CONCRETE SUSTAINABILITY CONFERENCE
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The Virtual Cement and Concrete Testing Laboratory: Application to Sustainability

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National Institute of Standards and Technology

NIST = National Institute of Standards and Technology

- Mission (Department of Commerce, 1901)
  - To promote innovation and competitiveness through measurement, standards, and technology to enhance economic security and quality of life.
- Vision
  - To be the global leader in measurements and in enabling new technologies.
- We're mostly physicists, chemists, materials scientists, and engineers

Sustainable Infrastructure Materials

- Service Life Prediction of High Performance Polymers and Composites
- Reduced Flammability of Materials
- Sustainable Concrete Materials (SCM !)
  - Material characterization
  - Rheology of concrete
  - Mitigation of early age-cracking in high volume fly ash concrete
  - Fundamental cement hydration modeling
  - Doubling service life of concrete
- **Outputs of our core research program include**
  - **New microstructure model for DOE durability of concrete for nuclear applications project**
  - **Proposed generic technology for mitigation of early-age cracking**
  - **the Virtual Cement and Concrete Testing Laboratory (VCCTL) software package**
  - **Measurement standards for rheology, X-ray diffraction, sulfate attack, etc.**

Sustainability of concrete

- Sustainability has important societal and systems engineering aspects - focus on materials in this talk
- The industry needs tools to help quantify the effect of new design decisions that attempt to make concrete *more* sustainable during the design, production, placement, and maintenance processes, by considering
  - energy
  - emissions
  - material sources
  - performance properties
  - construction waste
  - service life
  - maintenance schedule
  - ease of recycling

Virtual Cement and Concrete Testing Laboratory

VCCTL

Past and present members of VCCTL consortium

- Past: PCA, W.R. Grace, VDZ, ATILH, Holcim, Sika, BASF, Dyckerhoff, Cemex, NSSGA
- Present: FHWA, Mapei, RMC Foundation, Florida DOT
- ***We thank all of these for funding over 9 years that has made this research and software development possible***

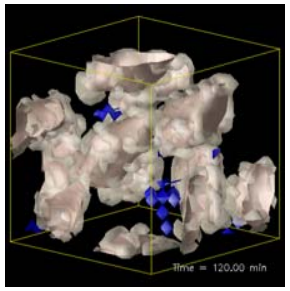
Fall 2009 Department of Commerce Silver Medal for VCCTL development

VCCTL Vision

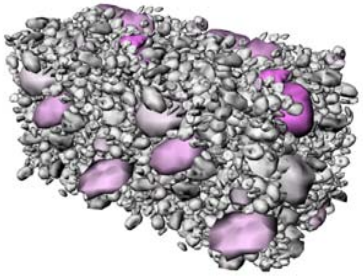
- ***Computer-design concrete just like structural engineers computer-design structures***
  - Performance prediction is a necessary foundation for effective use of performance-based standards and specifications
  - Since there is an increasingly wide class of materials going into concrete, can't simply rely on empirical testing – too many variables
  - Accurate materials-science-based **characterization** and **prediction** of performance is required so that
  - VCCTL will be an **effective tool** for **optimizing** the use of existing and new materials for existing requirements and new requirements **like sustainability**

3 parts of Consortium Research

- 3-D cement hydration modeling



- 3-D concrete rheology simulation



- Virtual testing lab (VCCTL) software

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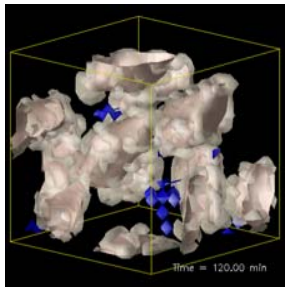

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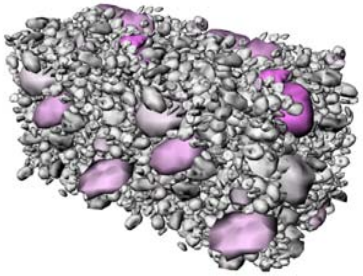


- ***Virtual testing lab (VCCTL) software***

Computing Resources

- NASA and DOE (Argonne) supercomputers

- NIST medium-size Linux cluster
- Powerful desk-tops (e.g. dual quad-cores) to run the VCCTL virtual lab software – can also use regular desktop or laptop for many applications

VCCTL analogy

- **Virtual** Testing Laboratory acts just like a **physical** testing laboratory
- Databases replace material hoppers and bins
- Material mixing models replace mixers
- Quantitative algorithms replace instrumented testing machines
- Software interface replaces lab cart

No magic involved…

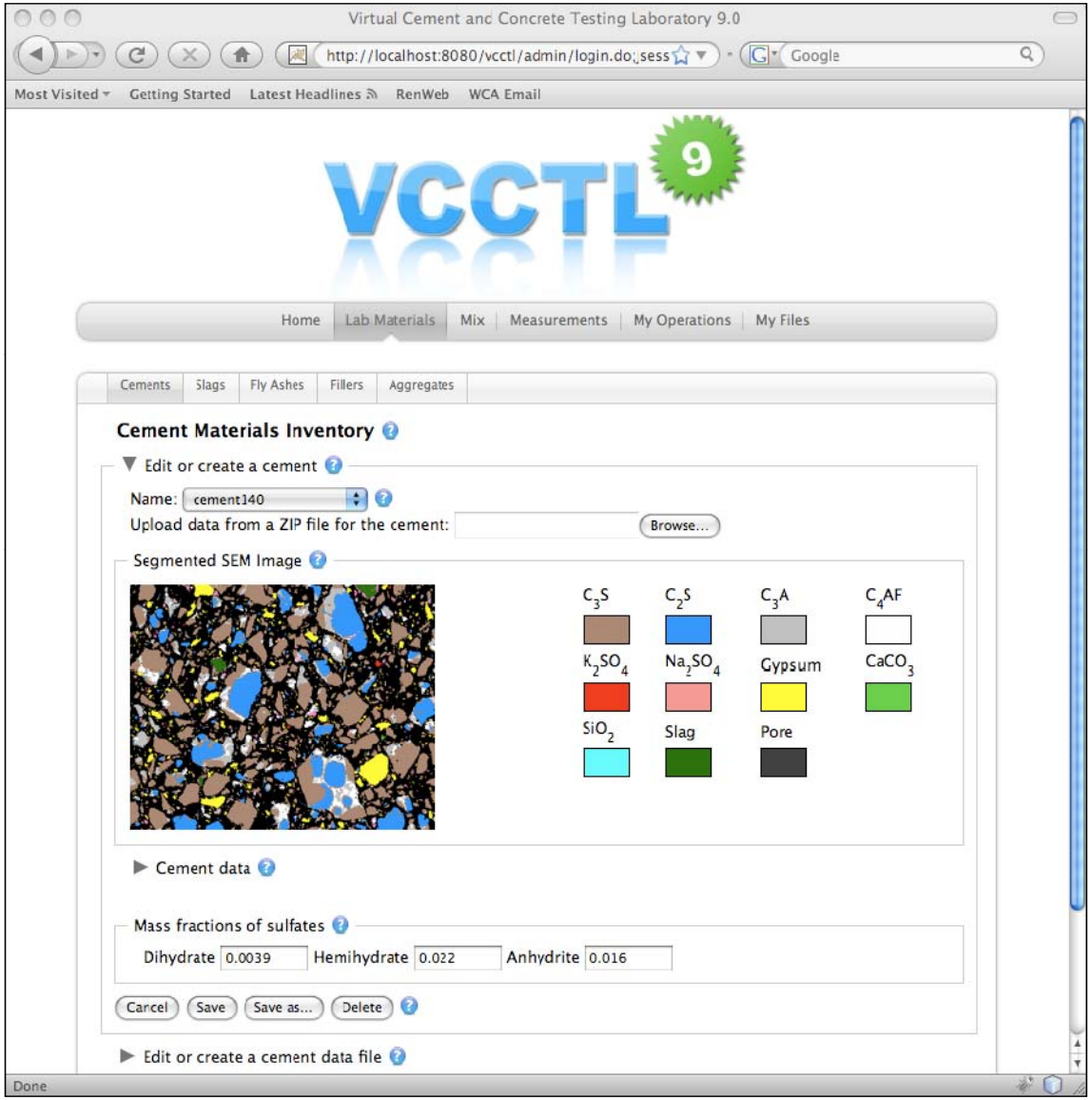
- No waving a wand and predicting the properties of anything…concrete is a complex material!
  - Material characterization – details of mineralogy, particle shape, and calorimetry
  - Must know chemistry (thermodynamics and kinetics) of complex reactions
  - Need to codify this knowledge into accurate models that give 3-D microstructures – otherwise property prediction is not accurate
- After all this hard work, the VCCTL tool becomes very powerful
- VCCTL has been designed using the computational materials science of concrete – based on fundamental chemistry and physics
  - potential of application to almost any material problem in concrete
  - sustainability
  - P2P

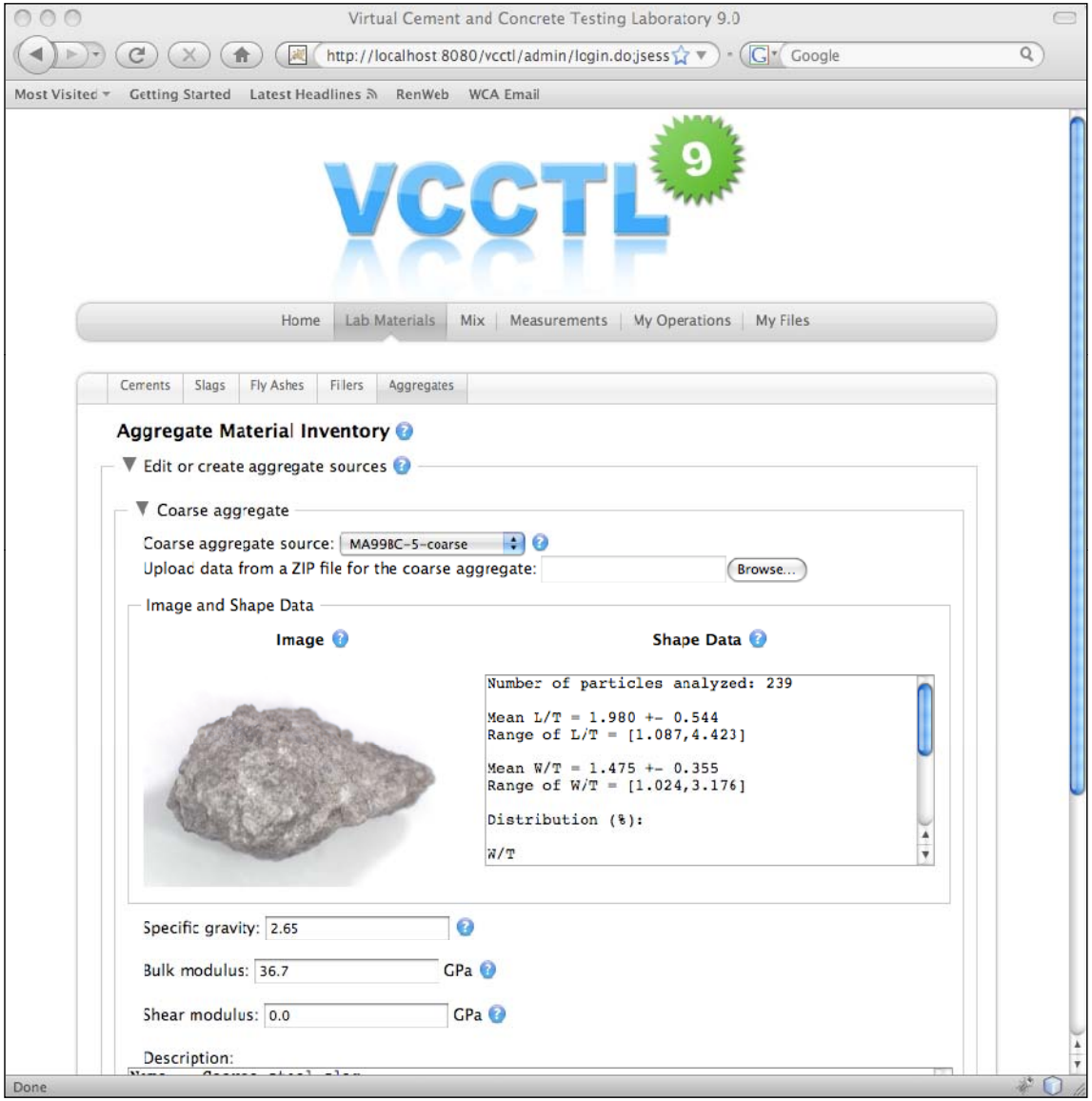
Where VCCTL is right now

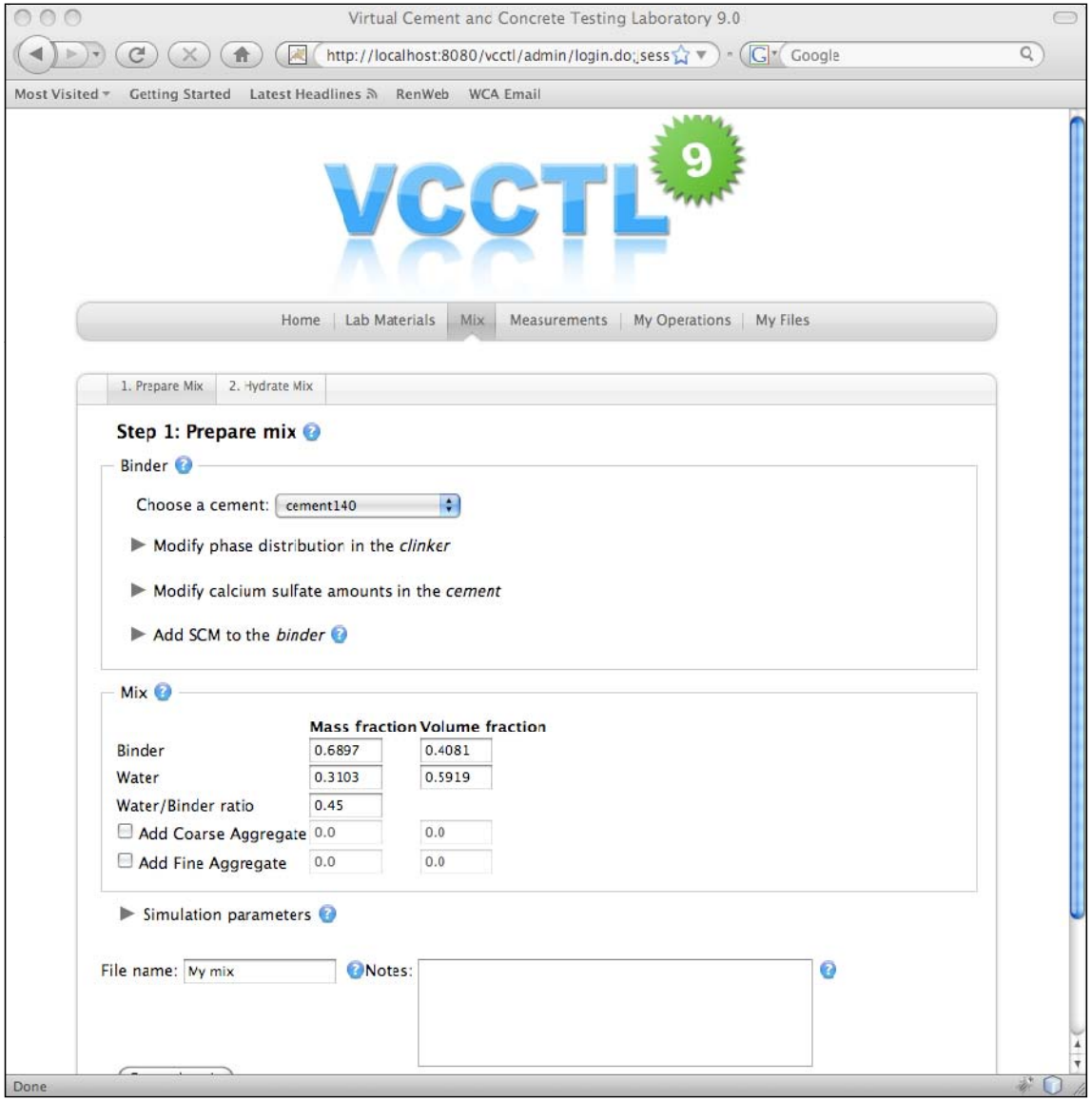
- Any portland cement, any aggregate
  - Can add new material sources as needed with characterization
- Any time of hydration, sealed or saturated, isothermal or adiabatic
- Can predict:
  - elastic moduli
  - chloride diffusivity
  - heat of hydration
  - compressive strength
  - rapid chloride permeability test

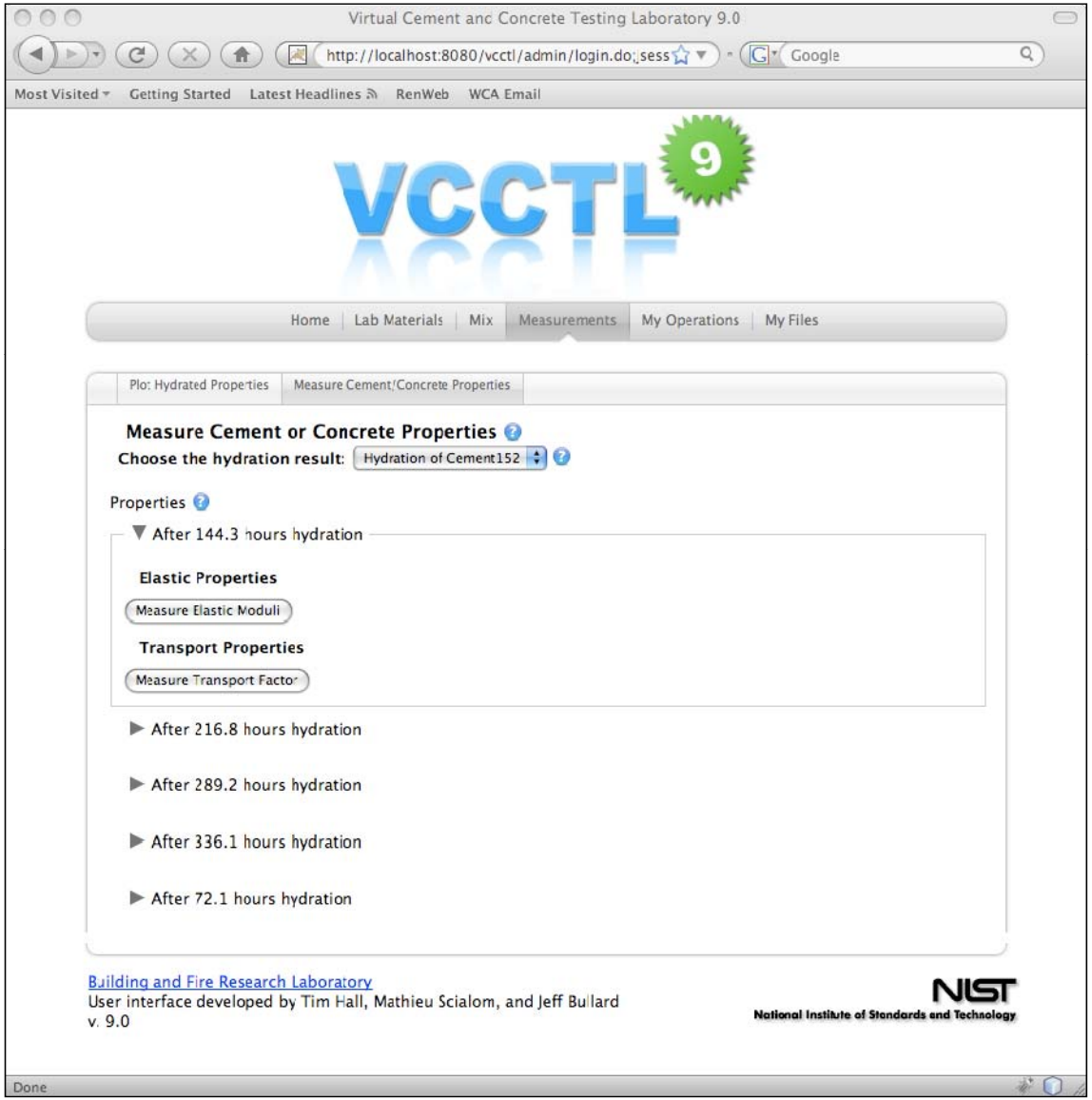
- Some ability to handle fly ash and slag, but not well-validated, and missing a lot of thermodynamic and reaction details

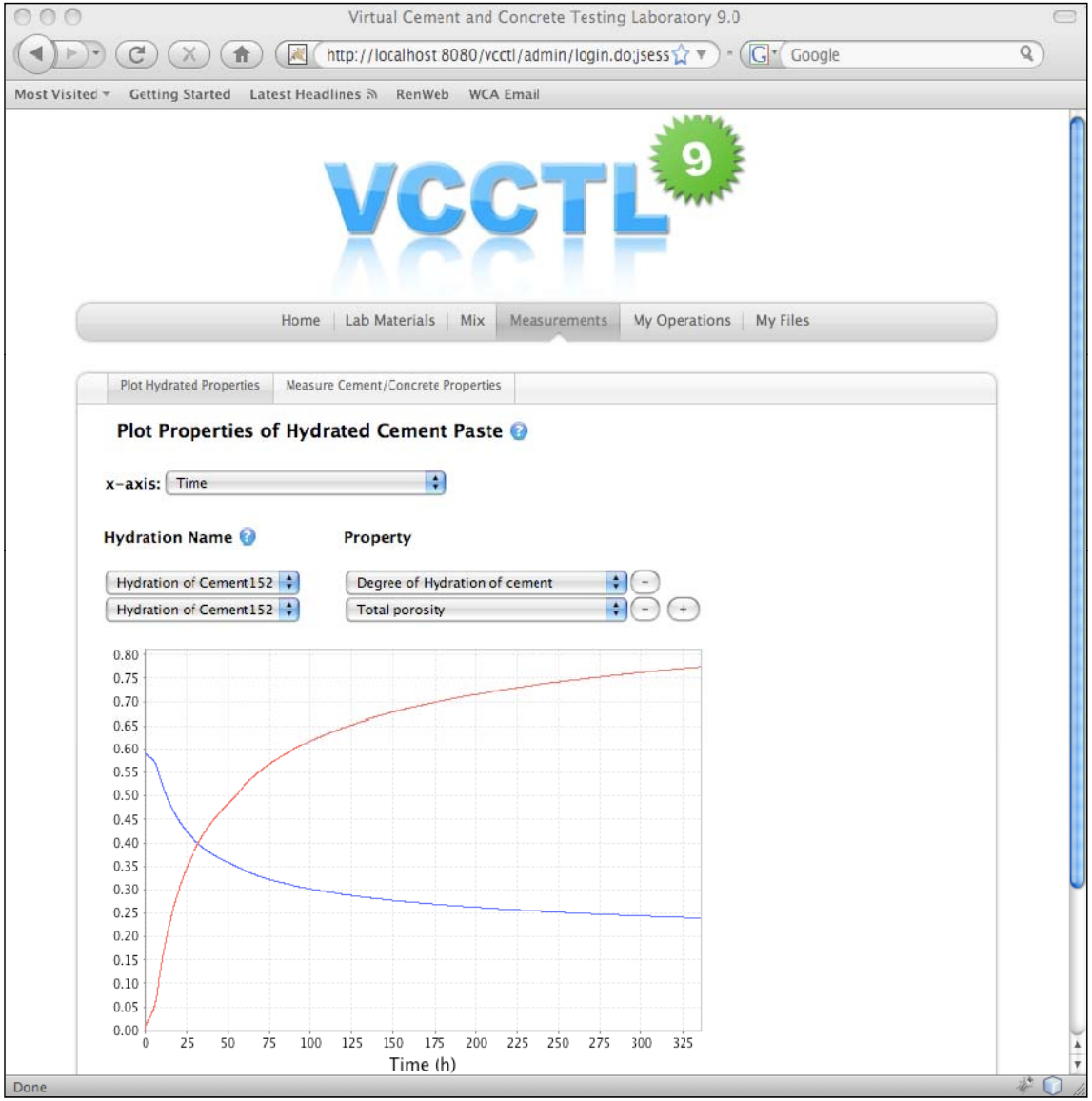
- Nine years of development have given a tool that can effectively be used right now, and which is poised for critical development for sustainability and other uses

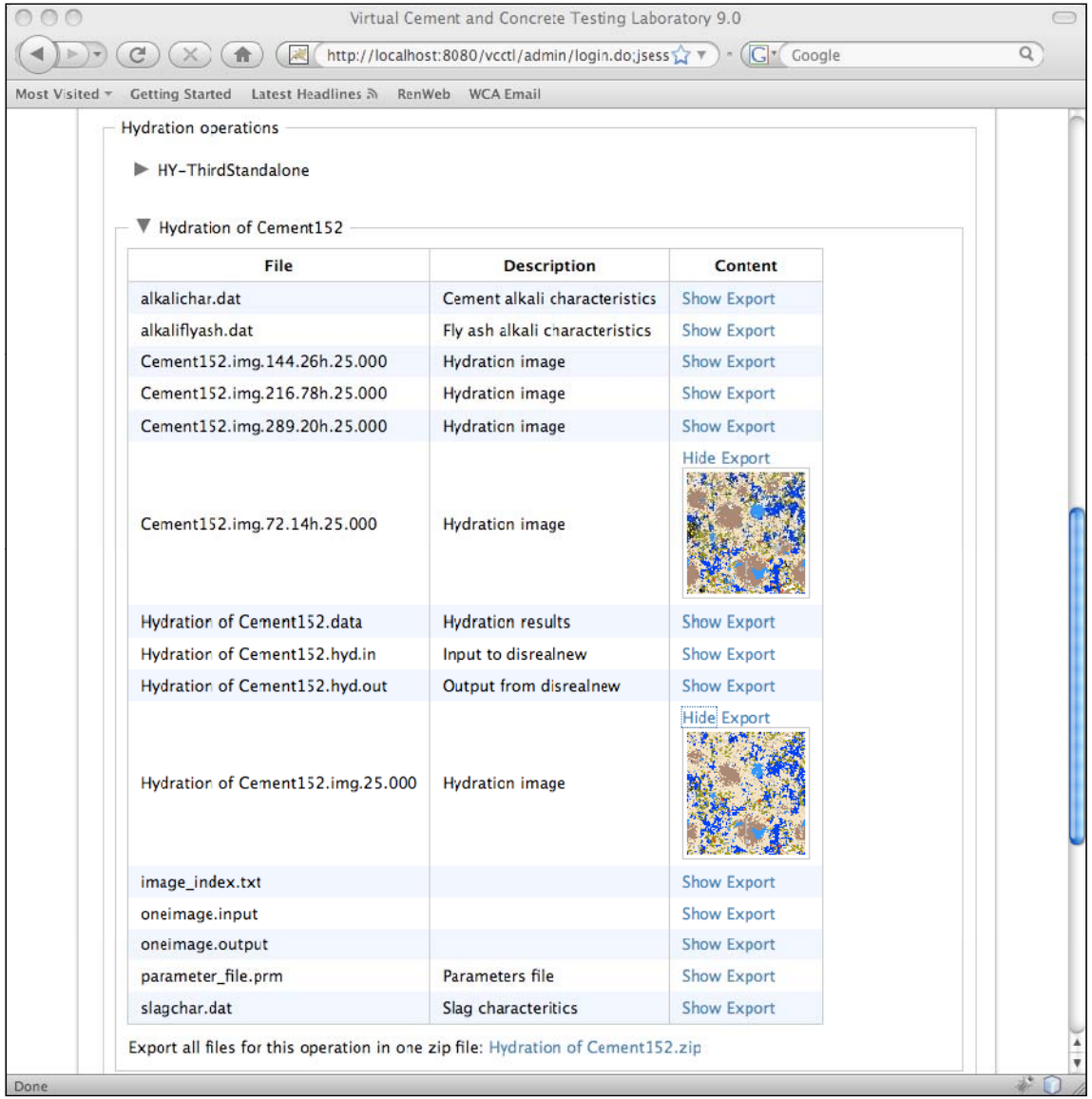


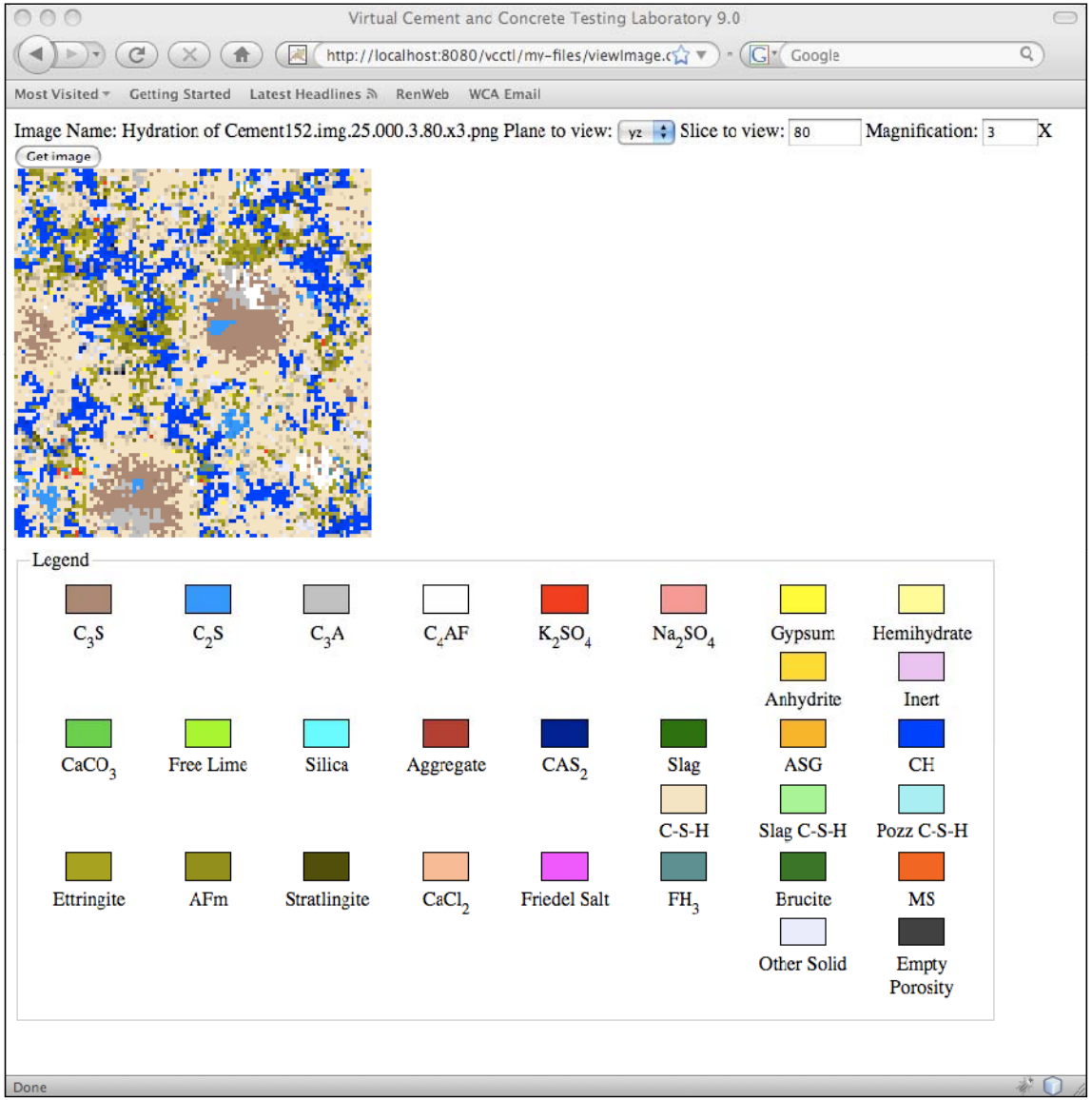












Possible uses right now

- Evaluate properties of concrete made from various portland cement sources with differing mineralogy (also added silica fume)
  - prediction of strength, elastic moduli, rapid chloride permeability test (= DC resistivity)
- Predict physical properties of concrete when coarse cement particles have been replaced with inert fillers (e.g. limestone powder)
- Compute variation of concrete chloride diffusivity when using various cements, aggregates, or mix designs

Possible uses right now

- Effect of variability in materials dispensed at batch plants on concrete performance
  - explore how material variation affects performance variation
- Virtual testing of the effect of cement changes, which come from changes in manufacturing conditions (e.g. lower T kiln, more or less grinding) on concrete properties
  - can associate any psd with any cement mineralogy
- Case studies showing differences between materials meeting prescription vs. performance specifications

Short-term improvements

- Prediction of coefficient of thermal expansion (CTE) to use in pavement design

- If user specifies costs of materials, software can output mixture costs (can include cost of chemical admixtures, but not full chemistry)
  - Other material accounting possible, too – e.g. embodied energy and CO_2 per volume of concrete

Short-term improvements

- Allow more than one cement (e.g. 1-10) to be included in virtual mix, so blending two or more different cements could be explored directly before investing in more silos
- Make links to NIST pervious concrete tools more usable and accessible
- Workability “critical points” – predict maximum packing fractions and how yield stress might be affected

Developmental needs related to sustainability predictions

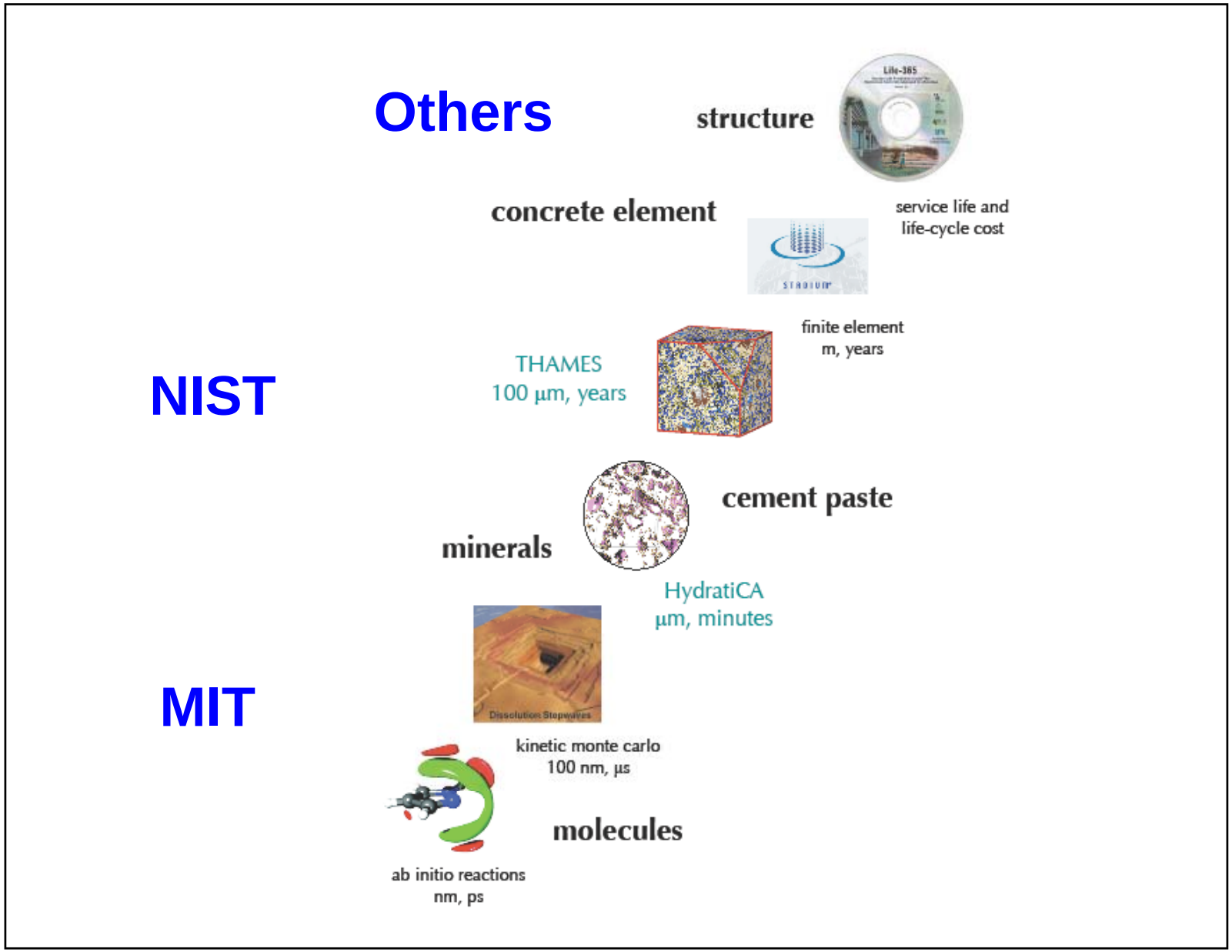
- Better mineralogical characterization of fly ash and slag, leading to $\rightarrow \rightarrow \rightarrow \rightarrow$
- Development of more realistic chemistry and physics of these materials in hydration models and VCCTL software
  - based on the thermodynamics of basic chemical reactions, which in many cases need to be measured (once and done)
- Durability test prediction
- Prediction of cracking and its effect on properties

VCCTL

- Performance prediction is a necessary foundation for
  - Performance-based standards and specifications
  - Optimization of concrete for criteria like sustainability

    That is what VCCTL is being designed to do

- Collaboration with MIT Concrete Sustainability Hub is being planned to be able to complete multi-scale picture of concrete from nanometers to meters (*see Prof. Ulm's talk later in the conference*)



Prospectus

- In 2010, 2011, and 2012, we will be working on
  - making the VCCTL software more usable and powerful
  - how to get this software into the hands of more users via workshops, cooperative agreements, commercialization, user groups, etc.

- Your ideas are most welcome!
  - Edward.Garboczi@nist.gov

Especially concerning sustainability!

Thank you!

