Virtual Testing of Ready Mixed Concrete

By Jeffrey W. Bullard[1] and Karthik Obla[2]

Besides being one of the most widely used construction materials of the modern era, hydraulic cement concrete is probably the most chemically and physically complex engineering material ever devised. For example, steel and other engineered metals typically are composed of three or four chemical elements distributed over two or three distinct chemical phases. In contrast, the binder of concrete alone, usually based on ordinary portland cement, contains 10 or more chemical elements, excluding chemical admixtures, which are distributed over 10–15 distinct chemical phases or compounds. The chemistry of concrete is further complicated by aggregates, which may be composed of multiple minerals that may or may not react with cement paste. From a micro structural viewpoint, concrete is a random, porous composite with important features that span length scales from nanometers to centimeters. All of these features have direct impact on the engineering properties of concrete. Further complicating the picture is the fact that concrete is processed in place, being cast as a viscous slurry and hardening over time as a result of complex hydration reactions in the binder.

This complexity makes concrete a unique construction material in its versatility, ease of processing and low cost. But a price is also exacted: our understanding of the underlying materials science is far from complete. Why is that important? In “high-tech” industries, such as aerospace and semiconductor sectors, the materials are less complex and their essential physics and chemistry are known. Materials in these industries are frequently designed “virtually” by using faster and less expensive computer models to identify promising formulations. For concrete, though, our incomplete understanding of the fundamental science has made it impossible to

1. Project Leader, Virtual Cement and Concrete Testing Laboratory,
Materials and Construction Research Division, NIST, Gaithersburg, Maryland.
2. Director of Research and Materials Engineering, NRMCA, Silver Spring, Maryland.

construct reliable computer models for design and optimization. The result is that mix design and optimization, guided by empirical rules, requires extensive trial-and-error physical testing that consumes large quantities of both materials and labor.

But that situation is now changing. Through support from the RMC Research Foundation, NRMCA is actively participating in a research consortium to accelerate the development and deployment of computer software for virtual testing of concrete. The consortium, called the Virtual Cement and Concrete Testing Laboratory (VCCTL™), is administered by the National Institute of Standards and Technology (NIST) and currently is comprised of NIST and 10 companies or industry organizations worldwide: NRMCA, Cemex Trademarks Worldwide Ltd., Holcim (US) Inc., W.R. Grace & Co., Sika Technology AG, Master Builders Technologies/Degussa, the Portland Cement Association (PCA), the International Center for Aggregates Research (ICAR), Verein Deutscher Zementwerke eV (VDZ) and the Association Technique de l'Industrie des Liants Hydrauliques (ATILH). The goal of the consortium is to develop a virtual testing system, readily used on a standard desktop computer that will reduce the amount of physical concrete testing needed and expedite the research and development process. Concrete performance such as rheology, strength and durability will be predicted from microstructural parameters such as cement physical and chemical properties, aggregate shape, size, curing conditions, etc. In some instances cement paste tests will replace more expensive and time consuming concrete testing. Achieving that goal could revolutionize the way that concrete mixes are designed and optimized.

The development of a virtual testing system is no small task. It requires fundamental scientific research into the physics, chemistry and materials science of concrete. The VCCTL consortium has identified three core competencies that are being addressed: 1) prediction of cement hydration behavior; 2) simulation of the rheological properties (i.e. flow behavior) of fresh concrete; and 3) prediction of the mechanical properties (elastic moduli, compressive strength) of hardened concrete.

The core computational tool for predicting the hydration behavior of cement paste is the NIST hydration model. Developed for the past 13 years, the NIST model generally is recognized as the most sophisticated and accurate model of cement hydration in the world. The model represents a cement paste at the microstructural level (1–100 µm) and simulates changes in the microstructure as hydration proceeds. The microstructure is encoded as a digital image, which enables the model to accommodate the full three-dimensional chemical and micro structural detail of the paste. Sophisticated experimental techniques for characterizing these details on real cements, also developed at NIST, are used to provide input to the hydration model. Full characterization requires knowledge of, among other things, the particle size distribution, the distribution of clinker and sulfate phases among particles and alkali content. An example of a fully characterized portland cement is shown in Fig. 1, with an original backscattered electron micrograph of the cement shown for comparison.

With this kind of three-dimensional chemical and micro structural information available, the hydration model simulates the development of microstructure by applying chemical reaction rules. As the simulation proceeds, the model directly calculates and records a wide range of properties, including heat release, degree of hydration, chemical shrinkage, pH, porosity and setting time.

Because cement hydration governs the microstructure development of the binder, which in turn influences all the physical properties of a concrete, research on hydration is critical for success of the VCCTL effort. Current research is focused on validating the model for a wide range of cements, on refining the kinetic mechanisms used by the model and on using the model to assess the effects of mineral admixtures such as slags and fly ashes.

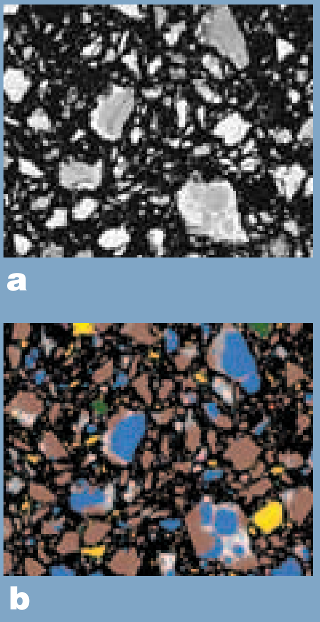
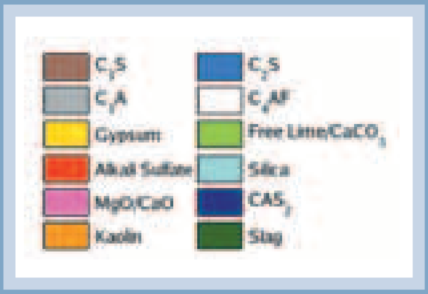


Figure 1. (a) Backscattered electron SEM image of a polished section of cement 140 from the Cement and Concrete Reference Laboratory proficiency sample program. (b) False color image of the same section, based on X-ray microprobe analysis. The meaning of each color is indicated in the accompanying legend. Images are 256 µm x 256 µm



The rheological properties of fresh concrete determine its workability, pumpability and finishability. Concrete flow properties are measured using field tests such as slump or using concrete rheometers. Complicating the issue is the fact that different types of rheometers measure different values for the viscosity of the same concrete mix and until recently it was unclear how these measurements on different rheometers could be related.

In response to this, VCCTL research on rheological properties is proceeding along two complementary paths. First, the measurement of fresh concrete flow is being placed on firmer scientific ground by developing standard, repeatable methodologies for testing mortars and concrete. These methodologies can be used to cross calibrate different concrete rheometers. Second, state-of-the-art computer models are being developed and tested for calculating flow behavior. These computational models currently are being used to predict the relative viscosity of concrete, i.e. the viscosity of fresh concrete relative to the mortar. In keeping with the philosophy of the VCCTL, the flow models incorporate three-dimensional, real-shape coarse aggregates and then directly track their motion under shear stress as they interact with the binder and with each other. The models are used to simulate flow under various geometries such as flow between rebars under gravity (self-compacting concrete) or in concrete rheometers (Figure 2). This approach will help in the optimization of concrete composition and fundamental understanding of the factors affecting concrete flow.

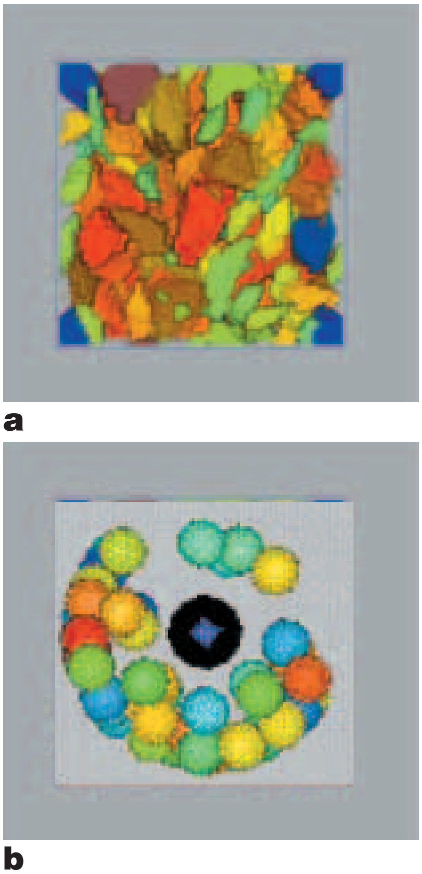


Figure 2. Static images from simulations of a) vertical flow of real particles through a system (grid) of four steel reinforcing bars, and b) flow of a suspension of spheres in a model rheometer with a coaxial geometry. Other visualizations are available at http://math.nist.gov/mcsd/savg/vis/concrete.

Based on these successes and its increasing acceptance by industry, computerized virtual tests are likely to be almost as common in the future as the slump test is today

The third major emphasis of the VCCTL consortium is to predict the mechanical properties of hardened concrete. With knowledge of its microstructure, the elastic properties of a cement paste are computed directly using well-known finite element methods. However, the wider range of important length scales in concrete make that method too computationally intensive to be practical on current desktop computers. Therefore, a different approach called Effective Medium Theory (EMT) is being employed to calculate the elastic properties (Young's modulus, Poisson ratio, etc) of hardened concrete. The EMT approach requires the elastic moduli of the cement paste, which is calculated as already described, and also the volume fraction, size distributions and elastic moduli of the fine and coarse aggregates. The EMT equations provide an excellent estimate of the elastic moduli of concrete and, in contrast to finite element methods, is extremely fast. Moreover, well-established, scientifically based correlations between elastic moduli and compressive strength are used to calculate the compressive strength of a concrete at any age based on the elastic moduli computed by the EMT equations. Once work is completed in these three core areas, efforts would be directed toward linking concrete durability properties to fundamental physical and chemical parameters of the various constituents in concrete.

The VCCTL consortium arrangement is proving to be remarkably effective at driving and accelerating the development of virtual testing of concrete in a way that is relevant and useful to industry. The virtual testing concept is gaining visibility and acceptance in the concrete community at large. The ASTM committees C.01 and C.09 Long-Range Strategic Planning Committee are working to adopt specifications for virtual tests to complement each of its standard test methods covering cement, concrete and aggregates. The American Concrete Institute has hosted several symposia on virtual testing and additional presentations on the concept are slated for the spring 2004 meeting. Based on these successes and its increasing acceptance by industry, computerized virtual tests are likely to be almost as common in the future as the slump test is today.

For more information on virtual testing of concrete or for details about VCCTL consortium, please visit the VCCTL web site at http://ciks.cbt.nist.gov/vcctl. Concrete producers interested in providing input toward the progress of this consortium should contact NRMCA's Karthik Obla at (888) 846-7622, ext. 1163 or by e-mail, kobla@nrmca.org. ■