Virtual Testing of Cement and Concrete—USA 2004

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A unique, multi-phase, random, complex, and composite material, concrete provides both strength and impermeability to engineered structures. Unlike most construction materials, the properties of concrete continue to develop over time and in place—assisting processing and fabrication. Testing and quality assurance, however, become more complicated. For instance, having to wait 28 days to ensure performance compliance is a unique, but not necessarily an attractive, feature of concrete.

Computer models today attempt to reduce the length of this waiting period through the prediction of cement and concrete properties by means of virtual testing. Based upon a detailed characterization of starting materials, such models predict a variety of properties of both fresh and hardening concrete. Successful prediction of properties with virtual testing will result in tremendous time and cost savings to the cement and concrete industry, and will play an important role in enabling the use of performance specifications. Virtual testing will also support the capability to rapidly perform a large number of "what-if" type computations to explore and optimize new material systems.

The successful prediction of properties through virtual testing is the goal of the National Institute of Standards and Technology (NIST)/Industry Virtual Cement and Concrete Testing Laboratory (VCCTL) consortium. Its members currently include two NIST laboratories (Building and Fire Research and Information Technology) and nine industrial members: Holcim (US) Inc., International Center for Aggregates Research, Portland Cement Association, National Ready Mixed Concrete Association, Sika Technology AG, Verein Deutscher Zementwerke eV, W.R. Grace & Co., Degussa/Master Builder Technologies, and Association Technique de l'Industrie des Liants Hydrauliques. A report on the progress of this consortium's work follows, along with a general overview of what virtual testing of cement and concrete actually is and what it aims to accomplish.

WHAT IS VIRTUAL TESTING?

Virtual testing is a fashionable name, given the ubiquity of "virtual" anything and everything around us today. But, what does it really mean in reference to cement and concrete materials? In condensed-matter physics, properties of simple materials are measured at a fundamental level. These measurements are then compared to quantitative predictions from condensed-matter theory that is based on valid mathematical principles applied to well-characterized atomic and molecular arrangements. In materials science, however, more complex materials are studied. These include random composites, biological materials, and concrete. For these and others like them, it is not possible to undertake analytical calculations. Thus, the field of computational materials science has been developed with the necessary condensed-matter mathematics solved on computer. Consequently, the virtual testing of cement and concrete is just computational materials science applied to cement and concrete.

An ideal model for concrete would be one that starts from the known chemical composition of the material. Beginning with the correct proportioning and arrangement of atoms, the modeling effort would build up the needed molecules, then the nanostructure and microstructure, and would eventually predict properties at the macroscale level. This idealized model, however, is still a long way off even with modern-day computers.

Science-based virtual models that do exist need high-quality data as input that emanate from careful characterization of the materials. The models can predict physical properties of interest to actual materials users, but are based on fundamental parameters and not on empirical testing. For example, measuring the Blaine fineness as a characterization of a cement powder does not provide useful data for a model. On the other hand, careful measurement of the cement particle size distribution (PSD) by, for example, laser diffraction

does give particle-level information vital to the successful modeling of how the cement hydrates and develops microstructure.

A functional VCCTL actually increases the need for physical testing and standards. Firstly, property predictions for a model can only be as good as the characterization of the starting materials. Thus, standardizedmethods for preparing and analyzing such materials will be critical. Secondly, measurements of fundamental properties are needed to validate the predictions. The VCCTL procedures will not eliminate standard tests, but will reduce their number. At the same time, the procedures will drive such testing away from empiricism to a firm basis in materials science.

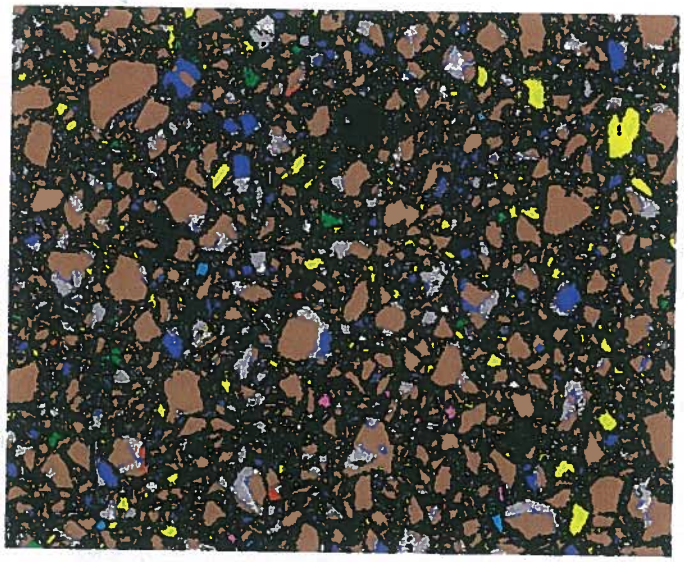

Fig. 1(a): This "false color" image, produced by scanning electron microscopy and x-ray microprobe analysis, illustrates the various chemical phases in individual cement particles. The image has been enlarged from its real size of 256 x 200 µm (10 x 8 mil)

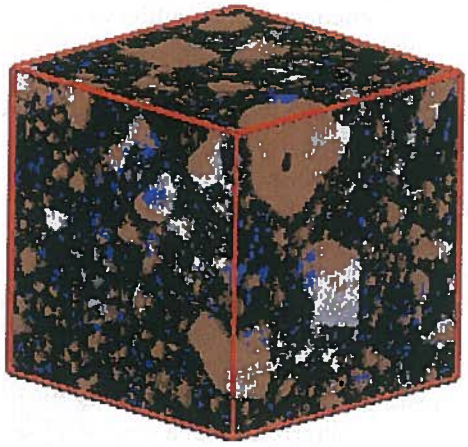

Fig. 1(b): This false color, three-dimensional image shows virtual cement particles mixed in water just prior to the start of hydration. The image is a cube, 100 µm (4 mil) on each side

IMPORTANT MATERIALS CHARACTERIZATION

The VCCTL models start at the level of the cement and mineral admixture particles. At this level, the most important needs include the cement PSD and where the various chemical phases of the cement are distributed within the particles. Accurate bulk measures of a cement's chemical phases using the Rietveld analysis of x-ray diffraction data, combined with particle-size distribution information, can capture most of the information necessary for experimental characterization of a cement's properties of hydration. Because cement hydration takes place at the individual particle level, correct particle level information is needed as input into the VCCTL virtual hydration model.

Use of a combination of back-scattered electron scanning electron microscopy (SEM) and x-ray microprobe analysis will identify the chemical phase belonging to each subregion (pixel) of each cement particle examined. Figure 1(a) displays, in false coloration, an image of cement particles after all of the major chemical phases have been identified. Cement databases containing this kind of information are being systematically built up and incorporated into the VCCTL software package. Figure 1(b), on the other hand, shows in a three-dimensional display how virtual particles, with realistic chemistry and shape, are arranged in a model cement-paste microstructure just prior to the start of hydration.

Aggregate in concrete, both fine and coarse, can be of many different mineralogical types, and is sieved or crushed to the desired size distribution. The aggregate's internal porosity, water absorption, mineralogy, and mechanical properties can vary greatly depending on its type. While these properties can be measured, to make a virtual concrete one must generally use aggregate having realistic shapes. For predicting some properties, such as chloride diffusivity, the shape of model aggregate does not seem to matter much. For other properties, however, like fresh concrete rheology and mechanical properties—especially at early ages—aggregate shape does mean a lot. Few standard tests address aggregate shape; none attempt to characterize the full three-dimensional aspects of aggregate shape necessary for understanding and predicting its effect on concrete properties.

The shape of real aggregates can be characterized by a combination of x-ray computed tomography and mathematical analysis. Figure 2 depicts a virtual reality modeling language (VRML) picture of a fine and a coarse limestone aggregate obtained from one of the proficiency samples of the American Materials Reference Laboratory (AMRL). Association of State Highway and Traffic Officials (AASHTO). Databases are currently being augmented for various aggregates and incorporated into the VCCTL software. Similar techniques can be employed to characterize cement particle shape. Cement particles

(usually about 10 to 20 μm [0.4 to 0.8 mil] in size) require x-ray microtomography to reach the diminutive length scales of approximately 1 μm (0.04 mil) per voxel necessary to capture their shape (a *voxel* is the term for "volume pixel," the smallest, identifiable box-shaped part of a three-dimensional digital image). Still, the three-dimensional shape of the very finest cement and admixture particles, 1 μm (0.04 mil) or less, cannot be so captured at the present time.

VIRTUAL TESTING OF CONCRETE

Testing of concrete performance starts with measuring concrete rheology, the assesment of how concrete flows into prepared forms before the setting point is reached. The well-known slump test is an empirical measurement of how concrete will flow in a given situation.

Work in the last few decades clearly indicates that concrete rheology must be characterized by at least two parameters: yield stress and plastic viscosity. The slump test only measures the yield stress. But plastic viscosity is needed as well to fully understand and predict the rheology of concrete, which in turn determines the workability and flowability of the material.

Because concrete is a mixture of materials crossing many length scales, spanning from micrometer-sized cement grains up to coarse aggregates 20,000 times larger, rheological investigation involves a multi-scale approach. The rheology of the cement paste greatly influences the time-dependent rheology of the concrete, and is itself non-Newtonian and complex in its physical attributes. Concrete's large fraction of aggregates, 60% or more (by volume), also has a very large effect on its rheology. Simultaneous modeling of the hydration process and cement paste rheology is beyond current computational capabilities. Therefore, a combined theoretical-experimental approach has to be taken. As a consequence, cement paste and mortar rheology is measured in a rheometer.

The effect of coarse aggregate on concrete rheology is modeled using a dissipative particle dynamics (DPD) approach. This is similar to a molecular dynamics technique for depicting the movement of atoms and molecules, but adapted instead for coarse-aggregate-sized particles. Figure 3 illustrates using the DPD model to show how realistic coarse aggregate particles arrange themselves under mixing forces. The rheological properties of the matrix of the suspension in Fig. 3 are supplied from cement paste and mortar measurements.

Experimental measurements of concrete rheology use different concrete rheometers. Several of these different designs are available, and test results are being compared in a current program sponsored partly by ACI. DPD simulations can analyze flow in different rheometer designs and extract fundamental parameters from empirical test results. Extracting fundamental rheological parameters like plastic viscosity and yield stress from such experimental measurements will permit their use for analyzing and predicting concrete flow under field conditions. Figure 4 plots the results of experimental and DPD simulations for relative viscosity of a concrete versus the volume fraction of coarse aggregate. Relative viscosity is the plastic viscosity of the concrete divided by the plastic viscosity of its mortar matrix. Figure 4 reveals good agreement between modeling and experimental results, with relative viscosity increasing as more coarse aggregate is added. There has also been work with DPD modeling undertaken

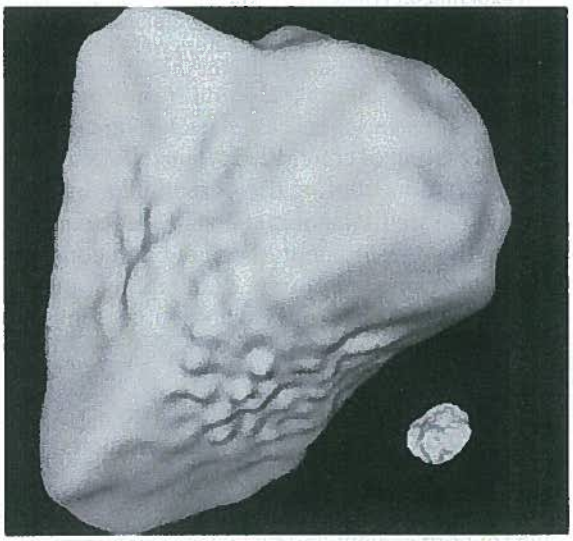

Fig. 2: Reconstructed VRML images of aggregates taken from AMRL proficiency samples. The large coarse aggregate (limestone), at left, is about 13 mm (1/2 in.) in size, and the fine aggregate (river sand), lower right, is about 1.5 mm (0.06 in.) in size

Fig. 3: A dissipative particle dynamics (DPD) simulation of coarse aggregate in a mortar matrix flowing under mixing forces

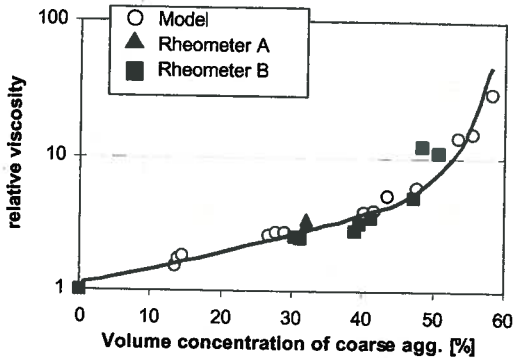

Fig. 4: Comparison of results using dissipative particle dynamics (DPD) with experimental rheometer data relating the dependence of relative viscosity of fresh concrete on the volume fraction of coarse aggregate. Two different rheometers were used. The solid line has been drawn in only as a guide for the reader's eye

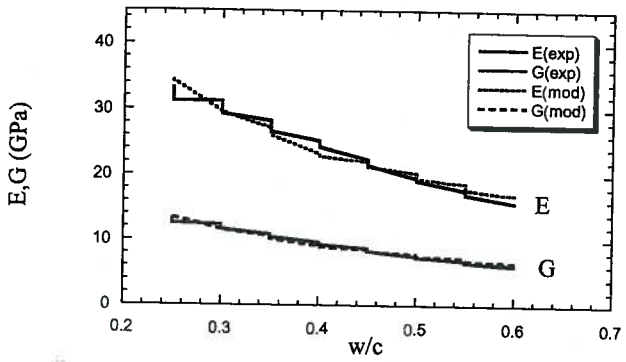

Fig. 5: Comparison of dynamic elastic moduli (Young's modulus E, shear modulus G) virtual testing predictions (dashed lines) to experimentally generated data (solid lines), versus *w/c*, for 28- and 56-day specimens of cement paste. For each *w/c*, the upper plot is for 56-day values and the lower is for 28 days. Note: 1 GPa = 145 ksi

for empirical testing of concrete flow in self-compacting concrete (SCC), thus offering the potential for basing these tests on more fundamental materials science.

To model the development of cement and concrete properties over time, a proper understanding (and model) of the hydration process is essential. While a complete understanding of cement hydration is still lacking, a significant knowledge base for it has been accumulated over the past 100 years of experimentation. The two most influential parameters for predicting properties of cement and concrete are water-to-cement mass ratio (*w/c*) and degree of hydration. If degree of hydration (of both cement and pozzolans) can be accurately predicted, many other properties can also be computed. The VCCTL hydration model operates on three- dimensional packings of cement particles having realistic shapes and chemical phase compositions, as was shown in Fig. 1(b). The model dissolves portions of the particles involved, allowing them to react with the surrounding water to produce a hydrated three-dimensional microstructural image of cement paste, where each three-dimensional voxel is occupied by a unique phase of the cement paste.

A hydrated image thus generated can be used to compute various property values, including set point, heat generation and temperature rise, chemical shrinkage and self-desiccation, and ionic diffusivity. In addition, values for mechanical properties can also be calculated. By treating each voxel as a tri-linear finite element, the overall elastic moduli of the cement paste model can be directly computed by using finite element techniques. Recently, investigators undertook careful testing of this combined algorithm. Figure 5 compares model and (experimental) dynamic moduli results for 28- and 56-day-old cement paste samples, graphed as a function of *w/c*. As can be seen, there is excellent agreement between virtual and experimental results for cement paste. Effective medium theory can then compute the contributions of the aggregates and any accompanying interfacial transition zones to the concrete elastic moduli. The effect of aggregate shape is taken into account quantitatively. This prediction for concrete is being validated at present.

Compressive strength is used more in the cement and concrete industries than is elastic moduli. Employing materials science to directly and fundamentally calculate compressive strength based on microstructure is a topic of research at present. The goal is to develop a multi-scale strength of materials technique that can give accurate, microstructure-based predictions of compressive strength. In the meantime, several semi-empirical approaches are possible for the prediction of compressive strength. The first is (based on) Power's gel-space ratio theory. The VCCTL cement hydration model can directly calculate this parameter using the theory, and for any degree of hydration for either portland or blended cements. With at least one experimental measurement of early-age compressive strength to calibrate the parameters of this semi-empirical theory, compressive strength can then be estimated at later ages. Normally, either a 3- or 7-day strength measurement is performed and the resulting strength prefactor is used to predict the 28-day and later strength.

While originally developed for portland cement systems, the theory has recently been applied successfully to blended cement systems. It would be preferable to predict compressive strength development directly without requiring an early-age measurement. Still, the previously mentioned procedure can result in considerable time and cost savings because it reduces the 28-day evaluation window to either 3 or 7 days.

Because elastic moduli development can be accurately predicted with VCCTL software, another semi-empirical approach for predicting compressive strength is to first compute elastic moduli. Compressive strength is then estimated based on a functional relationship between it

and elastic moduli. A convenient empirical equation relating Young's modulus and compressive strength, resulting from many experimental results, can be found in ACI 318.

An important area for virtual testing is the durability of concrete since conventional test methods tend to be very time consuming. Investigators are considering degradation mechanisms at the microstructural level, and the most recent versions of the VCCTL program permit simulations of sulfate or chloride attack at the level of the cement paste's microstructure. Discussions have also taken place about linking the VCCTL to the SUMMA™ durability project, headed by Jacques Marchand of Laval University, to bring durability prediction more closely into the scope of the VCCTL.

FUTURE PROSPECTS

While this article illustrates what virtual testing is and the wide variety of cement and concrete properties that can be predicted and studied using virtual testing at this point in time, there are still 2 more years left in Phase II of the VCCTL consortium. Thus, there will be continuous improvement beyond what is described here. The computer modeling efforts of recent years have clearly pointed out the need for new materials characterization standards and test methods. The performance of the modeling depends critically on high-quality input about the materials in question. Quantitative standards of high quality are also required for the experimental validation of the computer models. The models can only be proved, disproved, and improved based upon comparison to carefully measured experimental results.

Advances in the use of polymers, metals, ceramics, and pharmaceutical materials have been driven by the development of sufficient understanding of materials science to help explain puzzling experimental results, to point the way to new experimentation not thought of previously, and to optimize the manufacture and use of materials. Theoretical (or virtual) understanding of such materials have given their designers a whole new level of control that has lead to improvements and new opportunities for further advancement. Virtual testing, the authors believe, can and will supply the same benefits for cement and concrete manufacturers and users.

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Selected for reader interest by the editors.

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