Computational Materials Science on the Internet

by Edward J. Garboczi and Dale P. Bentz

The main idea of materials science is to create a material with desired properties by using processing to obtain a microstructure that will have those properties. This is carried out using a combination of experimental and analytical tools. However, a complex random material like concrete requires something more — computational materials science.

Computational materials science is essentially just materials science, except that computers are used to simulate and analyze microstructures and predict properties, in addition to doing experiments and solving analytical equations. This article describes an electronic monograph designed to present the background, techniques, and results to date in the computational materials science of concrete.

Computational materials science is a modern discipline, developing over the last 20 years because of the revolutionary advances that have been made in computer processing speed and memory capacity. Computational materials science is computers applied at the microstructural level, complementary to the already widespread use of computers at the structural scale, in finite element packages. The main application of computational materials science is to materials that have complex random microstructures, like concrete, which defy ordinary mathematical analysis. And concrete, in particular, has a *different* complex random microstructure at different length scales.

At the nanometer (10^{-9} m) length scale, the calcium-silicate-hydrate cement hydration product, the gel that holds concrete together, is a porous random material. At the micrometer (10^{-6} m) scale, cement paste is a different random porous composite material, made up of several different solid phases and capillary pores. At the millimeter (10^{-3} m) scale and above, concrete is another complex composite material made up of different size and shape aggregates, cement paste, and a complicated porous interface connecting the two, all randomly mixed together. So when trying to optimize concrete properties based on microstructure, the discipline of computational materials science is really needed.

In the 1990s, one of the main centers in the world for the computational materials science of concrete has been the National Institute of Standards and Technology (NIST), Gaithersburg, Md. Models of the microstructure and properties of concrete have been developed at all length scales of interest. Attempts have been made to link these models together to predict concrete properties as a function of mixture design, curing, and environmental exposure.[1-3] As part of the development of a Computer-Integrated Knowledge-Based System (CIKS) for building materials,[3,4] a monograph has been developed[5] that attempts to summarize and make available the current state of knowledge of the computational materials science of concrete. At present, the monograph focuses on the work done at, or in collaboration with, NIST. But many people outside of NIST have also contributed to the work, and are acknowledged within the monograph.

To aid in wider availability, this monograph has been prepared in electronic HTML format so that it is accessible via the Internet. It was prepared this way directly, rather than being written first as a book, and afterwards converted into HTML. Many parts are in color, which are easy and inexpensive to produce using the Internet, but still rather expensive in paper media. It

Chapter 1. Introduction
Chapter 2. Composite materials ideas, manual for finite element and finite difference algorithms
Chapter 3. Percolation theory
Chapter 4. Microstructure development of cement paste phases
Chapter 5. Cement paste percolation, transport, and elastic properties
Chapter 6. Mortar and concrete microstructure
Chapter 7. Transport and elastic properties of mortar and concrete
Chapter 8. The viscoelastic properties of concrete
Chapter 9. Modelling the degradation of mortar and concrete
Chapter 10. Sintering and curvature simulations
Chapter 11. General modeling: Electrical conductivity and fluid permeability, elastic properties, and mercury porosimetry

Appendix 1. Summary of concrete and concrete modelling for non-cement-based materials researchers
Appendix 2. Guide to Using CEMHYD3D: A three-dimensional cement hydration and microstructure development modelling package
Appendix 3. Digital images of porous materials and computer modelling: Description of a digital tool kit

Fig. 1 — Table of contents of the monograph.

is not designed to be printed out in its entirety to be read, but should be read with a browser directly at the website. Short parts can of course be printed out for reference, easier reading, etc. [5]

As can be seen in the table of contents (Fig. 1), the monograph, which is presently about 800 pages long with hundreds of figures, is quite comprehensive. It starts off with general ideas about random materials and then goes more explicitly into the details of concrete microstructure and properties. The main source of text in this monograph has been published papers. The monograph is more than just a collection of old research papers, however, although even that would be useful, as research results for a single area are often scattered among many different journals.

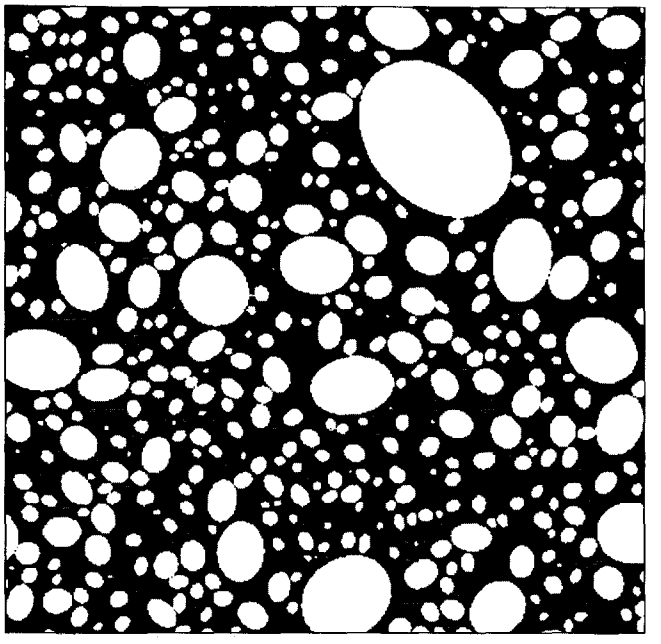

Fig. 2 — Example of a simple model for concrete, taken from the monograph. Gray is cement paste, white is aggregate, and black is the porous cement paste interface connecting the two phases.

In each chapter, text is arranged by sections, with an introductory paragraph for each section. For every section, there is a statement of approximately how many pages of text and how many bytes of figures there are for that entry. In each section, there are links going forward and backward to the next part of the section, as well as links going back to the chapter itself or the table of contents. The text itself is linked together via the references in each section.

A sample of what can be found in the monograph, Fig. 2 is a 2-D slice from a simple 3-D model of concrete, where ellipsoids were used to try and capture the shape of real aggregates. The aggregates are shown in white, the cement paste in gray, and higher porosity cement paste areas that connect the aggregates to the cement paste matrix are shown in black. Multiscale models of the chloride diffusivity of concrete have been developed based on more complex versions of this model.[1-3] These models and their application are all described in the monograph.

Since concrete is a prototypical random composite material, there is much that those who work primarily with other materials can learn from concrete. Many of the modelling techniques are also quite general, and can be used effectively on other random materials. For this category of reader, an appendix (Appendix 1) is included that introduces concrete as a material and summarizes many of the main modelling results obtained thus far. Appendix 1 can also serve as an appropriate introduction to the computational materials science of concrete for concrete technologists.

It should be emphasized that this monograph is an ongoing document, subject to frequent changes and additions. Old material will be removed when further research updates existing results, and material will be added as new research is completed. Since data quality is an important concern for technical data placed on the Internet, it should be noted that all information in the monograph at present has gone through the NIST internal review process, and all information that will be added in the future will also have been screened by the same review process.

More of the contents of the monograph could be described; it is best for the reader to access and read it directly. The hope is that the monograph will play two important roles:

- As a self-teaching guide to educate students and concrete technologists about the computational materials science of concrete, and
- An easily-accessible electronic resource, offering techniques and results to those doing basic and applied work in the materials science of concrete.

Acknowledgments

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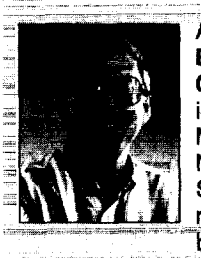
4. Clifton, J. R.; Bentz, D. P.; and Kaetzel, L. J., "Computerized Integrated Knowledge-Based System for High-Performance Concrete: An Overview," National Institute of Standards and Technology, *Internal Report 5947*, U. S. Department of Commerce, 1997.
5. Go to http://ciks.cbt.nist.gov/, and pick the entry marked *Monograph*. Other items of interest to CIKS users can be also found there.
6. For more information, see http://www.civil.nwu.edu/ACBM/

Selected for reader interest by the editors.



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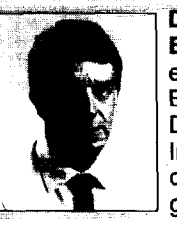

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