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Modeling and Assessment of Concrete and the Energy Infrastructure

George Guthrie* and James Carey

Abstract

This is the final report of a two-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). Concrete is an essential component of our energy infrastructure. The characteristics of concrete that determine its effectiveness in any application--be it construction (e.g., roads, bridges, dams) or waste isolation--result from the chemical and structural evolution of the particular concrete structure. Geochemical and mineralogical factors are among the most important, yet most overlooked, controls of this evolutionary process. This project is geared at using a combination of advanced geochemical and mineralogical experimentation, characterization, and modeling (much of which was developed to understand geological systems such as Yucca Mountain) to understand the evolution of concrete in a mechanistic way. Our goal is to develop a systematic approach to problems ranging from premature degradation of concrete to the design of next-generation concretes.

Background and Research Objectives

Improving the durability of concrete is a major national priority. Forty percent of the nation's bridges are structurally deficient or functionally obsolete, and traffic delays caused by inadequate roads will result in \$50B per year in wasted fuel and lost wages (CERF Report 94-5011.E). These are among the reasons that the National Science and Technology Council (NSTC) has singled out concrete in its plan for federal research in construction and building materials.

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These project addresses issues that related to modeling and assessing the durability and lifetime of energy-infrastructure materials including concrete. It is based on our belief that a multi-disciplinary geoscience and materials science approach can provide new solutions to many materials-related problems. Our ultimate goal is to develop a major initiative addressing a wide range of problems related to improved and specialized materials. However, our first step is to develop a program in a particular area related to the deterioration of concrete, the alkali-silica reaction (ASR). ASR is among the most vexing problems in concrete research, and it is responsible for the deterioration of bridges, roads, runways, dams, and other concrete structures. ASR is a major international concern, costing billions of dollars.

ASR results from the interaction of cement phases, pore solutions, and some constituents of the aggregate (principally silica phases). Understanding the mechanisms of ASR is critical to addressing such questions as: Which aggregate constituents will result in ASR? Can the cement chemistry be altered systematically to inhibit ASR? What measures can be taken to halt ASR in existing structures? By answering these questions, we can make a major contribution to improving the durability and lifetime of concrete structures. In addition, we hope to develop a non-invasive approach to monitoring the progression of ASR by adapting geophysical techniques used in the analysis of rock. This is a critical need for effective remediation decisions, which rely on early detection of ASR. Current methods to detect ASR are effective only after ASR has reached late stages (i.e., after cracks appear at the structure's surface) or require damaging the structure by drilling core for analysis.

Traditional approaches to addressing ASR are typically empirical, and the mechanisms by which the reaction occurs have remained elusive. However, federal regulations and the non-availability of prime aggregates have rendered the empirical approach inadequate. A mechanistic understanding of the reaction has become essential so that a predictive model of concrete evolution can be developed. Such a model will allow a systematic approach to predicting how a cement+aggregate+fluid system must be manipulated to achieve any desired final product (e.g., concrete that does not develop ASR). The geological modeling and experimental expertise at LANL can be exploited to

provide such a model, based largely on our expertise at understanding the properties and evolution of geological systems. This represents an innovative approach to solving a problem in concrete—no integrated geological modeling effort has been applied to the problem—and it is an approach that can be easily expanded into many other problems in materials science.

The thrust of this project is to develop a model that explains how ASR develops and progresses and that allows prediction of how this process is affected by changes in the composition of the concrete system. This model will consist of a geochemical modeling component with fine-scale mineralogical mechanisms to reproduce the petrological changes observed in a variety of concrete specimens. Once a successful model is validated, it will enable the prediction of how one can alter the initial cement composition systematically to control the final state of the concrete system. In other words, it will allow the determination of what must be added to cement to prevent ASR for each specific aggregate. Such a model will also represent an important scientific contribution to cement and concrete research.

We have three general applied research goals for this project:

- geochemical modeling of the evolution of a concrete system as a function of various parameters such as initial cement composition, aggregate mineralogy, water and fluid composition, temperature, and time;
- development of alternative methods for the identification of ASR, particularly ones that are environmentally friendly, can be implemented in the field, and can provide early detection of the onset of ASR (which is critical to remediation alternatives); and
- development of a non-destructive method for monitoring the onset and progression of ASR and the fractures that it helps develop.

To accomplish our objectives, we use a team approach and a combination of experimentation and modeling to: (1) determine the mechanisms of ASR, (2) develop a technique to detect ASR at an early stage using a non-invasive technique, (3) propose mitigation strategies, and (4) formulate a model for ASR that allows predictions over the wide range in conditions (e.g., cement composition, aggregate makeup, post-emplacement conditions) that occur for concrete. We intend to show that our

multidisciplinary team approach can work to provide new and better answers to this long-studied problem.

Importance to LANL's Science and Technology Base and National R&D Needs

The principal tactical goals addressed by this project are fundamental research and industrial partnerships. This project takes the innovative approach of applying geological expertise at LANL to solving problems traditionally considered non-geological. Collaboration with industrial partners and transfer of results of this program to the private sector will be a natural outcome of our work.

Hence, one major connection between these project and LANL goals is the development of industrial partnerships. The results of this project will be of interest to any industry associated with the production of concrete (e.g., the cement, aggregate, and ready-mix concrete industries) or with the use of concrete (e.g., the construction industry). Clearly, this represents major potential industrial ties, because concrete is the most common building material.

In addition, several LANL core competencies are embedded in this project, including complex experimentation and measurement; earth and environmental systems; analysis and assessment; and theory, modeling, and computing.

Finally, a potential link to DOE strategic directions involves interests in South Africa. South Africa faces the same problems with concrete and ASR as we do in the United States and its current focus on the development of infrastructure and inexpensive housing suggests an obvious tie with our interest in developing a program in geological approaches to concrete. We have begun to explore this opportunity, and we have identified interest within the South African government and industry. In addition, we are exploring potential funding sources for this particular application.

Scientific Approach and Accomplishments

Our overall approach is to treat concrete like other geological materials (i.e., rocks). We currently are focusing on three research goals as discussed above. Our work primarily involves several proof-of-principle efforts directed at the focus areas.

Most of our major milestones in the first year relate to doing preliminary investigations geared at proof of principle. These are:

- Obtaining core samples of degraded and non-degraded concretes from New Mexico and Iowa to use in bench-scale development of resonance techniques for the analysis of concrete integrity. We anticipate that the laboratory experiments will result in acoustic signals that will clearly differentiate degraded and non-degraded concrete.
- Obtaining similar core samples from concrete structures around LANL, including the potentially deteriorating concrete at the nuclear materials facility. These samples will also be analyzed in the bench-scale apparatus, and we will use these results to identify appropriate structures to use in the development of an in situ field technique.
- Initiating geological analysis of the degraded and non-degraded core. Analysis will involve scanning and transmission electron microscopies, quantitative x-ray diffraction (XRD) analysis (including micro-XRD), and petrological analysis geared at determining reaction mechanisms and at obtaining primary mineralogical and geochemical data on concrete constituents so that our geochemical model can be validated.

As part of scoping activities, we produced an inexpensive and environmentally friendly set of stains that can detect deleterious reaction products. This approach is in contrast to the current method used by highway departments that exploits uranyl acetate. We also obtained promising results using nonlinear resonance ultrasound spectroscopy as a method to evaluate fractures in concrete. We are developing this work in collaboration with the Alliance for Transportation Research (ATR), which recently conducted an independent, external review of our efforts with a national expert panel. The successful review will help our future program development efforts.

In the second year of the project we applied innovative geoscience methods to the development of high-performance concrete having enhanced strength and durability. We used proof-of-principle studies to demonstrate the applicability of geoscience methods to solving long-term problems in concrete. Our initial study addressed one of the most significant issues in concrete durability for the nation and, in particular, New Mexico: the alkali-silica reaction (ASR). This deleterious reaction occurs because of a geochemical

incompatibility between the rock-aggregate and the cement pore fluids. We successfully developed a staining method that allows ASR to be identified in concrete structure and also permits evaluation of the extent and point-of-attack of ASR. This work resulted in a patent application (50% of which has been granted to date); a paper in press; and an R&D 100 award. The test is a significant advance over existing technologies in that it is simple and has already yielded a new understanding of the mechanism of ASR.

We presented this work in a variety of forums including meetings of the Transportation Research Board, International Center for Aggregate, Strategic Highway Research Program (SHRP) High-Performance Concrete, and SHRP ASR; and in presentations to state departments of transportation (including Iowa and New Mexico) and the Federal Highway Administration. The response has been very positive and potential sponsors also expressed significant interest in other research programs we presented including a new nondestructive evaluation technique that uses nonlinear acoustic spectroscopy to reveal ASR and the development of high-strength and high-durability concrete using supercritical CO₂ treatment.

Publication

George D. Guthrie, Jr. and J. William Carey, "A simple, environmentally friendly, and chemically specific method for the identification and evaluation of the alkali-silica reaction," *Cement and Concrete Research* **in press** (1997).