COMPUTER MODELING OF CONCRETE MATERIALS AND STRUCTURES

J. E. Bolander
Department of Civil & Environmental Engineering, University of California, Davis, USA

D. Asahina
Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA

Keywords: Concrete, multi-scale material, computer modeling, discrete methods, durability mechanics, life-cycle analysis, model validation.

Contents

Summary

High performance concretes are being developed to produce stronger, lighter-weight structures and for numerous other applications that require improved concrete performance in the fresh or hardened states. Motivated partly by ecological factors, there has also been an increasing usage of alternative binders, as partial replacements for portland cement, and alternative sources of aggregates for concrete. Whereas conventional reinforced concrete design has been supported by decades of laboratory testing and observations of field performance, these newly emerging materials lack the database necessary for design and assurances of adequate long-term performance over the intended service life.

Computer modeling offers a precisely controlled environment for studying material composition and its relationships with structural performance. Such modeling stands to play a prominent role in the development of new concrete materials and their structural applications, complimenting results obtained through laboratory testing. Modeling supports the necessary shift from materials development based on empiricism to that based on the materials science of cement-based composites. Variations in the material composition, production processes, and exposure conditions (and the effects of such variations on life-cycle performance) can be simulated for large intervals on the length and time scales. This chapter highlights general concepts and trends in computer

modeling of concrete materials and structures, with coverage of some of the research needs and challenges.

1. Introduction

To a large extent, knowledge of conventional concrete materials has evolved through decades of laboratory testing and the monitoring of field performance. Structural mechanics and design concepts, such as no-tension design and plastic limit state design, have also played important roles in the application of concrete materials within structures. Although such methods continue to serve the structural design community well, it has become increasingly apparent that computer modeling is an essential component within the overall strategy to develop and improve concrete materials and structures.

Most of the advances in modeling capabilities have been accomplished within the framework of finite element methods. Indeed, roughly since the 1980s many of the techniques for structural analysis under mechanical loading had been developed and summarized in an American Society of Civil Engineers (ASCE) committee report. That ASCE document covers essential concepts such as constitutive modeling of concrete under multi-axial stress conditions, representation of cracking (including discussions of smeared versus discrete crack models), incorporation of reinforcement and its associated bond with the concrete, time-dependent effects including shrinkage and creep under sustained loading, and dynamic analyses. More recent literature contains a wealth of publications on the continued development of finite element and alternative modeling strategies. Notable amongst these publications are those produced by the FraMCoS and Euro-C conference series. Amongst this work, there has been growing interest in simulating microstructure development using models defined at the cement grain scale, as pioneered by researchers at the US National Institute of Standards and Technology (NIST).

Structural concrete design has traditionally involved the provision of safe and serviceable structures. For justifiable reasons, the most intense analysis efforts were first directed toward understanding load-induced failure of concrete structures, and thus their safety. As a result of several national programs on High Performance Concrete (HPC), which were formed in the early 1990s, research and development efforts have been extended to meet a broader set of objectives. Some of these objectives pertain to structural durability, which depends strongly on the mass transport properties of concrete and cracking behavior (e.g. crack spacing and opening) under service loading. Prolonging the maintenance-free service life is one objective. Furthermore, in recent years emphases on economy (e.g. efficient production technologies, such as self-consolidating concrete) and the keener realization of ecological constraints have fostered the development of new concrete materials, many of which involve alternative binders (usually as a partial replacement of portland cement) or alternative aggregates. Whereas portland cement has been the main binding agent in both conventional and newly emerging concrete materials, alternative binders (e.g. calcium aluminate cements and geopolymer cements) are receiving much attention. The role of computation has been strengthened and expanded by these recent shifts in interests. Along with stronger roles of computation comes increased needs for model validation at all scales of interest, and thus increased needs for collaboration with experimentalists.

This chapter reviews general concepts and motivations for the computer modeling of concrete materials and structures, assuming that the reader is familiar with most of the essential concepts, such as those outlined in previous state-of-the-art reports. Present research trends are directed towards the development of high-performance materials, alternative materials with lower environmental load, as well as non-traditional reinforcing materials (such as hybrid-fiber reinforcement and fiber-reinforced plastics). The totality of experimental data and field experience on these materials is limited and not sufficient for forecasting their service life performance, especially in severe environments. Many factors, such as component geometry, boundary conditions, degree of confinement, and size effects are important and complicate a comprehensive understanding of material performance within structural settings.

As a starting point for this chapter, we describe concrete as a multi-scale material. Discussions then center on the notion of model-based simulation, which can be viewed as a three-stage process of model construction, analyses, and results interpretation. For effective support of material and structural design, the three-stage process should be implemented within a fast-feedback loop that supports the creative abilities of the designer. This has been the intent of many earlier research works, but only now is computing technology meeting such needs within the three-dimensional frameworks necessary for addressing most research and practical problems.

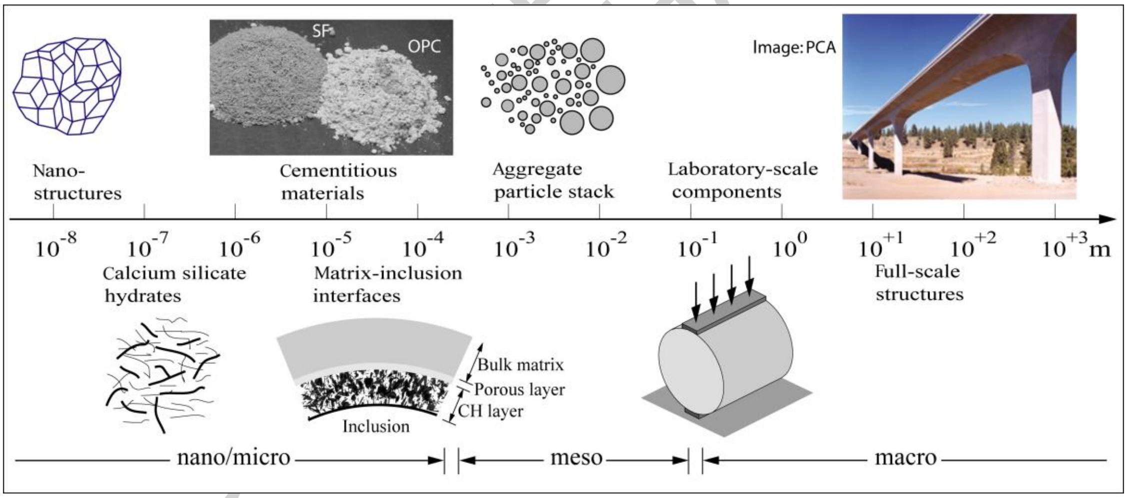

Figure 1. Concrete as a multi-scale material (adapted from van Mier (1997))

2. Concrete as a Multi-Scale Material

Concrete is a mixture of cementitious binder (which has been predominantly portland cement), aggregate inclusions, water, and an increasing variety of admixtures to modify the fresh and hardened properties of the product. Concrete is profoundly affected by structures and processes that reside within or span different (often disparate) length and time scales. Figure 1 depicts some of the relevant features and configurations that appear over the range of observation scales, from molecular structures and C-S-H morphology within the finer size intervals up to large-scale applications of concrete as a macroscopic continuum. The boundaries to what are often called the nano/micro/meso/macro-scales are not distinct and open to interpretation. The engineering of cement-based composites or concrete structures is occurring at all scales.

During concrete production, portland cement reacts with water to produce two main hydration products: calcium silicate hydrate (C-S-H) and calcium hydroxide. The calcium silicate hydrates are mainly responsible for the strength and stiffness of the cement paste, which develops over time due to continued hydration. Strength and stiffness are also affected by the packing efficiencies, and thus the particle size distributions, of both the cementitious materials and inert fillers. The desired trend toward stronger, less permeable materials follows from densification of the microstructure of the binder and at the interfaces of material/structural components. The amount, size distribution, and connectivity of porosity, and the introduction of cracks caused by volume instabilities or mechanical loading, affect the transport properties and thus the durability of structural concrete. Computer simulations at the fine scales are able to characterize evolving pore structures and study the role of phase interfaces on developing cracks.

The variety of potentially effective substitutions for portland cement is astounding, including materials that exhibit pozzolanic or latent hydraulic behaviors (e.g., industrial and agricultural by-products such as fly ash, ground granulated blast furnace slag, silica fume, and rice husk ash; and naturally derived materials, such as volcanic tuff and metakaolin). Whereas early age strength is generally lower due to dilution of the portland cement content, the addition of these mineral admixtures generally provides lower rate of heat production, increases longer term strength through secondary reactions, and improves the mass transport properties governed in large part by total porosity and its size distribution. Partial replacement of portland cement with these materials offers the added benefits of waste utilization and of reducing the CO_2 footprint of structural concrete. Indeed, such environmental benefits have become the central motivation in many concrete applications.

Micro-structural parameters		**Composite performance measures**
Fiber:	• Dimensions and geometry • Elastic modulus • Volume fraction • Orientation and distribution • Rupture strength • Electrical conductivity	• Pre-cracking strength • Elastic modulus • Post-cracking strength • Toughness • Fatigue life • Impact resistance • Crack size and spacing • Permeability • Electrical Properties
Matrix:	• Tensile strength • Pore size distribution • Defect size and concentration • Elastic modulus	
Interface:	• Porosity • Bonding properties	

Table 1. Basic elements within material-structure-property relationships for fiber-reinforced cement composites

There has been a growing appreciation of the multi-scale nature of concrete within the current movement toward performance-based designs of concrete materials and structures. Historically, however, studies of concrete materials and structures have been separated into different disciplines. This lack of integrated study has led to more or less distinct bodies of knowledge assembled at different scales of observation. The samplings of topics covered in this section, although mostly at the material scale, are highly relevant to the structural performance objectives, whether they concern safety, serviceability, constructability or economy. For the case of fiber reinforced concrete, Table 1 lists some of the basic elements within material-structure-property relationships that bridge the micro/meso-scales and the macroscopic continuum. Computer modeling provides the capability to quantitatively link such various factors that are defined over different length and time scales.

3. Motivations for Numerical Modeling

The motivations for developing computational models of concrete materials and structures are numerous. Some of the main motivations stem from:

- practical limitations of physical testing, especially considering the large ranges of relevant length and time scales that often need to be considered. Statistically significant and representative test results are generally cost-prohibitive for larger scale structural components and systems;
- potentially large variations in the properties of the source materials. Methods of processing often induce inconsistencies in the distributions of constituents, including variations in the positioning of reinforcing components;
- sensitivity of concrete properties to early-age thermal, chemical, and physical processes and their dependence on curing practice;
- aging and degradation of materials under the influence of multiple, possibly aggressive, environmental phenomena;
- three-dimensionality of material structure, transport mechanisms, and damage processes; and
- lack of quantitative links between actions occurring at different length and time scales.

An additional incentive for computer modeling comes from the thought exercises that go hand-in-hand with model development. Regardless of the predictive capabilities of the model, the thought processes used for program development differ from those involved in physical experimentation. The provision of unambiguous sets of instructions (i.e. the computer program) requires making formal connections between the various factors that affect concrete performance. Validated computer models offer a precisely controlled environment to study cause-and-effect relationships and the lack of practical constraints facilitates the exploration of design possibilities. Beyond the research capabilities and benefits, it can be argued that algorithm development has intrinsic educational value and should be promoted within the study of concrete materials and structures, and in engineering curricula in general.

4. Analysis Process and Modeling Strategies

Model-based simulation of materials and structures can be viewed as a three-stage process consisting of: 1) model selection and construction; 2) execution of the analysis routines; and 3) results interpretation. The analysis stage is mainly accomplished through the use of computer programs whereas, traditionally, model construction and results interpretation have involved significant human intervention and effort. Obviously, the overall process is largely affected by the material/structural type and analysis goals. These stages are now described with reference to concrete materials and structures, and particular emphasis on model selection and construction.

4.1. Model Selection and Construction

Model type should be carefully selected according to the objectives of the analyses, availability of data required for running and verifying the model, and adequacy of the available computational resources. Whereas the large majority of previous modeling studies have been conducted using two-dimensional analysis frameworks, most current research needs involve three-dimensional (material or structural) configurations, constraint conditions, and processes. The extension to 3-D can involve conceptual differences from the 2-D counterparts, but many of the challenges involve more practical matters, including the inherent difficulties in 3-D domain discretization, tremendous increases in computational expense, and difficulties in processing/interpreting the large amount of data generated by the analyses. Adequacy of available computational resources often becomes a controlling issue when modeling in three dimensions.

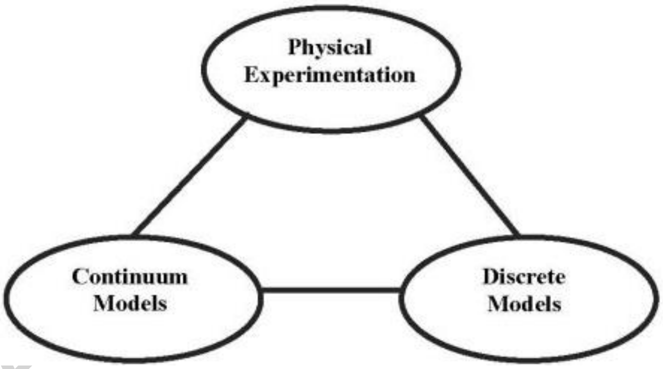

Figure 2. Complementary modes of investigation

The literature describes a multitude of different models for concrete materials and structures. This great variety makes their precise categorization difficult. Nonetheless, categorization is useful for discussing the commonalities and general capabilities of models. One broad categorization places models into one of two categories, depending on whether concrete is represented as a homogeneous continuum or as a collection of discrete elements. The utility of such models can be understood through comparisons with physical experiments (Figure 2). Both categories are described below with emphasis on discrete models as a growing trend, enabled by advances in computing technology. Recent research on fracture and damage has also involved the development of multi-scale models, many of which are a hybrid combination of continuum and discrete approaches.

4.1.1. Continuum Models

Continuum models provide an average description of material behavior for a representative volume element. Microstructure can be considered within the continuum description, through the use of homogenization and constitutive modeling techniques, but only in a mean field sense. A large set of parameters is needed to simulate complex behaviors and parameter values are typically calibrated through comparisons with experimental results. Nonetheless, this approach is attractive for engineering analysis, since sizable domains can be analyzed in a computationally efficient manner. Additional motivations come from the observation that the width of the fracture process zone in concrete can be large, roughly several times the maximum aggregate size. In some situations, damage is finely distributed over a region of a structural component and therefore its modeling via a continuum approach is attractive.

-

-

-

Bibliography

Baroghel-Bouny V., Mainguy M., Lassabatere T., and Coussy O. (1999). Characterization and identification of equilibrium and transfer moisture properties for ordinary and high-performance cementitious materials, *Cement Concrete Research* **29**, 1225-1238. [The equilibrium and transfer moisture properties of concrete strongly influence the durability of such materials.]

Bažant Z.P., Editor (1992) *Fracture Mechanics of Concrete Structures*. Proceedings of the First International Conference (FraMCoS-1), Elsevier, London, 1040 pp. [First in a series of international conferences on the fracture mechanics of concrete and concrete structures. The proceedings includes a state-of-the-art report on the fracture mechanics of concrete.]

Bažant Z.P. and Oh B.H. (1983). Crack band theory for fracture of concrete. *Materials and Structures* **16**, 155-177. [This paper presents an energy-based, continuum approach to modeling concrete fracture. Emphasis is placed on objectivity of the finite element solutions with respect to mesh resolution. Crack band theory, and its variants, has become the most extensively used approach for modeling fracture of concrete.]

Bentz D.P. (1997). Three-dimensional computer simulation of cement hydration and microstructure development. *J. American Ceramic Society* **80**(1), 3-21. [This feature article summarizes advances in the digital image-based modeling of cement hydration and microstructure development.]

Bentz D.P. and Garboczi E.J. (1991). Percolation of phases in three-dimensional cement paste microstructural model. *Cement Concrete Research* **21**, 325-344. [This paper presents a digital image-based model of cement hydration for the study of percolation of material phases as a function of hydration. The effects of water-to-cement ratio, degree of hydration, and substitution of inert or cementitious materials for cement on the connectivity of capillary porosity are simulated.]

Bolander J.E. and Berton S. (2004). Simulation of shrinkage induced cracking in cement composite overlays. *Cement Concrete Composites* **26**(7), 861-871. [A random lattice model is used to simulate shrinkage-induced cracking of an overlay material on a mature concrete substrate.]

Bolander J.E., Choi S., and Duddukuri S.R. (2008). Fracture of fiber-reinforced cement composites: effects of fiber dispersion. *International Journal of Fracture* **154**, 73-86. [A distinguishing feature of this work is the explicit representation of individual fibers within three-dimensional lattice models of fiber-reinforced concrete. This approach facilitates study of non-uniform fiber dispersions and their effects on structural performance.]

de Borst R., Bićanić N., Mang H., and Meschke G., Editors (1998). *Computational Modeling of Concrete Structures*. Proceedings of Euro-C 98 (Volumes 1 and 2), Balkema, Rotterdam. [This is the second in a series of influential conference proceedings on the computational modeling of concrete structures.]

Caballero A., López C.M., and Carol I. (2006). 3D meso-structural analysis of concrete specimens under uniaxial tension. *Computer Methods Applied Mechanics Engineering* **195**, 7182-7195. [This paper covers the development of interface finite elements and their effective use to model concrete fracture at the meso-scale.]

Constantinides G. and Ulm F.-J. (2007). The nanogranular nature of C–S–H. *J. Mechanics Physics Solids* **55**(1), 64-90. [This paper presents a technique and experimental protocol to assess the nanomechanical behavior of C–S–H based on a statistical analysis of nanoindentation tests.]

Cusatis G., Bažant Z.P., and Cedolin L. (2003). Confinement-shear lattice model for concrete damage in tension and compression: I. theory. *ASCE J. Engineering Mechanics* **129**(12), 1439-1448. [This lattice model is notable for its accurate reproduction of concrete behavior for a large range of multi-axial stress conditions. Lattice nodes correspond to the particle structure of concrete.]

DeJong M.J., Hendriks M.A.N., and Rots J.G. (2008). Sequentially linear analysis of fracture under non-proportional loading. *Engineering Fracture Mechanics* **75**, 5042-5056. [Sequentially linear analyses avoid the convergence problems often associated with nonlinear analyses of concrete fracture. In this paper, the sequentially linear analysis approach is extended to account for the common occurrence of non-proportional loading.]

Di Luzio G. and Cusatis, G. (2009). Hygro-thermo-chemical modeling of high-performance concrete. I: Theory. *Cement Concrete Composites* **31**(5), 301-308. [This paper presents a hygro-thermo-chemical model for high-performance concrete, which is suitable for transient analyses of moisture transport and heat transfer. The model accurately simulates early-age phenomena, including self-heating and self-desiccation.]

Gawin D., Majorana C.E., and Schrefler B.A. (1999). Numerical analysis of hygro-thermal behavior and damage of concrete at high temperature. *Mechanics Cohesive-frictional Materials* **4**, 37-74. [The thermal, hygral, and mechanical performances of concrete, including damage effects, are simulated within the framework of a coupled model, in which the nonlinearities due to high temperatures are represented.]

Grassl P. (2009). A lattice approach to model flow in cracked concrete. *Cement Concrete Composites* **31**(7), 454-460. [This paper introduces a dual-lattice approach for modeling crack-assisted flow in concrete. Elements within the flow lattice are aligned with potential crack directions, such that the local dependence of flow on crack opening is explicitly modeled.]

Hansen E.J. and Saouma V. (1999). Numerical simulation of reinforced concrete deterioration: Part II - Steel corrosion and concrete cracking. *ACI Materials J* **96**, 331-337. [This paper presents a mechanics-based model for simulating reinforcing steel corrosion and associated concrete cracking, with applications to concrete bridge decks.]

Herrmann H. and Roux S. Eds. (1990). *Statistical Models for the Fracture of Disordered Media*. Elsevier, Amsterdam. [This book summarizes developments in modeling fracture of disordered media from the perspectives of statistical physics. This work inspired the development of lattice models of concrete fracture.]

Jennings H.M. (2000). A model for the microstructure of calcium silicate hydrate in cement paste. *Cement Concrete Research* **30**(1), 101-116. [The model described in this paper provides a quantitative description of the microstructure of C-S-H between 1 and 100 nm. Amongst several notable features of the model, it accommodates the presence of low-density and high-density C-S-H.]

Jirásek M. (1998). Nonlocal models for damage and fracture: Comparison of approaches, *International J. Solids Structures* **35**(31-32), 4133-4145. [This paper classifies and analyzes notable nonlocal constitutive models for simulating damage and fracture of quasi-brittle materials. The phenomenon of stress-locking, exhibited by some of the models, is examined.]

Jirásek M. (2000). Comparative study on finite elements with embedded discontinuities, *Computer Methods Applied Mechanics Engineering* **188**, 307-330. [This paper reviews the development and application of finite elements with embedded discontinuities. Various diverse formulations are classified with respect to the types of kinematic enhancement and internal equilibrium condition used.]

Jun P. and Mechtcherine V. (2010). Behaviour of strain-hardening cement-based composites (SHCC) under monotonic and cyclic tensile loading: Part 2 – Modelling. *Cement Concrete Composites* **32**(10), 810-818. [This paper derives constitutive relations for strain-hardening cement-based composites under tensile loading. The derivations are based on a multi-scale approach in which the actions of individual fibers are considered.]

Lackner, R., Hellmich Ch., and Mang H. (2002). Constitutive modeling of cementitious materials in the framework of chemoplasticity. *International J. Numerical Methods Engineering* **53**(10), 2357-2388. [This paper describes a multi-surface plasticity model for chemically reactive media with attention to shotcrete. Applicability of the model is demonstrated through analyses of shotcrete tunnel shells, where creep is of significant influence.]

Landis E.N. and Bolander J.E. (2009). Explicit representation of physical processes in concrete fracture. *J Physics D: Applied Physics* **42**(21), 214002. 17pp. [This paper reviews opportunities for advancing knowledge of concrete fracture through combined physical testing and numerical modeling. Attention is given to coupling direct measurements of concrete fracture, acquired via x-ray microtomography, and discrete modeling approaches.]

Maekawa K., Chaube R., and Kishi T. (1999). *Modeling of concrete performance: Hydration, microstructure formation and mass transport*, E & FN Spon, London. [This book provides an integrated, physically-based approach for concrete life-cycle simulation. The authors are pioneers and significant developers of this subject area.]

Ožbolt J., Balabanić G., Periškić G., and Kušter M. (2010). Modeling the effect of damage on transport processes in concrete. *Construction and Building Materials* **24**, 1638-1648. [This paper presents a three-dimensional numerical model for transport of capillary water, oxygen, and chloride ions through concrete. The model is used to investigate the effects of concrete cracking on the depassivation of steel reinforcement.]

RILEM Technical Committee 130-CSL (1996). Durability Design of Concrete Structures, *RILEM Report* 14, eds. A. Sarja and E. Vesikari, E&FN Spon. [This publication outlines key concepts in the durability design of concrete structures, including the use of probabilistic frameworks for service life estimation.]

Roelfstra P.E., Sadouki H., and Wittmann F.H. (1987). Le béton numérique. *Materials and Structures* **18**, 327-335. [This is widely regarded as the first publication involving the numerical modeling of concrete at its meso-scale, at which the mortar matrix, aggregate inclusions, and their interface are represented as distinct entities.]

Sanchez F. and Sobolev K. (2010). Nanotechnology in concrete - A review. *Construction and Building Materials* **24**, 2060-2071. [This review paper covers basic definitions, advances in instrumentation and computational materials science, and the nano-engineering of concrete materials.]

Schlangen E., Koenders E.A.B., van Breugel K. (2007). Influence of internal dilation on the fracture behavior of multi-phase materials. *Engineering Fracture Mechanics* **74**, 18-33. [A multi-scale model, which couples hygral and structural behaviors, is used to simulate the effects of concrete mixture design and heterogeneity on cracking behavior.]

Schlangen E. and van Mier J.G.M. (1992). Experimental and numerical analysis of micromechanisms of fracture of cement-based composites. *Cement Concrete Composites* **14**, 105-118. [This paper introduced the lattice modeling of concrete materials and has become the most highly cited article in that subject area.]

Task Committee on Finite Element Analysis of Reinforced Concrete Structures, State of the Art Report on Finite Element Analysis of Reinforced Concrete, *American Society of Civil Engineers*, New York, NY, 1982, 545 pp. [This is a landmark publication on the finite element analysis of reinforced concrete structures.]

Ulm F.-J. and Coussy O. (1995). Modeling of thermochemomechanical couplings of concrete at early ages. *ASCE J. Engineering Mechanics* **121**(7), 785-794. [This paper describes early-age concrete as a thermomechanical chemoreactive porous media. Hydration of cement is considered in the formulation of constitutive equations, from which autogeneous shrinkage and aging are modeled.]

Ulm F.-J., Bažant Z.P., and Wittmann F.H., Editors (2001) *Creep, Shrinkage and Durability Mechanics of Concrete and Other Quasi-brittle Materials*. Proceedings of the Sixth International Conference (ConCreep-6), Elsevier, Amsterdam, 811 pp. [This is the sixth of an influential set of conference proceedings noted for its emphases on creep and shrinkage, and more recently the durability mechanics of concrete materials.]

van Mier J.G.M. (1997). *Fracture Processes of Concrete: Assessment of Material Parameters for Fracture Models*, New Directions in Civil Engineering, CRC Press, Boca Raton. [This book offers important insights regarding concrete fracture, with emphasis on the integration of physical testing and discrete modeling of concrete at the material scale.]

van Vliet M.R.A. and van Mier J.G.M. (1999). Effect of strain gradients on the size effect of concrete in uniaxial tension. *International Journal of Fracture* **95**, 195-219. [Strain gradient effects on concrete fracture are studied through tensile testing of specimens over a large size range.]

Yip M., Li Z., Liao B., and Bolander J.E. (2006). Irregular lattice model of fracture of multiphase particulate materials. *International Journal of Fracture* **140**, 113-124. [The toughening mechanisms of concrete fracture are studied using a three-dimensional lattice model of the material meso-structure. The event-by-event solution procedure is accelerated through low-rank updating of the system stiffness matrix.]

Biographical Sketches

John Bolander obtained a Ph.D. degree in Civil Engineering from the University of Michigan, Ann Arbor. He is currently a professor within the Department of Civil and Environmental Engineering at the University of California, Davis. His research work centers on the computational modeling of concrete materials and structures.

Daisuke Asahina obtained a Master of Science (M.S.) degree in Oceanic Architecture and Engineering at Nihon University, Japan, followed by a Ph.D. degree in Civil Engineering from the University of California, Davis. He is currently a post-doctoral researcher in the Earth Sciences Division of Lawrence Berkeley National Laboratory, Berkeley, California, U.S.A.