical properties of the cementitious materials could be important for the modeling of cementitious materials over long time frames.**

Verification and Validation
General Limitations of the CBP Software

Limited validation exercises

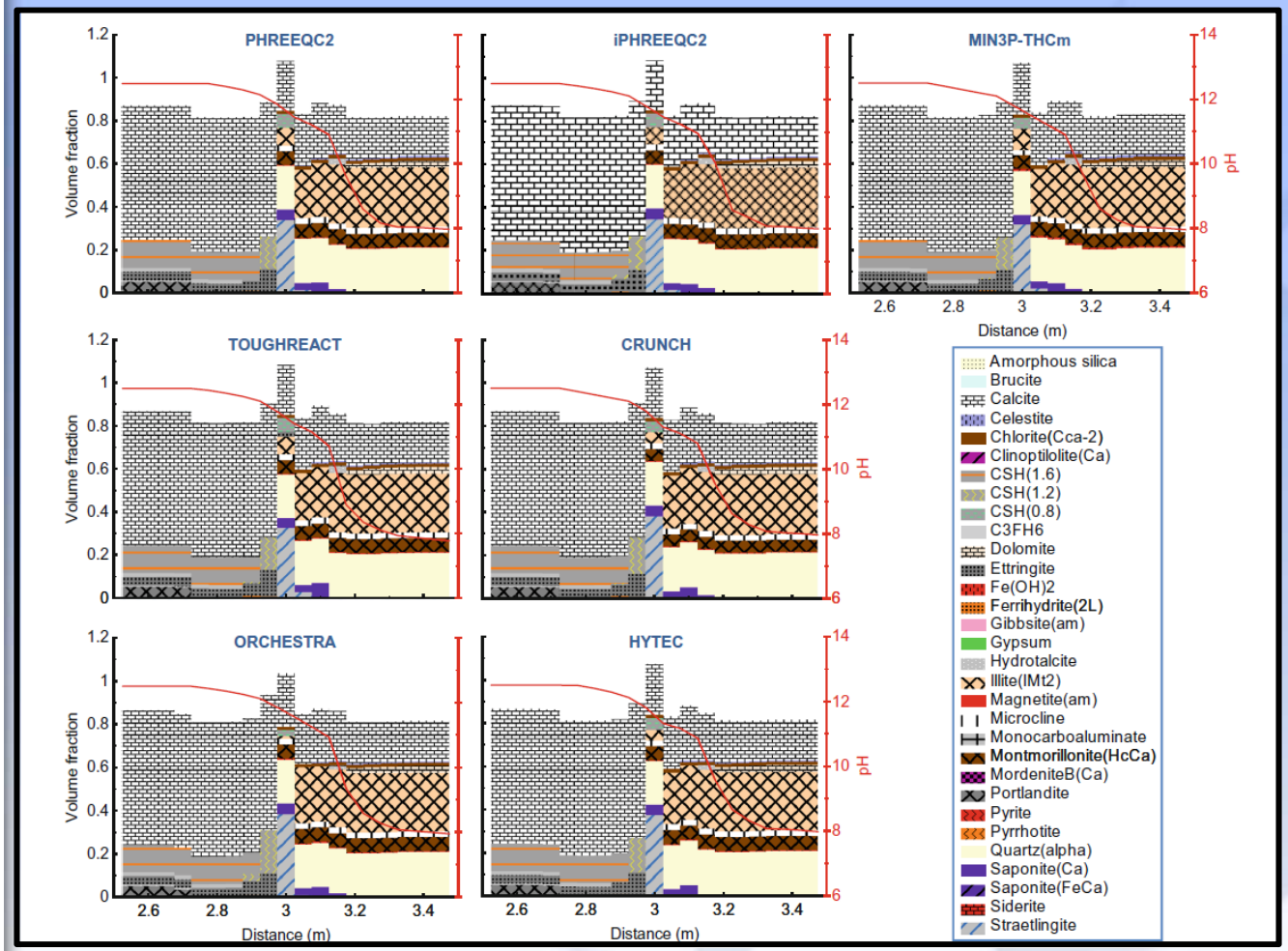
- **Additional validation test cases would improve confidence in the Toolbox**
- **Validation test cases should include flow and transport of deleterious species through degraded cementitious materials**

Verification and Validation General Limitations of the CBP Software

Insufficient support for modeling damage due to sulfate attack

- **The technical basis for sulfate ingress and resultant chemical reactions and mineralogical changes is well-supported.**
- **Support is more limited for several assumptions related to the approach and parameterization of the modeling of damage due to sulfate attack.**
- **Without additional support for these assumptions, confidence in damage progression due to sulfate attack is limited.**

Verification - ORCHESTRA Model-to-Model Comparison

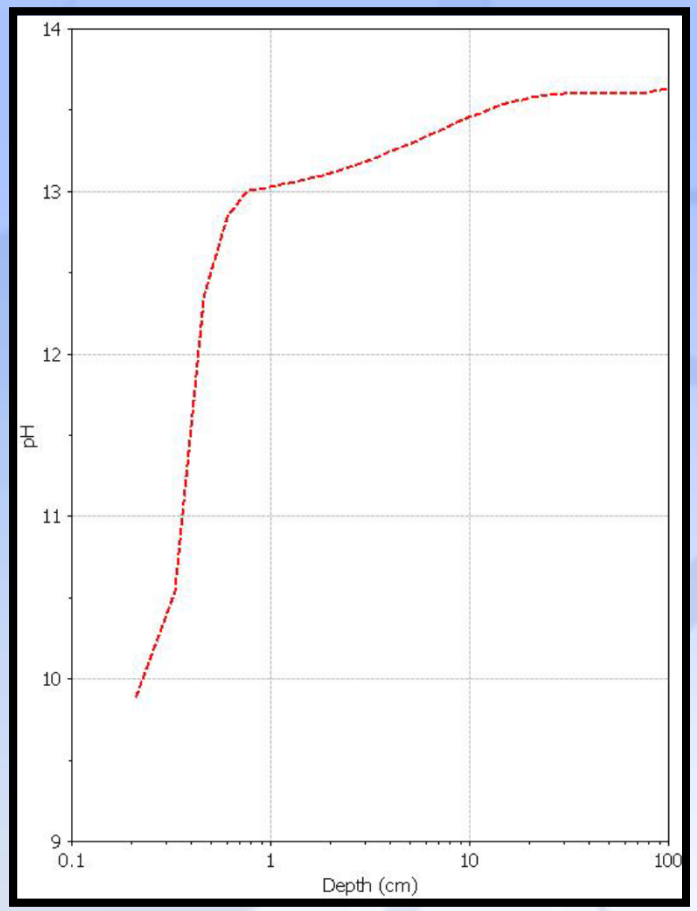


International peer-reviewed benchmarking study

- **Efficient**
- **Demonstrates inter-model consistency**
- **Builds model confidence**

Marty et al., 2015; Meeussen and Brown, 2015

Validation - ORCHESTRA Carbonation



Comparison of LeachXS/ORCHESTRA output against measured carbonation depth from a dome core (241-C-107) sample after approximately 65 years

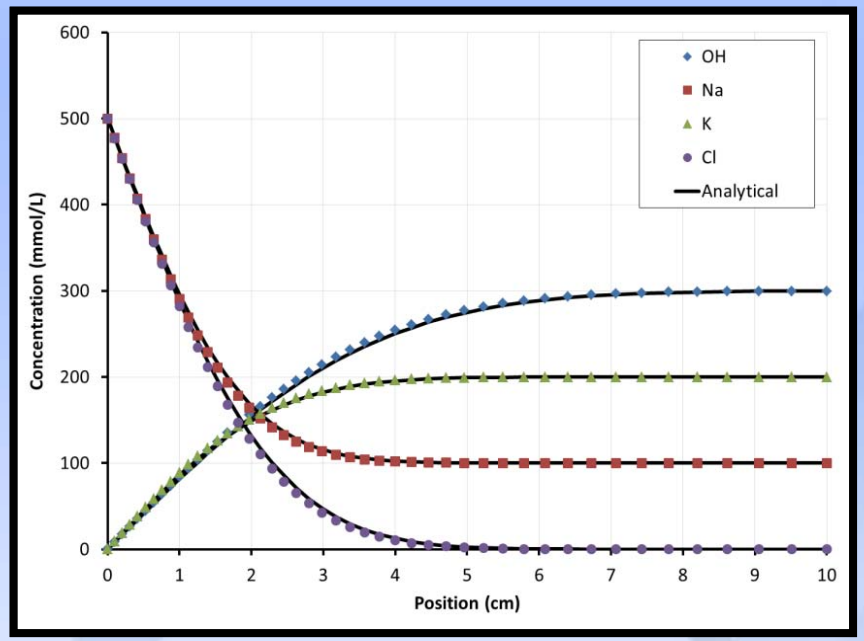
WRPS-51711-FP; Meeussen and Brown, 2015

Verification & Validation LeachXS/ORCHESTRA

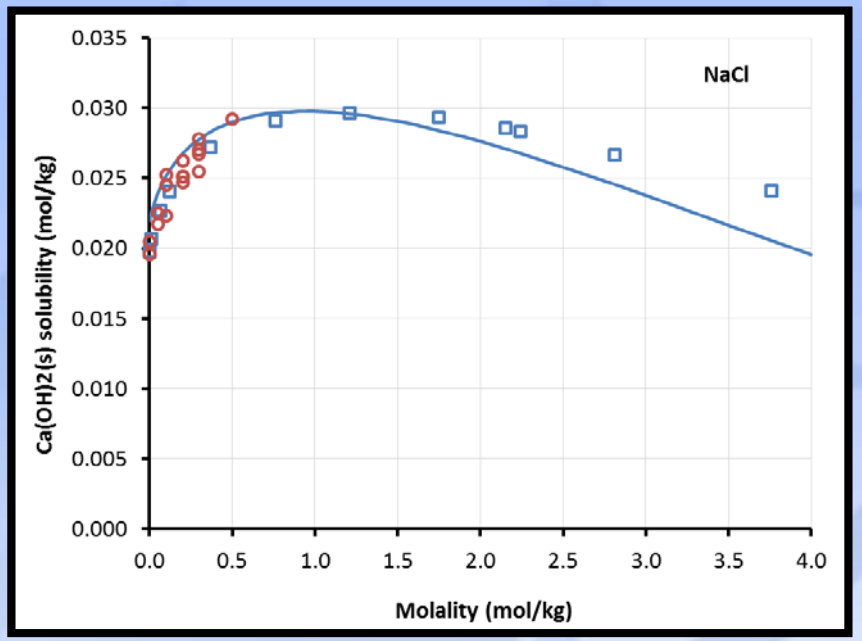
NRC Recommendations

- **Discuss the limitations of using test methods (e.g., representativeness of test methods for field conditions)**
- **For the purposes of validation of diffusive transport through an intact matrix, the C-107 test case is appropriate.**
- **Additional information on the selection of parameters would be helpful to verify that this test problem is consistent with model validation rather than model calibration.**
- **Carbonation-induced corrosion could occur in a much shorter period of time if advective transport occurs through cracks.**
- **CBP should conduct a literature search to gather additional field studies for similar validation exercises under a range of environmental conditions.**

Verification & Validation
STADIUM



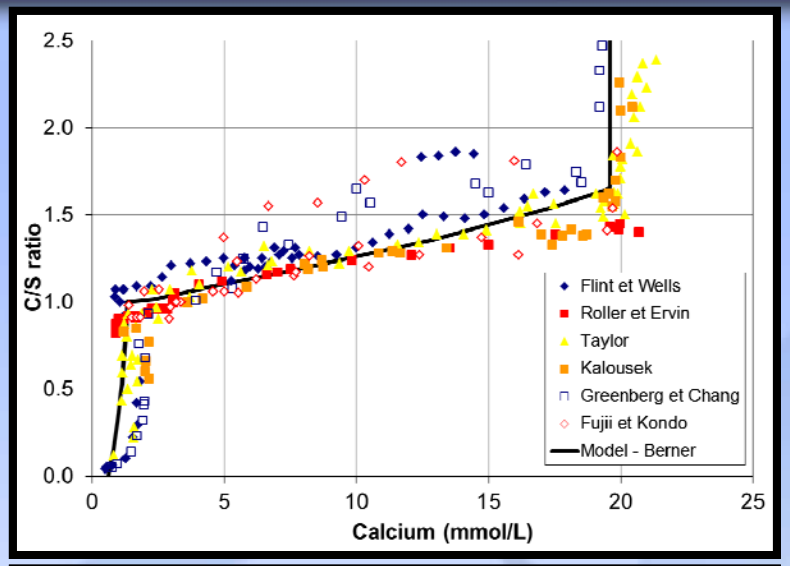
Comparison of STADIUM output against analytical solution for diffusion

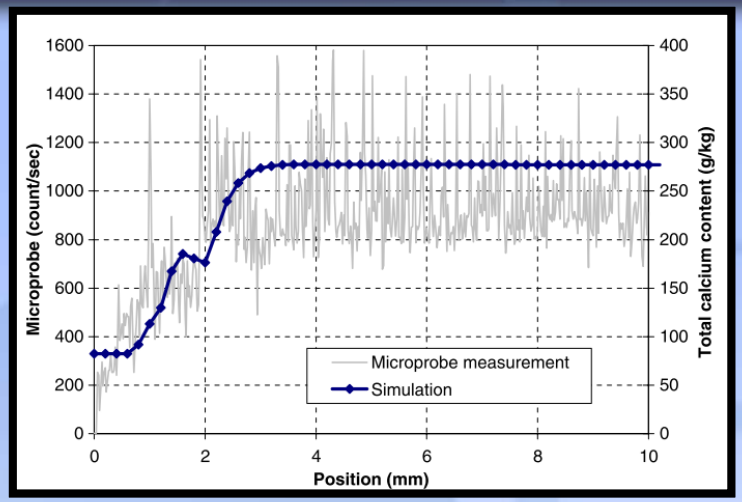


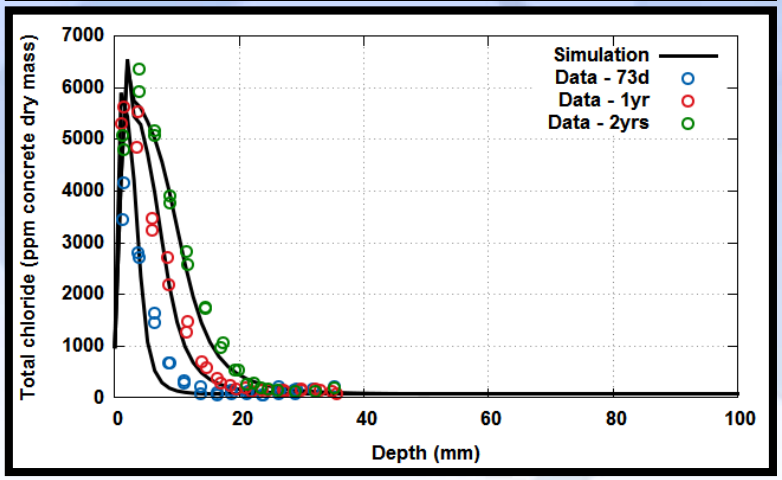
Comparison of STADIUM output against experimental studies for the solubility of portlandite in NaCl solution (data from Johnston, 1931 and SIMCO [red])

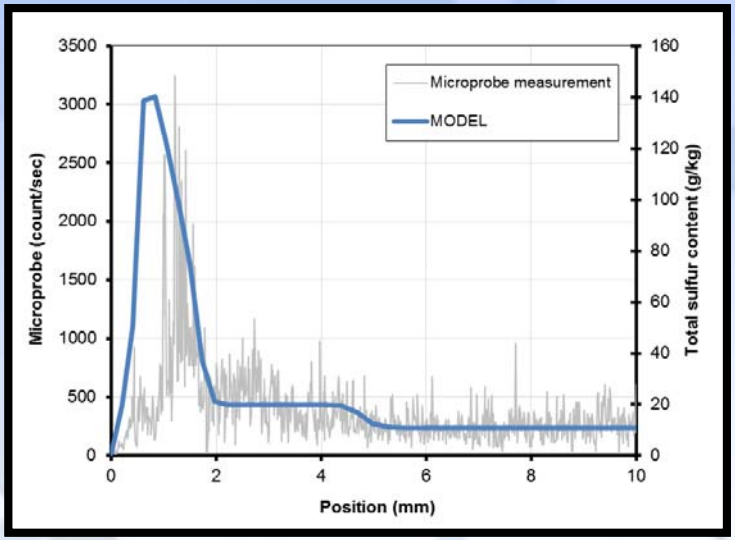
Samson, 2015

Verification & Validation
STADIUM



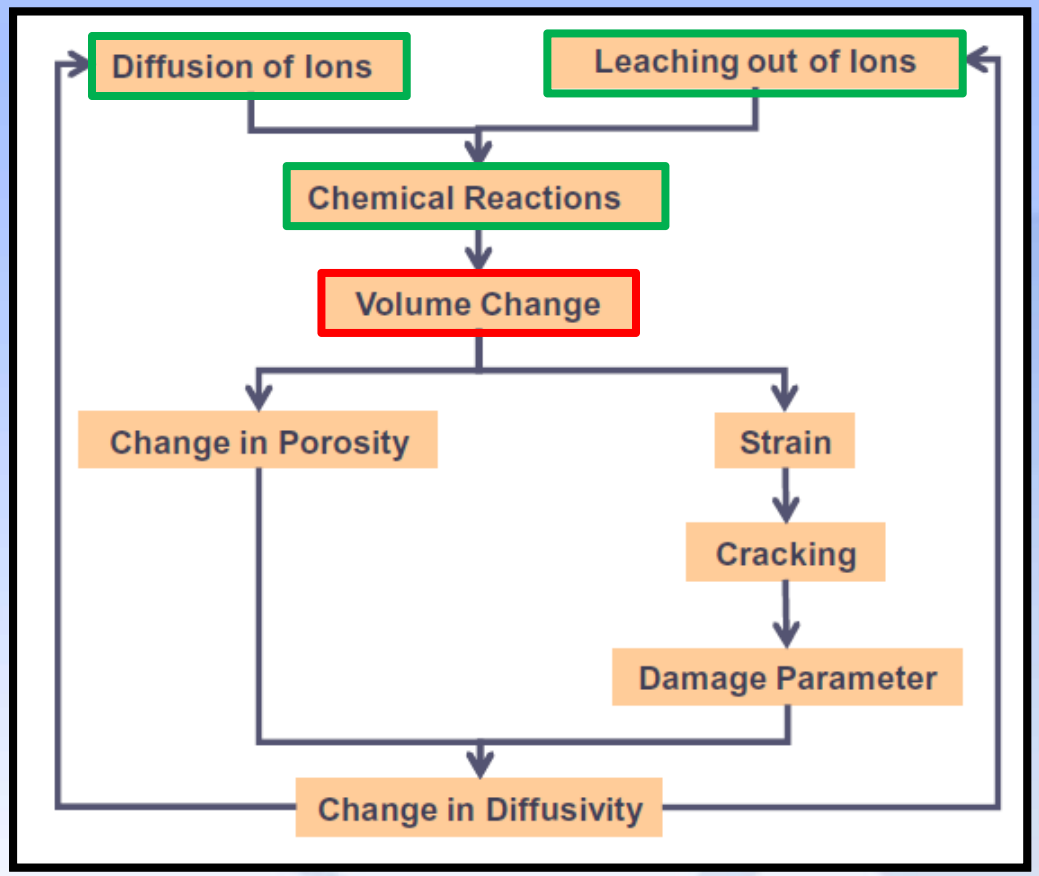






Samson, 2015

Validation – ORCHESTRA & STADIUM Sulfate Attack



Technical basis

- \+ Diffusive transport
- \+ Leaching
- \+ Formation of expansive phases
- \- Volume increase based on equilibrium thermodynamic calculations
- \- Parameterization of volume change calculation
- \- Additional experimentation and validation needed

Sarkar, et al., 2010; Meeussen and Brown, 2015

Conclusions

Toolbox documentation should include additional discussion of the limitations of the software, including:

- **Incomplete set of degradation mechanisms**
- **Limited coupling of mechanisms**

Future work to address limitations

- **Additional degradation mechanisms and coupling of mechanisms, including mechanical damage**
- **Additional support for modeling damage due to sulfate attack**
- **Additional validation exercises**

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