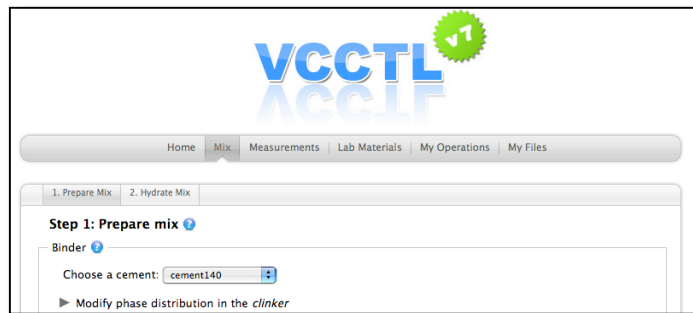**(3-17-09) Virtual Testing of Concrete Using Computational Materials Science**

Do you ever dream about having an accurate idea how a new source of cement or aggregate will affect concrete pumpability without doing lots of slump tests (and slump tests may not give you the right answer, anyway)? Or have you ever wished for a tool that could give you advanced warning of chemical incompatibilities in concretes made with blended cements? These wishes are a reality in the pharmaceutical, metals, and semiconductor industries, where quantitative theory based on fundamental materials science has been successfully applied to guide research and development of new materials. This is the way science works best – ever since the time of Tycho Brahe, Johannes Kepler, and Sir Isaac Newton, the greatest advances in science have involved the close cooperation of experiment and theory.

Unfortunately, quantitative theory for concrete materials has not advanced to the level of sophistication it has in these other industries because construction materials like aggregates, Portland cement, and supplementary cementitious materials such as slag and fly ash are much too complicated for straightforward application of basic materials science. For example, the packing of random-shaped particles like aggregates is still a very hard, unsolved mathematical problem. Fortunately, a new branch of materials science has arisen in the last thirty years, called computational materials science, which has allowed direct application of materials science theory to complicated materials like construction materials via the power of modern computers. Computational materials science has grown in accuracy and range of applicability as ongoing advances in information technology have yielded better hardware and faster algorithms.

The leading computational materials science tool in the US today for concrete is the Virtual Cement and Concrete Testing Laboratory (VCCTL), which is being developed at NIST with the active cooperation of six leading corporations and associations in the concrete field: the Ready-Mixed Concrete Research and Education Foundation, the Federal Highway Administration (FHWA), BASF, Mapei, Sika Technology AG, and W.R. Grace. This large, integrated software package mimics a complete physical testing laboratory, with databases of cement and aggregates instead of bins and hoppers, material combination and concrete curing models instead of mixers and molds, a software interface instead of a cart to take materials and samples around the laboratory, and accurate models for performance prediction instead of instrumented testing machines.

The driving force behind the VCCTL is to be able to reduce the need for much routine testing, especially in the material development process, and make the remaining testing

"smarter" by measuring fundamental material quantities that are needed by these kinds of models to be able to unleash their predictive power. An example of such a "sea-change" for a Portland cement concrete test would be measuring fundamental rheological quantities with a rheometer instead of running (ad infinitum…) empirical slump tests.

To unlock the power of fundamental models, however, requires a higher level of material characterization than has heretofore routinely existed. The VCCTL cement database is a good example of the kind of prerequisite information. In this database, we have not only the cement composition (mass fractions of each mineral component), but we also have the spatial distribution of those minerals in the cement powder, the readily soluble alkali fractions, the particle size distribution and the actual 3-D particle shapes recorded mathematically. Using the information in this database, we can reconstruct cement pastes with prescribed water-cement ratio, composition, volume and surface area fractions, and real particle shapes. The figure below shows a 3-D image of such a paste with a resolution of 1 micrometer, along with an image of the same paste that has been "virtually hydrated" for several hours. This combination of reality and model gives us an extraordinary ability to accurately predict real behavior for portland cement concrete and someday for more complex formulations that include supplementary cementitious materials and chemical admixtures.
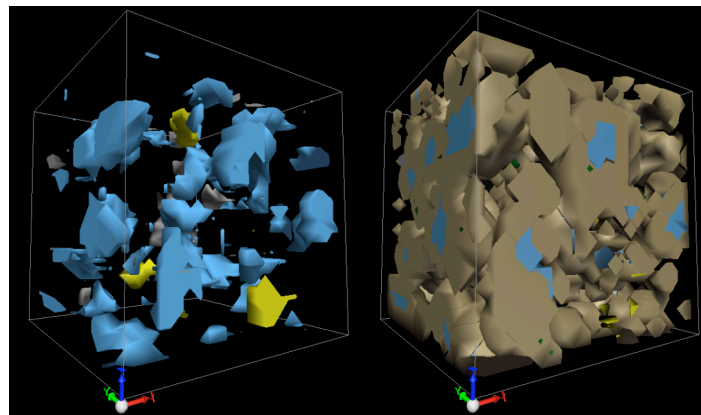
What are the real-world implications of virtual testing? To give one example, NIST researchers have used VCCTL in recent years to simulate the influence of replacing coarse cement clinker particles with a cheap filler such as limestone. Such a mix adjustment would reduce overall cost and also would produce a greener mix (limestone has zero carbon footprint, while clinker generates about 1 metric ton of carbon dioxide for each ton of clinker). But would such a change compromise concrete properties? VCCTL simulations helped determine a limestone grading and replacement level that it predicted to have no significant negative impact on the 28-day compressive strength, and subsequent experiments confirmed the accuracy of the virtual tests. (You can find more information on this study at http://concrete.nist.gov/~bentz/cemrepl). As another example, a cement manufacturer in the VCCTL consortium used virtual testing to troubleshoot a cement formulation problem leading to "out of spec" 28-day concrete compressive strength. The VCCTL indicated how to change the clinker chemistry of the cement to bring the strengths back within specifications. Again, only a small number of

physical tests were needed to confirm the prediction, and the company realized over $1M in cost savings by replacing most of the physical tests with virtual tests.

In eight years of cooperative work, VCCTL software has progressed from version 1.0 to version 7.1. The VCCTL is a challenging undertaking, because all its predictions are intentionally based on fundamental materials science and not empirical correlations. Only in that way can the VCCTL be flexible enough and accurate enough to accommodate changes in materials that come about for various reasons, e.g. changes in supply or standards. Although some of the companies in the consortium have made effective economic use of the software already, we expect to have a version that is even more widely usable and practical in a few years. We also hope to develop and release, in 2009, an educational version of VCCTL, eVCCTL, which can be used by students across the US and the world as part of their construction material training.

We are only beginning to realize the potential of applying computational materials science to construction materials. Materials scientists around the world are making great strides in understanding the fundamental physics and chemistry that govern the behavior of cement and concrete. As these new insights are used to construct ever more accurate and sophisticated computer models, and as these modeling tools become more widely used in industry, concrete materials research, testing, and quality control will change dramatically. The scenarios that were listed at the start of this article are only dreams now, but their fulfillment, via computational materials science and the VCCTL, is not that far away.