Model-Based Simulation of Durability of Materials and Structures

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Insufficient long-term durability of civil engineering infrastructure, especially concrete structures, has been a major problem causing enormous economic loss to many countries. Concrete structures are plagued by reinforcement corrosion, cracking due to drying shrinkage and nonuniform creep, alkali-silica reaction, sulfate attack, carbonation, leaching, freeze-thaw, etc. Short-term resistance of concrete structures exposed to fire has become a major question for high-strength concrete in recent years. At the same time, it would be highly beneficial to devise ways of incorporating into concrete certain industrial wastes, such as blast furnace slag and crushed bottle glass from curbside recycling.

A rational approach to all these problems requires realistic mathematical models and computer simulations of chemical reactions, diffusion processes for heat and transport of various chemical agents, expansive processes in the microstructure, and fracture and long-term deformations of the material. Since durability problems generally involve large uncertainties, stochastic modeling and predictions of statistical scatter are very important.

The durability problems represent a major challenge for mathematical modeling. The diffusion processes involved are generally nonlinear and coupled. Along with the diffusion process, complex chemical reactions take place at reaction fronts as well as in the bulk. Characterization of reaction rates as functions of pressure, temperature, and concentrations can be accomplished only by comprehensive models, which must capture capillarity as well as adsorption phenomena on the surfaces of nanopores, calling for the use of surface thermodynamics aside from bulk thermodynamics. In addition, volume changes caused by chemical reactions, surface adsorption, etc., are sensitive to pressure, and the volumetric changes result in damage in the form of distributed microcracking. In the case of chemical reactions on surfaces, the reaction rates depend not only on pressure but also on such surface stress components as crystal growth pressure, which gives rise to reaction anisotropy. Ion transport gives rise to electric current and electrochemical cells.

The damage localizes into macrocracks. This causes interaction of the diffusion-chemical reaction problem and ion transport with structural stress analysis, and calls for the use of energy methods of fracture mechanics. In fact, fracture mechanics is generally coupled with the diffusion and chemical reaction problems. Furthermore, all these phenomena exhibit considerable randomness, which makes it necessary to approach the problem probabilistically and take into account both the randomness of the process and the uncertainty in the properties of the material and the reacting chemical involved.

Complete solutions to the long-term durability problems can be obtained only by numerical simulation based on a realistic mathematical model. The numerical approach, though, does not help understanding very much. One must equally strive for simplified analytical solutions, which have to be based on asymptotic methods and exploit the technique of asymptotic matching. Such asymptotic approaches are essential to master the problem of scaling—i.e., the problem of how to extrapolate short-time reduced scale laboratory tests to long-time and real structure sizes, how to design accelerated tests, how to infer damage in one kind of structure from observations on another. Without robust mathematical models, understanding of their asymptotics and scaling, a major progress in the durability problems cannot be achieved. So far, progress has been hampered by the lack of mathematical approaches among the classical durability researchers, and by the lack of understanding of the complex mechanisms of durability problems among mathematicians and mechanicians.

A workshop entitled "Model-Based Simulation of Durability of Materials and Structures," sponsored by the National Science Foundation, was held at the Czech Technical University, in Prague, during July 4–6, 2002. The workshop was aimed at stimulating a dialogue between these two groups of researchers, leading to synergistic efforts having a better chance of success. The workshop gathered the leading researchers with the goal of promoting crystallization of ideas, appraising recent progress and its applicability in engineering practice, and identifying the main problems for future research. There were 40 invited participants in the workshop; 19 participants were from the United States, and 21 from Europe and elsewhere.

In this Special Issue of the *J. Mater. Civ. Eng.*, ASCE contains a partial collection of the papers presented in the workshop, consisting of nine papers selected to cover different aspects of the research area (two other papers from the workshop were published in 2003 in the fall issue of *International Journal for Restoration*).

The first paper in this special issue, titled "Challenges of Mechanics and Materials Research in the Twenty-First Century," is written by two NSF program directors, and provides a broad overview for needed future research directions and opportunities. The second paper, titled "Shotcrete Elasticity Revisited in the Framework of Continuum Micromechanics from the Submicron to the Meter Level," is a comprehensive presentation of multiscale models for a special concrete, the shotcrete. The third paper, "Accelerated Assessment and Fuzzy Evaluation of Concrete Durability," focuses on an important topic—how to evaluate accelerated test data for long-term durability. A fuzzy synthetic evaluation method was developed for this purpose. The fourth paper, "Nonlinear Coupling of Carbonation and Chloride Diffusion in Concrete," presents a numerical simulation model for coupled diffusion processes of carbon dioxide and chloride in concrete. The numerical simulation is based on previously developed materials models. The fifth paper, "Thermal Degradation in Heterogeneous Concrete Materials," describes theoretical and numerical models for concrete under high temperature, especially the damage process due to the high temperature. The sixth paper, "Composite Damage Models for Diffusivity of Distressed Materials," is devoted to the effect of damage on the diffusivity of composite materials. A newly developed theory called composite damage mechanics was applied to the transport properties of concrete. The seventh paper, "Model-Based Simulation for Maintaining the Reliability of Deteriorating Structures," evaluates the time-varying performance of deteriorating materials, and its effect on structures is measured by the reliability index profile, addressing three specific aspects. The eighth paper, "Does Calcium Leaching Increase Durability of Cementitious Materials?—Evidence from Direct Tensile Tests," addresses an important problem for concrete. Observation of test data and micromechanical analysis show that calcium leaching makes concrete more ductile. The last paper, "Deterioration of Reinforced Concrete Structures Due to Chemical-Physical Phenomena," develops mathematical and numerical models encompassing several coupled effects, such as humidity diffusion, pollutant transport, and heat transport, taking into account the effect of the mechanical damage on the transport properties in concrete.

During the last session of the workshop, the participants identified the following as profitable research directions:

- Scaling effects in time and space need to be addressed, multiscale models developed, and gaps between temporal and spatial scales bridged. New developments in experimental techniques and testing results for different scales should be exploited. Most of the examples used for simulation have been limited to two dimensions, while three-dimensional simulations with the time factor should be emphasized in the future.
- Multiphysics problems, such as chemo-thermo-hygromechanical coupling and transport problems in distressed media, will gain in prominence.
- Since many models are being developed to simulate durability of various materials, round-robin tests and validations of the simulation models need to be conducted. Criteria should be established to uniformly evaluate model simulations. Better experimental techniques and testing methods are needed to validate models and their parameters.
- Virtual manufacturing needs to be developed as an engineering tool to simulate manufacturing processes, and virtual testing methods need to be developed as a design tool for modelers. Simulation models are especially needed for extreme events, such as fire damage and collapse of structures.
- Repair science and technology are an important future direction for model-based simulation. Sensors, adaptive models, and active control should be established as an entire engineering system.
- Interaction among scientists, modelers, and practitioners should be enhanced, while practical applicability of simulation models should be emphasized.
- The essential effects of microstructural features should be included as quantitative inputs to the simulation models.
- Probabilistic-based life-cycle design methods will be important for providing rules and recommendations for engineers.
- Mechanistic integration of corrosion initiation and propagation needs to be mastered. Not many modelers are focusing on this topic.
- Sustainable development of materials and structures will be an important new direction for model-based simulation.