# Tools for Improving the Sustainability and Durability of Concrete

## Modeling Hydration and Performance

Exploratory Advanced Research . . . Next Generation Transportation Solutions

How does hydration affect the performance of concrete, including its setting, strength, and durability? Can advanced hydration models be developed that will allow practitioners to input the composition of cement, supplementary cementitious materials, and admixtures, combined with temperature, and receive guidance on a pavement's expected performance? Answering these questions is the goal of the Exploratory Advanced Research (EAR) Program project "Mechanisms of Hydration and Setting of Ordinary Portland Cement in Simple and Complex Systems." Princeton University is conducting this research, which is funded by the Federal Highway Administration (FHWA). Research partners for the project are the National Institute of Standards and Technology (NIST); Oklahoma State University; Rice University; University of California, Santa Barbara; and W.R. Grace and Company.

### Innovations in Measurement and Modeling

Until recently, the primary obstacle to advancing the control of hydration in cement has been the inability to observe, measure, and model the process at the material's length scales, which can range from nanometers to millimeters. This project's innovation is that it focuses precisely on these length scales by using cutting-edge, experimental measurement techniques combined with computer-modeling approaches. Researchers have been conducting the study in two phases: The first phase focused on the mechanisms of cement hydration, including the influence of aluminate and sulfate ions, and the second phase is currently investigating the influence of organic admixtures.

### Cutting-Edge Techniques

For this study, researchers have been using both experimental measurement and modeling to reveal how chemical and surface interactions affect the kinetics of hydration reactions at early ages. The aim of the study is to establish findings that will lead to an unprecedented understanding of which chemical reactions occur, where they occur, at what rate, and how they can be modified. This comprehensive understanding will ultimately enable development of tools that engineers can use to predict the complex physical and chemical processes that control the setting, early-age and long-term strength, and durability of concrete. The end result will lead to important improvements in concrete durability, economy, strength, and sustainability, all of which will lead to better mix designs and longer lasting pavements.

Researchers identified mechanisms to include in the new models by using experimental techniques such as vertical-scanning interferometry, tomography-assisted chemical correlation, and nuclear magnetic resonance spectroscopy. These techniques also provide previously unobtainable data to verify model predictions and to validate models at the nano-, micro-, and macroscopic length scales. During the course of the study, the researchers discovered new breakthrough techniques, which include combining nano-computed tomography and nano-x-ray fluorescent data to gather 3D chemistry data, allowing researchers to obtain even more information from a single scan of concrete materials. Because this technique can be used on a range of materials in which obtaining data on structure and chemistry is important, it holds great promise for the broader x-ray imaging community.

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### Breakthrough Advances

This project's breakthroughs in the measurement and analysis of concrete materials are matched by modeling advances that help researchers better design and interpret experiments. The resulting new understanding of hydration mechanisms and development has been used by the project researchers to improve the HydratiCA model developed by NIST, which is currently the most sophisticated tool for simulating hydration. The improved model will be able to generate both microscale and macroscale predictions of hydration behavior under a much wider range of conditions than previously possible. Researchers have also developed SimBNG, a boundary nucleation and growth model that is powerful but also fast enough and simple enough to be used in the field.

### Gold Standard for Data

The project's data will serve as the "gold standard" of hydration mechanism data for years to come. Following the conclusion of this project, FHWA will make data readily accessible to use in future modeling or experimentation undertaken by other researchers. A user-friendly database will allow researchers to access relevant data by technique, mineral, additive, and other key words. Data will include raw and processed images of concrete microstructures and nanostructures, combined with the techniques and specific settings used to obtain them. Data from the project are already being used to advance today's pavement technology, including contributing to papers that have appeared in such publications as the *Journal of the American Chemical Society, Cement and Concrete Research*, and *Acta Materialia*.

### Importance to FHWA

The 2009 Summit on Cement Hydration Kinetics and Modeling in Quebec, Canada, stimulated the concrete research community to take a fresh look at hydration. U.S. sponsors of the summit included FHWA and the National Science Foundation. Following the summit, NIST and FHWA issued a joint publication outlining their vision for needed research, *NIST Special Publication 1138: Paving the Way for a More Sustainable Concrete Infrastructure: A Vision for Developing a Comprehensive Description of Cement Hydration Kinetics.* This project advances the joint research vision and addresses the modeling needs identified at the summit, including improving the ability of HydratiCA to predict hydration kinetics and infrastructure and developing SimBNG for use in the field. The SimBNG model in particular is a major step forward in meeting FHWA's goal to improve models so that they give field engineers more agility in concrete materials selection and mixture qualification.

EXPLORATORY ADVANCED **RESEARCH**

### What Is the Exploratory Advanced Research Program?

FHWA's Exploratory Advanced Research (EAR) Program focuses on longer term, higher risk research with a high payoff potential. The program addresses underlying gaps faced by applied highway research programs, anticipates emerging issues with national implications, and reflects broad transportation industry goals and objectives. To learn more about the EAR Program, visit the EAR Web site at www.fhwa.dot.gov/advancedresearch. The site features information on research solicitations, updates on ongoing research, links to published materials, summaries of past EAR Program events, and details on upcoming events.

### Learn More

For more information on this project, contact Richard Meininger, FHWA Office of Infrastructure Research and Development, at 202-493-3191 (email: richard.meininger@dot.gov).



Researchers conducted x-ray nano-computed tomography and nano-x-ray fluorescent imaging using the Beamline 26 x-ray nanoprobe at Argonne National Laboratory in Illinois.

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