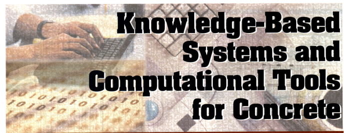
Knowledge-Based Systems and Computational Tools for Concrete



by Edward J. Garboczi, Dale P. Bentz, and Geoffrey J. Frohnsdorff

Within the Building and Fire Research Laboratory at the National Institute of Standards and Technology (NIST), the HYPERCON Partnership for High Performance Concrete* Technology [(PHPCT) http://ciks.cbt.nist.gov/phpct/] program is working to develop the materials science knowledge necessary for making high-performance concrete (HPC) a usable, well-understood, and durable material, thus enabling the reliable application of high-performance concrete in buildings and civil infrastructure. This work involves the combination of experimental and computational materials science research, that is needed to address the complex nature of concrete.

The delivery of the output of this research is focused on developing computer-integrated knowledge systems (CIKS), that are a synergistic combination of databases, models, and computational tools. This article describes the current status of such systems presently available for use by concrete technologists.

The NIST research that is going into the computational systems and tools to be described in this article is divided into six themes within HYPERCON:

1. Processing of HPC — addressing methods for selecting and proportioning ingredients, determining the rheological properties, and selecting the mixing, placing, and consolidation procedures and the curing conditions to ensure a product of the desired performance and uniformity;
2. Characterization of concrete and concrete materials — providing techniques needed for characterizing the composition and properties of concrete materials, and the composition, structure, and uniformity of an HPC produced by any process or from any source;
3. Performance prediction — developing a suite of models for simulating and predicting transport and other durability-related properties of HPC;
4. Structural performance of high-strength HPC in a fire — developing methods for predicting the effects of fire on the performance of high-strength HPC;
5. Structural performance — providing knowledge needed to allow for more rational use of HPC and taking account of its performance; and
6. Economics of HPC — developing models for calculating the life-cycle costs of HPC in civil infrastructure applications, beginning with bridge decks and then proceeding to other structures.

Clearly, NIST research alone cannot generate all the knowledge that is needed to go into the CIKS systems. The remainder of the knowledge that is needed must be generated by partners from industry and government who have joined with NIST in HYPERCON. Partners include the Portland Cement Association; Holnam Inc.; Lafarge; Dyckerhoff; Cemex; the Federal Highway Administration; Fibermesh Co.; W.R. Grace and Co.; Master Builders Technology; and the National Ready-Mixed Concrete Association. New partners are always welcome and can contact: geoffrey.frohnsdorff@nist.gov; edward.garboczi@nist.gov; or dale.bentz@nist.gov.

An early CIKS was designed to predict the chloride diffusivity and service life of plain portland cement concrete where corrosion of the steel reinforcement is the major degradation mechanism.[1] This article describes new systems, such as the Virtual Cement and Concrete Testing Laboratory (VCCTL), which is a CIKS that integrates many NIST models into a seamless package for using computational models to hopefully replace much of the testing that is done to develop and verify new concrete mixtures. Other available computational tools are also described.

The Virtual Cement and Concrete Testing Laboratory

Figure 1 shows a schematic view of the structure of the VCCTL. This is a computer-based virtual laboratory whose

* ***High-Performance Concrete*** (HPC) is concrete that meets special combinations of performance and uniformity requirements that cannot always be achieved routinely using conventional constituents and normal mixing, placing, and curing practices. Thus, a high-performance concrete is a concrete in which certain characteristics are developed for a particular application and environment. Examples of characteristics that may be considered critical in an application are: ease of placement, compaction without segregation, early age strength, long-term mechanical properties, permeability, density, heat of hydration, toughness, volume stability, and long life in severe environments. *(Editor)*

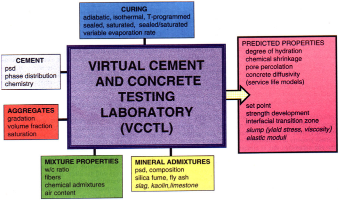


Fig. 1 — Schematic overview of the structure of the Virtual Cement and Concrete Testing Laboratory. Italics indicate a capacity that is planned but not currently available.

goal is to reduce the number of physical concrete tests, whether for quality assurance or for expediting the research and development process. Many of the models developed at NIST over the last 10 years are at the stage where their predictions are quantitative and accurate. Many standard tests can be replaced by computer models right now and many more may be replaced in the future, so that, for example, a cement company that develops a new cement will be able to immediately predict many facets of the performance of concrete made from the new cement. Models available now can handle the effects of:

1. Different kinds of curing, which involves cement particle-size distribution and composition, mineral admixtures, and temperature and moisture conditions; and

2. Aggregates, which include the particle-size distribution (as given by a sieve analysis), volume fraction, degree of saturation, and shape.

These models can now, or soon will be able to, predict degree of hydration, chemical shrinkage, heat release, diffusivity, set point, strength development, elastic properties, and slump (yield stress and plastic viscosity). Databases are also becoming available for using the cement hydration model for various cements, which are an important component of the VCCTL (http://ciks.cbt.nist.gov/phpct/database.html).

The earlier CIKS for predicting chloride diffusivity of concrete has been integrated into the VCCTL. The VCCTL consists of a WWW-based menu-driven interface (front end) that controls the execution of the underlying models and returns plots of the quantitative results back to the user. Version 1.0 of the VCCTL will be available by the time this article appears (http://vcctl.cbt.nist.gov). A consortium of industrial companies is being formed to do the computational and experimental research needed to improve and extend the VCCTL to make it more powerful and usable.

Other computational tools

Electronic Monograph

The VCCTL will incorporate, as a key part, many sophisticated materials science models. To be able to use it as more than a black box, however, there must be a strong education component available to any user. This component is the Electronic Monograph.[2,3] This is a web site set up like an electronic book, with chapters and sections, organized by a linked table of contents. Right now, the text in this monograph is the equivalent of over 1900 pages of single-spaced, 12-point-font text. The monograph covers most of the computer modeling work on concrete carried out at NIST over the last 10 years (and some of the experimental work) and could be classified as a virtual textbook on the computational materials science of concrete (http://gemini.tntech.edu/~jbiernacki/Multi_Scale_Syllabus.html). It is regularly revised so as to stay up to date with new research developments at NIST, which is the world leader in the computational materials science of concrete. Many programs, written primarily in C and FORTRAN 77, are available for downloading. Planned growth of the monograph in the year 2001 includes the addition of more educational software and incorporation of an electronic index (search engine).

4Sight Software

Research conducted for the Nuclear Regulatory Commission over many years has resulted in the development of a software package called 4Sight,[4] which incorporates the materials science of concrete degradation into a computational tool for predicting the service life of underground concrete vaults for storage of low-level radioactive waste. This package unites the chemistry and transport properties of concrete to give estimates for how long a concrete vault will serve as an effective barrier for the containment of radioactive waste.

At present, 4Sight is being validated experimentally and modified to allow for the effects of cracking. Proposed work involves including more radionuclide-chemistry.

Concrete Optimization Software Tool (COST)

A concrete specifier or researcher may want, with a given concrete system, to choose the components that optimize a certain property or combination of properties. For more than one parameter, this is almost impossible to do by trial and error. The preferred way to do the optimization is to conduct a statistically designed experiment, analyze the results, and quantitatively predict where the optimal point will be. Many concrete technologists do not have expertise in the statistics of designed experiments, which is why COST (Concrete Optimization Software Tool) is being developed under Federal Highway Administration auspices (http://ciks.cbt.nist.gov/~bentz/fhwa/homepage.html).

COST is an on-line design/analysis system, whereby concrete specifiers and researchers may compute optimal settings of mixture proportions for concrete. It does this by specifying a statistically designed experiment for the user, and then, after the user carries out the experiments, analyzing the results and giving the optimal settings of the parameters that were varied.[5]

The inputs to COST include:

1. Desired performance criteria (1 to 5 criteria);
2. Desired number of variable mixture components (2 to 5 components); and
3. Desired limits on the proportion of each component.

The outputs from COST include:

1. An optimal experimental plan for the analyst to run to determine the best proportions;
2. An optimal statistical analysis of the data (after the analyst has run the plan); and
3. The optimal concrete mixture proportion settings, along with values of the performance criteria at these best settings.

Concrete Microscopy Library

The Concrete Microscopy Library is a new web site that contains micrographs and captions that cover many aspects of concrete microstructure (http://cee.ce.uiuc.edu/lange/Micro/). It is a resource for students and professionals who are interested in the microstructure of cement-based materials. The images have been gathered mainly from the collections of Paul Stutzman of NIST and David Lange of the University of Illinois at Urbana-Champaign, although they welcome contributions from other researchers. This web site is an educational tool and, as such, it serves a complementary purpose to the Electronic Monograph by providing pictures of real microstructures with which to compare model results.

Other tools

Two other computational tools have recently become available. The first is a tool for properly proportioning a lightweight aggregate component of a concrete mixture design to aid curing and minimize the effects of self-desiccation and autogenous shrinkage, which are a significant problems for low water-cement ratio (*w/c*) high-performance concrete materials.[6] The second is a tool that helps examine a concrete mixture to evaluate its susceptibility to spalling in fire conditions.[7]

VCCTL, CIKS, Computational Tools, and ACI

In addition to its practical uses, the VCCTL is intended to be an example of the way knowledge of concrete technology could be disseminated in the future. In the U.S., the main source of information on concrete technology is ACI and will remain so for the foreseeable future. Therefore, NIST is working with ACI and its committees to encourage and facilitate the dissemination of future ACI committee documents in the form of interoperable computer-integrated knowledge systems, rather than as simple hard copy and CD-ROM representations of knowledge.

At the same time, NIST is striving to increase recognition within ACI of the benefits of providing concrete technology, as represented in the committee documents, with a strong basis in materials science, and reducing dependence on empirical knowledge. For example, NIST played a major role in the recommendations that led to the establishment of ACI Committees 126, Database Formats for Concrete Materials Property Data; 235, Knowledge-Based Systems and Mathematical Modeling of Materials; 236, Materials Science of Concrete; and 365, Service Life Prediction; and in organizing the Workshop on Cement and Concrete Standards of the Future,[8] of which ACI was a cosponsor.

Also, NIST has recently proposed that several ACI materials committees should cooperate with Committee 235 in a pioneering effort to make a substantial body of information on concrete materials available in a coherent form as an interoperable computer-integrated knowledge system. There seems little doubt that the benefits would be great in making reliable and comprehensive knowledge available in a user-friendly format that could be interrogated by the user to almost any depth desired.

Training

Training in the use of these CIKS and computational tools, and in how they work, so that they are not a black box is provided in the annual ACBM/NIST (ACBM = Center for Advanced Cement-Based Materials) Computer Modeling Workshop. The Year 2001 workshop will be Jue 11-14. This is a four-day workshop, or tutorial, that provides intensive lectures on the materials science behind these models. This workshop would be beneficial for concrete technologists working in the areas of either modeling or experimental investigations dealing with cementitious composites.

Acknowledgments

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Selected for reader interest by the editors.

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This article is based on a presentation made at the 1999 ACI Fall Convention, in Baltimore, Md., during the technical session on "Computerized Knowledge Bases for Concrete," sponsored by ACI Committees 235, Knowledge-Based Systems and Mathematical Modeling for Materials, and 126, Database Formats for Concrete Materials Properties (now discharged).

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