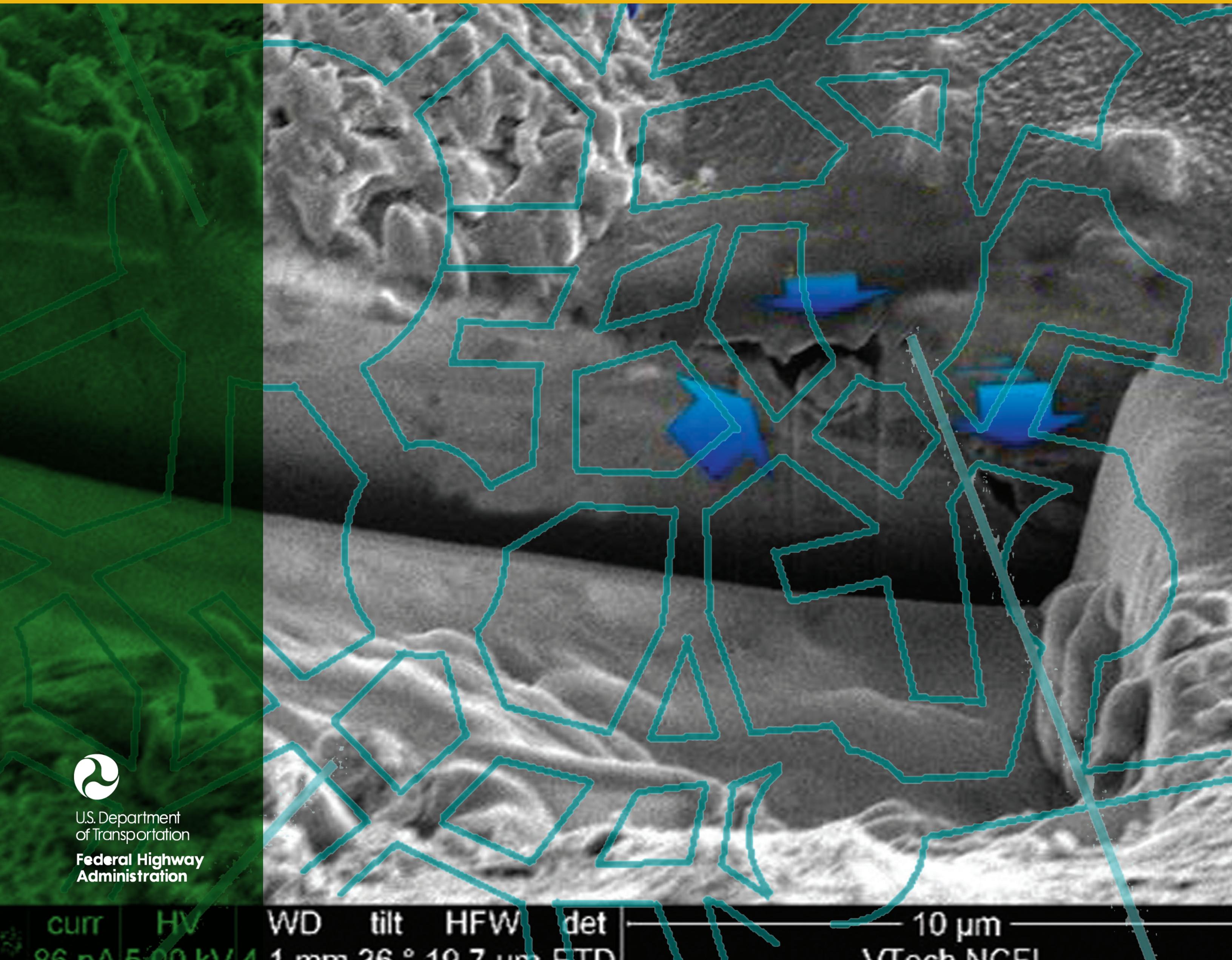
EXPLORATORY ADVANCED RESEARCH

The Exploratory Advanced Research Program

Multiscale Materials Modeling

WORKSHOP SUMMARY REPORT • April 23–24, 2013



U.S. Department
of Transportation
Federal Highway
Administration

Foreword

Breakthrough concepts in material science is one of the focus areas of the Federal Highway Administration's (FHWA) Exploratory Advanced Research (EAR) Program and is a critical area of investment to create longer-lasting, more resilient, roadways and structures and preserve existing highway system assets under increasing demands.

While industry has an interest in better performing and more cost-effective materials and academics have and will continue to study material properties, there is a clear government role for encouraging an environment where experimental results and models can be compared and investigators can build on each other's results. Developing an understanding of the complex materials used in highway infrastructure requires an enormous amount of research. Developing models is hard and software to test and apply the models harder. Integrating analytic approaches from multiple researchers is a whole new ballgame. Yet, that is exactly why and where government leadership is needed to connect the science to applications that will save money and time and provide materials with whole new properties for a next generation highway system.

The EAR Program is taking advantage of new scientific approaches for measuring and modeling materials across multiple length and time scales. It is becoming possible to characterize the chemical and mechanical properties in new ways necessary for controlling and designing complex materials used in roadways and structures. Accordingly, the EAR Program is funding research on multiscale material modeling across multiple institutions and coordinating the results with others conducting similar research. Based on this workshop and similar activities, FHWA is working through the EAR Program with other government agencies and is considering continued investment in moving scientific advances in materials characterization and modeling into the design and use of radically new materials.

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Notice

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16. Abstract

This report summarizes a 2-day workshop held to share information on multiscale material modeling. The aim was to gain expert feedback on the state of the art and identify Exploratory Advanced Research (EAR) Program opportunities for multiscale material modeling as it applies to the optimization of properties, durability, and construction of asphalt and cementitious pavement and construction materials. The workshop provided an opportunity for researchers who develop material models and engineers who use the results of material models to discuss multiscale modeling of cementitious and asphaltic materials. Discussion topics included the purposes and audiences for current and future models, the state of the art in approaches to model degradation mechanisms across length scales, and technical and programmatic approaches to advance multiscale modeling methods. These discussions will form the basis for transition of results from research on multiscale material modeling and new plans for EAR Program activities.

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SI* (MODERN METRIC) CONVERSION FACTORS

APPROXIMATE CONVERSIONS TO SI UNITS

Symbol	When You Know	Multiply By	To Find	Symbol
		LENGTH		
in	inches	25.4	millimeters	mm
ft	feet	0.305	meters	m
yd	yards	0.914	meters	m
mi	miles	1.61	kilometers	km
		AREA		
in^2	square inches	645.2	square millimeters	mm^2
ft^2	square feet	0.093	square meters	m^2
yd^2	square yard	0.836	square meters	m^2
ac	acres	0.405	hectares	ha
mi^2	square miles	2.59	square kilometers	km^2
		VOLUME		
fl oz	fluid ounces	29.57	milliliters	mL
gal	gallons	3.785	liters	L
ft^3	cubic feet	0.028	cubic meters	m^3
yd^3	cubic yards	0.765	cubic meters	m^3
	NOTE: volumes greater than 1000 L shall be shown in m^3			
		MASS		
oz	ounces	28.35	grams	g
lb	pounds	0.454	kilograms	kg
T	short tons (2000 lb)	0.907	megagrams (or "metric ton")	Mg (or "t")
		TEMPERATURE (exact degrees)		
^{o}F	Fahrenheit	5 (F-32)/9 or (F-32)/1.8	Celsius	^{o}C
		ILLUMINATION		
fc	foot-candles	10.76	lux	lx
fl	foot-Lamberts	3.426	candela/m^2	cd/m^2
		FORCE and PRESSURE or STRESS		
lbf	poundforce	4.45	newtons	N
lbf/in^2	poundforce per square inch	6.89	kilopascals	kPa

APPROXIMATE CONVERSIONS FROM SI UNITS

Symbol	When You Know	Multiply By	To Find	Symbol
		LENGTH		
mm	millimeters	0.039	inches	in
m	meters	3.28	feet	ft
m	meters	1.09	yards	yd
km	kilometers	0.621	miles	mi
		AREA		
mm^2	square millimeters	0.0016	square inches	in^2
m^2	square meters	10.764	square feet	ft^2
m^2	square meters	1.195	square yards	yd^2
ha	hectares	2.47	acres	ac
km^2	square kilometers	0.386	square miles	mi^2
		VOLUME		
mL	milliliters	0.034	fluid ounces	fl oz
L	liters	0.264	gallons	gal
m^3	cubic meters	35.314	cubic feet	ft^3
m^3	cubic meters	1.307	cubic yards	yd^3
		MASS		
g	grams	0.035	ounces	oz
kg	kilograms	2.202	pounds	lb
Mg (or "t")	megagrams (or "metric ton")	1.103	short tons (2000 lb)	T
		TEMPERATURE (exact degrees)		
^{o}C	Celsius	1.8C+32	Fahrenheit	^{o}F
		ILLUMINATION		
lx	lux	0.0929	foot-candles	fc
cd/m^2	candela/m^2	0.2919	foot-Lamberts	fl
		FORCE and PRESSURE or STRESS		
N	newtons	0.225	poundforce	lbf
kPa	kilopascals	0.145	poundforce per square inch	lbf/in^2

*SI is the symbol for the International System of Units. Appropriate rounding should be made to comply with Section 4 of ASTM E380.
(Revised March 2003)

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List of Acronyms and Abbreviations

General Terms

3D	three-dimensional
CNT	carbon nanotube
CTE	coefficient of thermal expansion
DOT	Department of Transportation
DVS	dynamic vapor sorption
EAR	Exploratory Advanced Research
ERDC	Engineer Research and Development Center
FHWA	Federal Highway Administration
FIB	focused ion beam
ICME	integrated computational materials engineering
I-QSAR	inverse-quantitative structure activity relationships
MD	molecular dynamics
MGI	materials genome initiative
nm	nanometer
NIST	National Institute of Standards and Technology
NSFC	naphthalene sulfonate superplasticizer
NSF	National Science Foundation
QMM	quantum mechanical methods
QSAR	quantitative structure activity relationships
SMM	structural materials and mechanics
TFHRC	Turner-Fairbank Highway Research Center
TPF	transportation pooled fund
UCLA	University of California, Los Angeles
UTPA	University of Texas–Pan American
VCCTL	Virtual Cement and Concrete Testing Laboratory

Introduction

On April 23–24, 2013, at the Turner-Fairbank Highway Research Center (TFHRC) in McLean, VA, the Federal Highway Administration's (FHWA) Exploratory Advanced Research (EAR) Program and Office of Infrastructure Research and Development convened a 2-day workshop to share information on multiscale material modeling.

The workshop was held to gain expert feedback on the state of the art and identify EAR Program research opportunities for multiscale material modeling as it applies to the optimization of properties, durability, and construction of asphalt and cementitious pavement and construction materials.

The "Multiscale Material Modeling" workshop provided an opportunity for researchers who develop material models and engineers who use the results of material models to discuss multiscale modeling of cementitious and asphaltic materials.

Discussion topics included the purposes and audiences for current and future models, the state of the art in approaches to model degradation mechanisms across length scales, and technical and programmatic approaches to advance multiscale modeling methods. These discussions will form the basis for transition of results from research on multiscale material modeling and new plans for EAR Program activities.

Part One:
Presentations

Measurement, Modeling and Interpretation of Sorption Isotherms: Directions Towards Predicting Material Properties and Degradation Phenomena

Gaurav Sant
University of California, Los Angeles (UCLA)

Gaurav Sant, at the University of California, Los Angeles' Department of Civil and Environmental Engineering, examined the problems of concrete degradation and durability and discussed possible solutions to these problems.

Sant initially explained that binding liquid water results in an inherent volume reduction and a nano-porous nature results in the development of large stresses as water enters and leaves a material. The consequence of this is shrinkage and microcracking which leads to locations of instability and possible macro-cracking. Sant highlighted that it is possible to predict and estimate the level of volume change and the implications of these changes using modeling and analysis of water sorption isotherms.

Workshop participants were informed that for any given partial pressure a relationship exists between water absorbed and partial pressure of water vapor. This equilibrium relationship is known as the sorption isotherm. Sant explained this is important because water uptake and release directly relate to shrinkage, the nature of a microstructure, potential for fluid transport, and the saturation state.

According to Sant, water sorption isotherms can be measured using dynamic vapor sorption (DVS) analyzers. It then becomes possible to estimate volume change, moisture transport behavior, porosity, and dimensions. With information on damage and porosity available, it is possible to infer how damage during drying would influence material properties. Sant explained there are lots of models that will fit sorption spectra but there is some difficulty in modeling an evolving structure. Workshop participants were told there needs to be a way to also introduce the effects of an evolving structure and the accompanying damage and porosity changes. Sant noted that modeling structure evolution requires the ability to reliably predict water sorption isotherms and history effects, to consider the kinetics of sorption, and to consider the role of interfaces and aggregates.

In summary, Sant explained that although at this time it is possible to model equilibrium effects, in reality it is necessary to also account for non-equilibrium states. It is currently possible to estimate a worst-case scenario but what is really desired is a means to determine real-life behavior and account for the effects of kinetics of water uptake and release, the role of cracks and inclusions, and cyclic absorption and temperature effects.

Moving forward, Sant believes the development of multiscale modeling is critical. For example, Sant would like to see how microcracking, macrocracking, and alterations in microstructure and properties would change sorption behavior and deterioration. He also noted it would be useful to describe how moisture effect, volume change, and damage evolve at the field scale and how to correlate sorption response to volumetric change experienced by material.

Water Sorption in Cement Paste: A Link Between Meso-Pore and Properties: Reversible and Irreversible Deformation

Hamlin Jennings
Massachusetts Institute of Technology

Hamlin Jennings, at Massachusetts Institute of Technology, began by mentioning there is overwhelming evidence for “colloid” behavior—where a substance is microscopically dispersed throughout another substance. Jennings stated the challenge ahead is direct measurement and developing a colloid model that comes from complex analysis of neat cement paste. He noted an easier method is required to evaluate structures.

Jennings informed workshop participants that a conceptual picture of grains and water is emerging, as shown in figure 1; however, Jennings questioned how a structure changes with chemistry and deformation. One method put forward was a technique called *water isotherm*. This method probes all pores but is very difficult to interpret. Jennings suggested the problem should be divided into parts, starting with low pressure hysteresis and reducing the problem to solid and pores. Other parts of the problem put forward by Jennings included a model of a structure with gel pores, high- and mid-pressure hysteresis, irreversible dimensional change, and development of an analytical tool. Available techniques outlined by Jennings included *molecular dynamics (MD)*—a technique involving computer simulation of physical movements of atoms and molecules that can be used to determine macroscopic thermodynamic proper; *grand canonical Monte-Carlo*—a powerful modeling technique that accounts for density fluctuations at fixed volume and temperature; *density functional theory*—a modeling method for investigating the electronic structure of atoms, molecules, and condensed phases; and *Langmuir–Kelvin.*

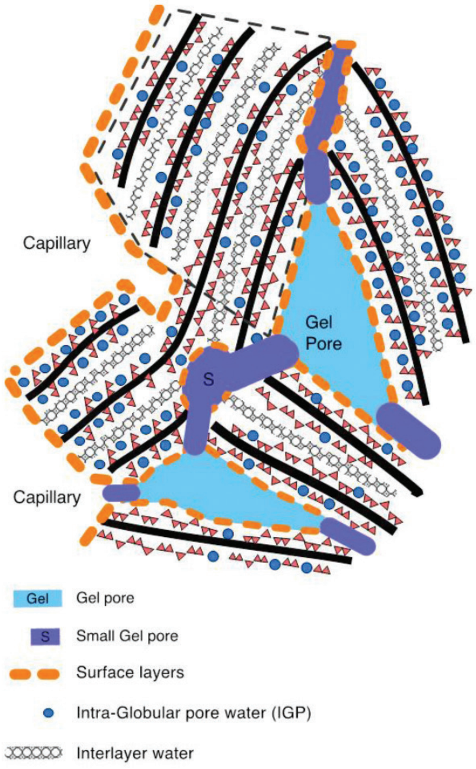

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Figure 1. Conceptual picture of grains and water.

Jennings provided workshop participants with an overview of water content at the atomic scale, highlighting adsorption isotherms and comparing adsorption experiments. He noted atomistic simulations cannot address the meso-scale directly; however macroscopic models cannot achieve this either because the sub-micron scale is affected by discrete molecular interactions that macro-scale continuum theory cannot capture.

Workshop participants were then informed about atoms and particle interactions at the colloidal scale—where atoms are treated implicitly and lumped into nanoparticles. Jennings explained the nanoparticles interact with force potentials parametrized on mechanical properties at the molecular scale. Jennings noted a bottom-up philosophy is employed to obtain effective interactions at the colloidal scale. Additionally, Jennings covered *polydispersity*—where a sample of objects have an inconsistent size, shape and mass distribution; *meso-porosity*—involving a material containing pores with diameters between 2 and 50 nm; a *lattice-gas model*—a type of cellular automaton used to simulate fluid flows; sorption of water in gel only; and the concept of a network of pores, as shown in figure 2.

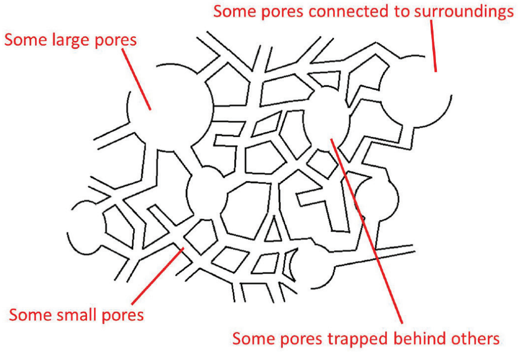

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Figure 2. A network of pores.

In conclusion, Jennings stated models are required to interpret certain experiments, including isotherms. He also noted it is possible to characterize the microstructure of new materials and changes in microstructure, including deformation, deterioration, and durability.

Porous Material Under the Nanoscope

Roland Pellenq
Massachusetts Institute of Technology

Roland Pellenq from the Massachusetts Institute of Technology provided workshop participants information about isothermal molecular models for cements with varying amounts of calcium and silicate. The models are important for understanding material strength and elasticity. Two-dimensional models can provide information about crystalline structure, and three-dimensional for amorphous glassy structure, both of which can be found in cement. Pellenq also said it is important to validate models with experimentation.

Multiscale Modeling of the Performace of Cementitious Materials

Florence Sanchez
Vanderbilt University

Florence Sanchez, at Vanderbilt University School of Engineering, provided workshop participants with an overview of the "International United States–Poland Workshop on Multiscale Computational Modeling of Cementitious Materials," which took place in Krakow, Poland, in October, 2012. Participants from eight countries, including Japan, Spain, France, Austria, Poland, United States, Switzerland, and The Netherlands met with representatives from Purdue University, Georgia Institute of Technology, UCLA, Virginia Polytechnic Institute and State University, Massachusetts Institute of Technology, Tennessee Technological University, Rice University, and Vanderbilt University.

Sanchez explained the purpose of this international workshop was to meet a need for more sustainable concrete and develop alternative cement systems and a wide range of supplementary cementitious materials. The international workshop participants were motivated by a need for concrete with superior and multifunctional "smart" properties; however, Sanchez noted development requires extensive testing and large costs which restrict the industry's ability to achieve innovative solutions.

Sanchez highlighted the concept of complex multiscale interaction with the environment and how this leads to an increase in the deterioration process. As shown in figure 3, mechanical loads combine with weathering forces, including temperature, radiation, and water. This leads to internal chemical changes, such as decalcification and alkali–silica reactions. These changes cause internal stresses, such as loss of alkalinity and shrinkage, and ultimately lead to material damage, including loss of compressive and tensile strength.

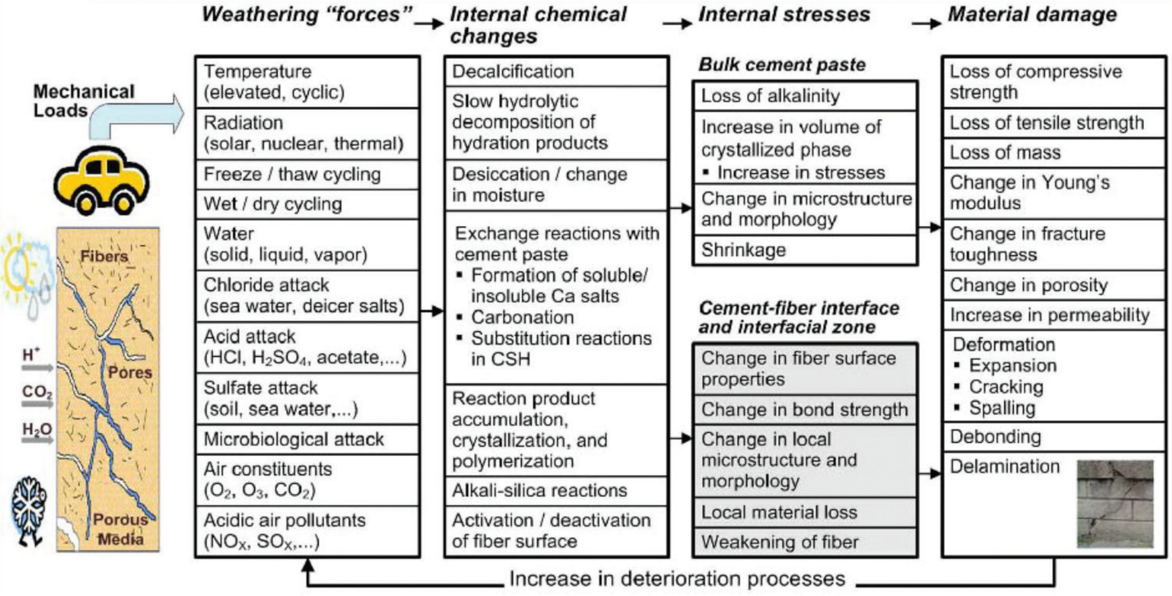

Figure 3. Multiscale performance of carbon microfiber reinforced cement-based composites exposed to a decalcifying environment.

© Reprinted from *Materials Science and Engineering: A, Vol. 527, Issue 13–14*, Sanchez, F. & Borwanker, A., "Multi-Scale Performance of Carbon Microfiber Reinforced Cement-Based Composites Exposed to a Decalcifying Environment," Pages 3151–3158, Copyright 2010, with permission from Elsevier.

Sanchez went on to explain that computational modeling represents a promising avenue. Such a tool provides an opportunity to simulate complex behavior and model systems over many lengths and timescales. Sanchez stated there is a need for unified methods capable of bridging the length and timescales for simulating and predicting material performance. Some of the objectives of the international workshop were to review state-of-the-art knowledge of computational modeling of cementitious materials, from the atomistic to the macroscopic scales, and define the gaps currently missing to develop a comprehensive and predictive multiscale computational framework.

As Sanchez explained, the results of the international workshop indicated current efforts for multiscale computational modeling of cementitious materials are disjointed. Sanchez stated that existing models do not bridge all scales and noted many research gaps and challenges to overcome. These include linking nano- and mesoscale models, connecting top-down macroscopic approaches with bottom-up models, identifying appropriate mechanisms at each scale, modeling damage evolution at multiple scales, and a lack of multiscale bridging methods for coupling between multiphysics and mechanical behaviors. Sanchez informed workshop participants that there is a need for new approaches to integrated modeling and a coordinated global research effort.

Sanchez went on to provide an overview and several examples of top-down and bottom-up approaches to computational modeling. One featured top-down approach aimed to develop tools to predict the performance of cement-based materials over extended time frames with potential applications in nuclear waste management. Another example of a bottom-up approach aimed to develop a fundamental understanding of chemo-mechanical interactions at fiber-matrix interfaces and design the macroscale failure of fiber reinforced cement composites by engineering the fiber-matrix interface. Potential applications included the design of structural and multifunctional materials tailored to specific civil, medical, and military applications.

Sanchez concluded by summarizing the main challenges to multiscale modeling of the performance of cementitious materials. These include mechanisms and parameter estimation, linking the models from one scale to another, and multiscale bridging methods coupling multiphysical information and mechanical behavior.

For more information on the International United States–Poland Workshop on Multiscale Computational Modeling of Cementitious Materials and to view the virtual collaboration environment, visit http://www.multiscalemodelingofconcrete.com/.

Why Would Engineers Want to Use Multiscale Modeling: General Thoughts and the Example of Virtual Cement and Concrete Testing Laboratory

Edward Garboczi
National Institute of Standards and Technology

Edward Garboczi, at the National Institute of Standards and Technology (NIST), began with some general remarks and context regarding multiscale modeling. Garboczi explained that other materials are already taking advantage of the integrated computational materials engineering (ICME) and materials genome initiative (MGI) approach, which link data and models to develop new materials. Garbocazi questioned why this approach could not also be applied to concrete.

Garboczi explained that the current level of success is largely based on the measurements of the past. Now that this "seed corn" has been used up, models cannot progress further or make new multiscale links without an influx of basic experimental data. Garboczi asked what will allow research funders to have the patience to wait for longer-term results. He suggested that all the experimental information could be placed into a concrete materials data repository. Workshop participants were told validated experimental data from all over the world could feed into it. Although a useful resource, Garboczi cautioned the repository would need long-term, sustained, and coordinated support.

Garboczi proceeded to compare simple models to complex models; for example, a desktop computer versus a supercomputer model. Workshop participants were advised not to disparage one by insisting the other is the only valid approach. Garboczi noted there is a difference between models that help industry on a daily basis and models that help improve understanding of complex and fundamental issues. He suggested one method could be to build simple, valid, non-fitting models by abstraction from validated, realistic, and complex models.

Next, Garboczi discussed concrete rheology and combining multiscale models and measurements. Workshop participants were informed of measuring and computing rheology parameters for cement and mineral admixture particles in water, sand grains in cement paste, and gravel in mortar fluid. Garboczi explained there are several lessons to be learned by linking multiscale models and experiments between cement paste, mortar, and concrete. Lessons include: (1) simultaneous measurements and models are crucial; (2) standard reference materials and measurements are leading the way to practical use; and (3) in order to move forward and compute cement paste rheology, inter-particle forces must be measured to input into a model.

Garboczi went on to give workshop participants an overview of the multiscale modeling endeavors of the Virtual Cement and Concrete Testing Laboratory (VCCTL). The VCCTL offers an integrated package to predict microstructure and properties, providing a link between micro- to millimeter scales for chloride transport and elastic moduli. The multiscale modeling at VCCTL also represents a crossover between desktop computing and supercomputing. Garboczi noted as computing power increases and offers multicores, increased processing power and memory, VCCTL also becomes more effective and practical.

Some of the specific lessons outlined by Garboczi included: (1) to use a cement paste microstructure model to give data needed for transport and elastic moduli of interfacial transition zones and matrix in mortar models; (2) to reserve lots of time and funding for information technology work; (3) to have an implementation plan for how people can use your models; and (4) to have experimental data.

Finally, Garboczi noted a large investment for research is a small investment for industry and government. For example, $20 million per year is a relatively small amount but will have a big payoff compared to the market size for cementitious materials, he pointed out. Garboczi concluded by saying the only way this research effort can be successful is for it to be centrally run, as a high-level basic science effort, and to draw from the entire materials science research community. Next steps suggested by Garboczi include putting together a trial multiscale model, identifying areas that require work, and identifying a systematic process for abstracting simple, accurate models from more complex and basic multiscale models.

A Practioner's Thoughts on Modeling

Larry Roberts
Roberts Consulting Group

Larry Roberts, at Roberts Consulting Group, addressed industry progress made without the use of models. Roberts used the example of the first naphthalene sulfonate superplasticizer (NSFC) technology application on Route 1 in Avon, MA, in 1931.

According to Roberts, at this time the Cabot Corporation was supplying carbon black in an attempt to make the center section of Route 1 black but was experiencing poor results. The company founder, Godfrey L. Cabot, recognized the problem was a dispersion issue and knew that his nephew, Charles Almy of the Dewey and Almy Chemical Company, was working on dispersing agents for emulsion polymerization. Roberts explained that an acquaintance of his, Maynard Renner, was subsequently called in to a meeting with Cabot Corporation and the Dewey and Almy Chemical Company. The plan was to try to disperse carbon black in NSFC and then make up some material in concrete to see if it was black.

After Renner made some mortar and showed it was indeed black, the road was built; however, one of the unexpected side effects of this process was that the road was unexpectedly strong. Recognizing the expense of NSFC at the time, Dewey and Almy went on to develop water reducer technology based on lignin and triethanolamine, which is still used today. Roberts reminded participants that no advanced models were used at this time, yet huge progress was still made.

Roberts noted this success was down to a simple inspiration, centered on the idea that something that can disperse emulsions would also disperse carbon black in concrete. Laboratory and field work resulted in data which can be reviewed and discussed and although the road was expected to be black, the stronger concrete result differed from expectations. A whole division of the company was subsequently formed to pursue opportunities based on dispersion in concrete. Roberts highlighted that progress is not equal to acceptance or agreement; for example, the fact that NSFC was too expensive in that era was not accepted and a workable, less-expensive alternative was sought and found.

Roberts informed workshop participants that models allow an idea to be stated very precisely which allows researchers to clearly design the work to test the ideas as efficiently as possible. The difference between the model prediction and results provides clarity and identifies things that need to be changed to improve the model so it better represents reality. Roberts noted that in modern times, where low hanging fruits have already been harvested, it is unlikely that researchers will happen upon easy solutions to durability and sustainability challenges facing road construction. It is therefore necessary to work smarter—something made easier by the analytical technologies available today.

Roberts went on to analyze some of the negative sides of over reliance and misuse of models. He reminded workshop participants of the importance of not settling for a successful model and no longer advancing development. He stated researchers must commit to continue the pursuit of progress; for example, if a model is agreed to fully represent reality, progress will cease and current understanding will be locked in place. Another danger highlighted by Roberts is the expectation of accurately recreating reality on a tablet device with clear and executable answers and next steps laid out. If a model is a “black box,” it does not fully explain its assumptions and, without any opportunity to fully understand its internal logic, it becomes impossible to learn when it fails and to trace whether a failure was due to an incorrect variable for material or exposure condition, or a faulty calculation of output variable. Roberts concluded that it is always important to ensure a model has encompassed all variables and not to push models into the field too early.

Multiscale Packing Algorithm for Modeling of Mechanical Response of Concrete: Educational Top-Down Module

Konstantin Sobolev
University of Wisconsin–Milwaukee

Konstantin Sobolev, at the University of Wisconsin–Milwaukee, began by informing workshop participants that portland cement concrete is a complex, nano-structured, multiphase, multiscale composite material that evolves over time.

Sobolev proceeded to outline the following modeling objectives: (1) develop multiscale aggregate packing for concrete in a virtual environment by varying the aggregate packing parameters; (2) create a numerical three-dimensional (3D) model of a particulate composite, real-life aggregate distribution and multiscale packing architecture; and (3) finite element modeling in multiscale to characterize stress-strain material response with various aggregate properties, matrix properties, and spatial distribution. Multiscale modeling methods highlighted by Sobolev included virtual aggregate packing, computer aided design representation and processing, finite element stress analysis, and finite element modeling. Additionally, Sobolev noted the use of an educational module for virtual aggregate testing.

Sobolev described a packing model and explained how the developed algorithm begins with the random generation of a center for the first sphere. This means a sphere of the maximum diameter, known as *Dmax*, is packed. Packing is followed by the placement of spheres with a diameter larger than or equal to the minimum diamater. Sobolev explained that overlaps between spheres are not allowed and a sphere can only be packed if its center is located inside the container. If the generated coordinates are not suitable for the placement of a sphere then the sphere is discarded and new coordinates are generated, as shown in figure 4. Likewise, Sobolev explained if parts of the accepted sphere are located outside of the container, the corresponding reduction of the volume is provided. Following adjustments, Sobolev confirmed he has developed a quick pseudo-dynamic packing strategy.

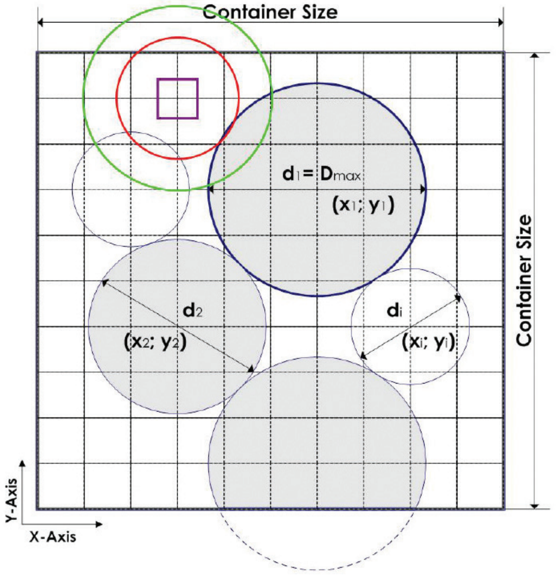

Figure 4. Description of a packing model.

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Sobolev went on to explain the concept of a suspension packing model, where all spheres are placed with separation rules. Sobolev also described packing into a container with periodic boundaries to represent the elementary volume of particulate assemblies and eliminate the wall effect. Workshop participants were told that all packing parameters were tuned to meet the grading of real-life concrete aggregates. Sobolev provided an overview of virtual aggregate packing and illustrated the results of two-dimensional and 3D packing, shown in figure 5. Sobolev noted that stress results obtained from larger scale models are applied as input pressures to the next level scale.

In conclusion, Sobolev told workshop participants that a pseudo-dynamic packing algorithm has been created that is capable of packing 25 million spheres and is enhanced with multiscale capabilities. The next level can be further packed and used for finite element simulation. Additionally, Sobolev noted that a top-down multiscale model can be used to link the micro- and nano-structure to macro tests used in the laboratory.

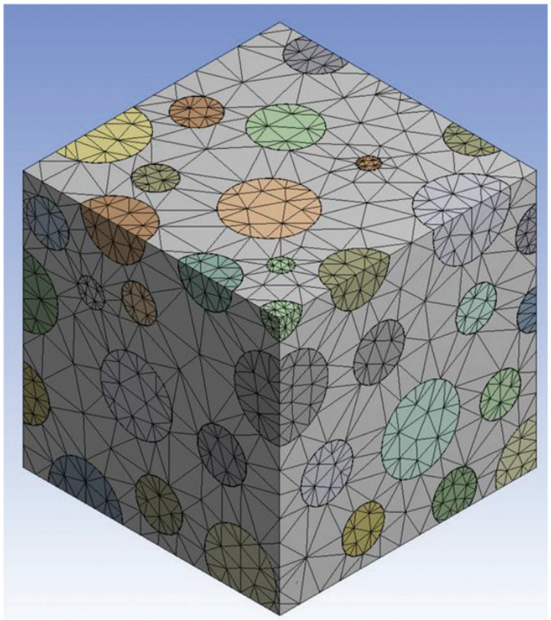

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Figure 5. An example of virtual aggregate packing showing the suspension packing model separation rule.

A Multiscale Computational Model for Predicting the Response of Asphaltic Pavement to Cyclic Loading

David Allen

Pavement Scientific International (formerly of University of Texas–Pan American)

David Allen, at Pavement Scientific International (formerly at the University of Texas–Pan American's (UTPA) College of Engineering and Computer Science), began by outlining the daunting challenge ahead in developing a multiscale computational model for predicting the response of asphaltic pavement to cyclic loading.

Allen explained there are many roadway design inputs to account for. Inputs include environmental conditions—such as surface temperature and moisture; moving tire loads—including tire configurations, inflation, and axle weights; geometry factors—such as roadway thickness, aggregate size, distribution and angularity, and roadway width and slope; and material properties—such as asphalt type, aggregate properties and volume fraction, additive properties and volume fractions, and fracture toughness. Allen noted these inputs exist on three different scales: global, local, and microscale.

Allen made several observations about asphaltic pavement. He noted that roadway failure is inherently time dependent and that the critical energy release rate can be time dependent, with no stress singularity. Additionally, Allen stated that macroscale failure of the roadway is generally preceded by a variety of microscale energy dissipative phenomena—a feature he noted is ideal for multiscaling. Allen also told workshop participants that a robust design methodology requires that microscale variables be accounted for in the model, which is also considered ideal for multiscaling.

Allen explained that UTPA's approach to multiscale analysis is to perform microscale analysis, followed by homogenization with successively larger scale analyses. He noted that local homogenization techniques work when the length scales are widely separated so that macrocracks do not interact with each other. Allen also highlighted these techniques work when the damage at the local scale remains distributed statistically homogeneously and the microcracks do not localize.

According to Allen, localization requires that the mean solution be modified. He mentioned it is necessary to monitor the higher order terms in the global stress expansion as a function of the local stress. Additionally, he noted any higher order terms must be included in the global analysis or macrocracks must be inserted. Allen also went on to discuss other items, including homogenized kinetics, fibrillation in asphalt, and homogenization of a cohesive zone (see figure 6).

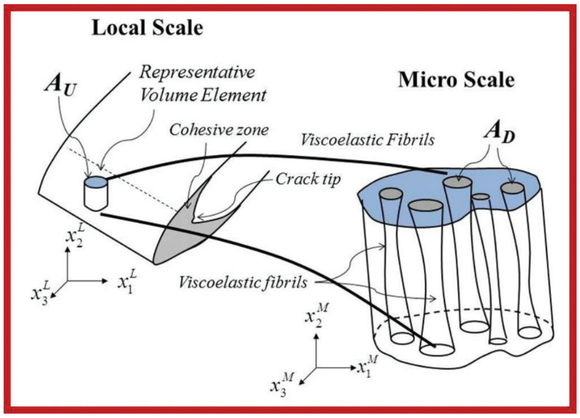

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Figure 6. Homogenization of a cohesive zone.

As part of his presentation, Allen also provided an overview of a viscoelastic cohesive zone model, homogenization of local scale constitutive equations, a computational algorithm for viscoelasticity, and multiscale pavement analysis (see figure 7). Additional topics Allen presented to workshop participants included a dynamic multiscale tapered uniaxial viscoelastic bar, a multiscale response to a projectile, and a roadway subjected to tire and cyclic loading, crack transition, and global cracking.

Allen concluded with a brief overview of alternatives to multiscale modeling. Single-scale phenomenological and single-scale micromechanical modeling have many similar advantages to multiscale modeling but do not allow control of local design variables, do not enable simplified experiments, and are not physically based. In summary, Allen noted UTPA currently has a multiscale model capable of predicting the evolution of damage and deformation in asphaltic pavement. Although further development is required, this patented model can control micro, local, and global input variables in the design process.

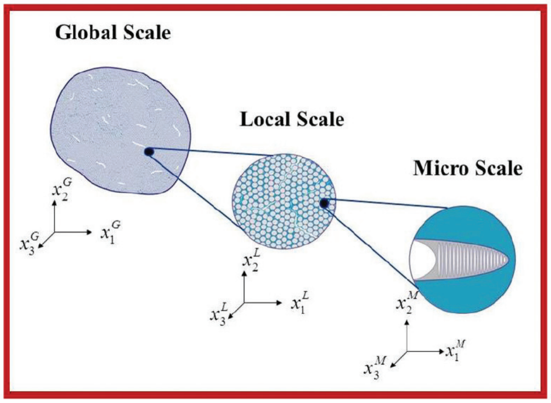

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Figure 7. Multiscale pavement analysis.

U.S. Army Engineer Research and Development Center's Advanced Materials Initiative—Super Fibers and Super Structural Ceramics

Bob Welch
U.S. Army Engineer Research and Development Center

Bob Welch, of the U.S. Army Engineer Research and Development Center (ERDC), provided an overview of ERDC's advanced material initiative program. The advanced material initiative program is developing the generation after next "super" structural materials—fibers and structural ceramics—to technology readiness level four, which will involve a laboratory demonstration.

The philosophy and approach of the ERDC program is to use atomistic and multiscale simulations to guide both material design and material synthesis. Welch defined this concept as *design first, then build* and went on to highlight that simulations are closely related to experiments for validation and proofing. Welch explained that the material development paradigm is changing from one that is largely empirically-based to one that uses atomistic and larger-scale simulations. This is coupled to multiscale material diagnostics and material response experiments, as well as advance material design and material synthesis. According to Welch, ERDC adopted this approach in 2005 for the development of "super" carbon nanotube (CNT) fiber design and is now employing it in the development of a "super" structural ceramic composite.

Welch explained that much of the technology supporting this approach is being developed as it is being used—for example, nanoscale material response and atomistic and multiscale simulations. Welch then proceeded to list the advanced materials research and development techniques ERDC currently employs. These include atomistic and multiscale simulations to guide material design and synthesis, carbon nanotubes and other "super" molecules or crystals as strength members, multiscale material response measurements and diagnostics to validate simulations, and advanced material synthesis.

Welch informed workshop participants that the goal of the initial super materials program, to develop CNT-based filaments to the point of a laboratory demonstration, would be a major accomplishment. Success would result in a material with twice the strength-to-weight ratio of Kevlar and five times the strength of very high-strength steel. According to Welch, successful development would inaugurate a paradigm shift in material development and lay the technical foundation for rapid development of other "super" materials and materials by design.

Welch proceeded to describe some of the effects of molecular defects on CNT tensile strength. Welch confirmed that CNTs display amazing strength and stiffness even with defects. Additionally, he stated that most CNTs suffer brittle failure at room temperature. Workshop participants were then shown how over a million simulations were used both in CNT fiber development and to study the effects of CNT length on CNT fiber response. Welch stated that these simulations were possibly the first to identify a scalable molecular design and predict mechanical properties for a "many-million-psi" fiber.

Another material project Welch presented to workshop participants was the development of an ultra-lightweight "super" structural ceramic for use in civil infrastructure, buildings, and transportation systems. The goal here is to improve tensile strength and toughness of silicon carbide, by employing CNTs, graphene, or fibers, to produce a super silicon carbide composite. Welch stated that, although very challenging, this goal is not considered impossible and would ultimately lead to a two-thirds weight reduction for aluminum and steel structures and equipment.

Welch concluded by highlighting some of the factors nanoscale phenomena can control or influence in the field of engineering, from material strength to corrosion and weathering protection. Welch stated that nanotechnology is the big frontier for engineering technology advancement for the next several decades and will allow unprecedented opportunities for enhanced materials, improved energy efficiency, and reduced maintenance.

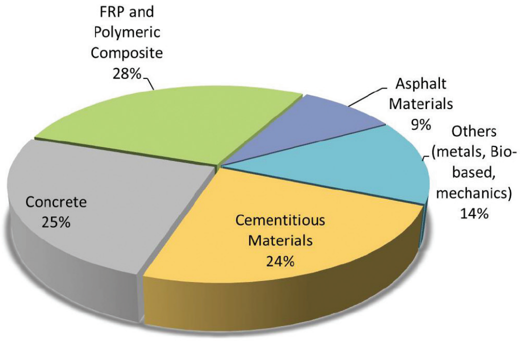
The Role of Multiscale Modeling in Advancing Infrastructural Materials

Grace Hsuan
National Science Foundation

Grace Hsuan, at the National Science Foundation's (NSF) Division of Civil, Mechanics and Manufacturing Innovation, provided an overview of the Structural Materials and Mechanics (SMM) Program as part of her presentation on multiscale modeling in advancing infrastructural materials. Hsuan began with a general organizational overview before focusing on specific areas of interest.

Areas of interest include mechanics and engineering materials research—aimed at advances in the transformation and use of engineering materials efficiently, economically, and sustainably; and resilient and sustainable infrastructures research—designed to advance fundamental knowledge and innovation for resilient and sustainable civil infrastructure and distributed infrastructure networks.

According to Hsuan, the SMM Program supports fundamental research to understand the behavior of civil infrastructure materials in responding to mechanical, hydrothermal, and time-dependent loads in the build environment. Hsuan stated the program also investigates material life-cycle performance and sustainability. Particular emphasis areas are new materials and methods to enhance sustainability and model-based simulation of aging and deterioration mechanisms. Hsuan noted the program predominantly serves the civil, mechanical, and materials engineering community and aims to integrate materials science and engineering to create innovative infrastructural materials. As shown in figure 8, research areas supported include fiber-reinforced plastic and polymeric composite, concrete, cementitious materials, asphalt materials, and other materials.



Source: Grace Hsuan, National Science Foundation

Figure 8. Research areas supported by the Structural Materials and Mechanics Program.

Hsuan went on to highlight specific program directions. These include sustainable alternative cementitious materials and asphalt binders, bio-based composites and functional graded materials, incorporating modeling to accelerate materials design, and linking chemistry and mechanics to model materials life-cycle performance. Workshop participants were informed that 20 projects have been funded in the past 10 years, examining cementitious and concrete materials, and asphalt. Hsuan also highlighted several other relevant programs within NSF, including Mechanics of Materials, Materials Surface Engineering, Designing Materials to Revolutionize and Engineer the Future, and Computational and Data-Enabled Science and Engineering.

Some Observations About Modeling—Highway Pavement and Structural Materials

Richard Meininger
Federal Highway Administration

Richard Meininger, at FHWA's Turner-Fairbank Highway Research Center (TFHRC), continued the presentations by examining modeling in relation to highway pavement and structural materials. Meininger began by outlining some problems to avoid, such as an example of delaminating and shallow cracking 2–3 in (5–8 cm) deep on I-90 in New York. A section of concrete approximately 7 in (18 cm) long was cut from I-90 for a coefficient of thermal expansion (CTE) test. Figure 9 shows the exposed coarse aggregate particles on the wearing surface of this section of concrete.

Figure 9. Photograph showing the top and bottom ends of a section of concrete from I-90.

According to Meininger, FHWA infrastructure research areas focus on pavement and structures. *Pavement* research aims to emphasize performance and includes safety, rideability, durability, and sustainability. Asphalt layers, concrete pavements, and aggregates are also focus areas. *Structure* research focuses on fighting corrosion in metals and examines safety, durability, and sustainability in addition to precast and post-tensioned concrete and structural performance of steel.

Meininger went on to explain some ways to encourage multiscale model use. Methods include designing for performance and then assuring performance through models, tests, and service. He noted it is also important to consider long-term design–build involvement where bidders are more interested in using models. Meininger suggested another way to encourage multiscale model use is to provide demonstration packages for FHWA and State Departments of Transportation (DOT) to use in FHWA's mobile asphalt and concrete laboratories. Models could also be used in forensics to understand why a failure occurred.

Workshop participants were informed about the characterization of materials for model inputs. Some may be more regional in nature depending on aggregate quality and availability, climate and soils, and cementitious sources and preferred blends. Meininger noted sophisticated measuring tools may not always be available to all practitioners and also highlighted that standardized methods and reporting is needed. Additionally he suggested advantages should be demonstrated to State DOTs.

Meininger provided an overview of the laboratories housed at TFHRC. These laboratories provide a vital resource for advancing the body of knowledge to help address national transportation goals. Meininger informed workshop participants that existing concrete research at TFHRC includes rheology of pastes and mortars, calorimetry to characterize reactions, petrography of polished and thin sections, chemistry laboratory and asphalt research, high-volume fly ash mixtures, and ground limestone. Additionally, Meininger explained that two cooperative research and development agreements exist on alternative cementitious materials: *Solidia*—a cement based on carbonation; and *Ceratech*—a cement based on Class C fly ash.

Meininger also discussed FHWA's Aggregate and Petrographic Laboratory at TFHRC. One featured case study involved using petrography as a tool for investigation of source of lime in hot mix asphalt cores. Workshop participants were shown photographs of asphalt cores containing lifts per core.

Meininger noted there is support for hydration modeling and development of a roadmap. Examples of this support include the VCCTL, International Summit on Cement Hydration Kinetics and Modeling, and an ongoing Princeton University–NIST project. Meininger also mentioned some specific examples of ongoing research at the TFHRC Concrete Laboratory, including the examination of rheology, calorimetry, and time of set. Additional research highlighted by Meininger examines how high fly ash content concrete performance is improved with powdered limestone included in a ternary cementitious blend.

Next, Meininger highlighted some potential FHWA goals over the next 50–100 years. For example, goals for pavements over the next 50 years could include design and analysis for truck traffic, with a move from mechanistic and empirical toward performance. Pavement goals could also focus on durability, specifically loadings, climate, and de-icing chemicals. An economic means of restoring friction and ride and best use of regional aggregates and binders were other pavement goals put forward by Meininger. Over the next 100 years, goals for structures could include effective inspection and mitigation of problems; solving tendon and cable chloride and corrosion; and using high-quality precast sections with durable grouts and mortars to join together the sections.

Meininger also discussed some existing EAR Program and modeling projects already underway. These projects involve aggregate research—including the blending of fine aggregates in concrete, the interface of asphalt and aggregate, and modeling of granular aggregate base. Meininger also explained there is support for researching basic asphalt properties as demonstrated by research undertaken by the Asphalt Research Consortium and Western Research Institute. Meininger went on to highlight another EAR Program project exploring high-performance stress-relaxing cementitious composites.

Finally, Meininger provided an overview of some of the transportation pooled fund (TPF) projects in this field. The TPF allows Federal, State, and local agencies and other organizations to combine resources to support transportation research studies. According to Meininger, there are 169 TPF records on concrete, 103 records on asphalt, and 60 records on base.[1] Specific projects

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[1] http://www.pooledfund.org/

include studying the permeability of concrete at Indiana DOT, effects of different de-icing and anti-icing chemicals on concrete at South Dakota DOT, and ternary blends in concrete at Iowa DOT.

The presentation concluded with an opportunity for questions and an overview of the TFHRC infrastructure research teams.

Multiscale Modeling of Multiphysics: From Atoms to Continuum

James Lee
George Washington University

James Lee, at George Washington University's Department of Mechanical and Aerospace Engineering School of Engineering and Applied Science, outlined some of the motivations for multiscale modeling of multiphysics. Lee stated that nanomaterials manifest fascinating and beneficial properties, which can be exploited for a variety of applications. These include sensors, actuators, and energy harvesters. Lee noted that from design and synthesis to application of nanomaterials, theoretical modeling of multiphysics is at the core of the broad field of nanoscience.

Lee proceeded to explain two avenues of multiscale modeling: (1) sequential or hierarchical multiscale modeling—where separate calculations are made at each scale and results are passed between scales, as shown in figure 10; and (2) concurrent multiscale modeling—where calculations are integrated and solved simultaneously to include different resolutions and physical descriptions.

Lee's presentation also explored MD and the interatomic potential, non-equilibrium MD, re-formulation of the Nosé-Hoover thermostat,[2] Maxwell's equations at the atomic scale,[3] and the Lorentz force of a charged particle.[4] Lee also discussed induced electromagnetic quantities, coarse-grained MD simulation, multiple length scale modeling, and multiple time scale algorithms. Several sample problems were also put forward to workshop participants. These problems included mechanical wave propagation, heat conduction, electromagnetic waves, and failure behavior.

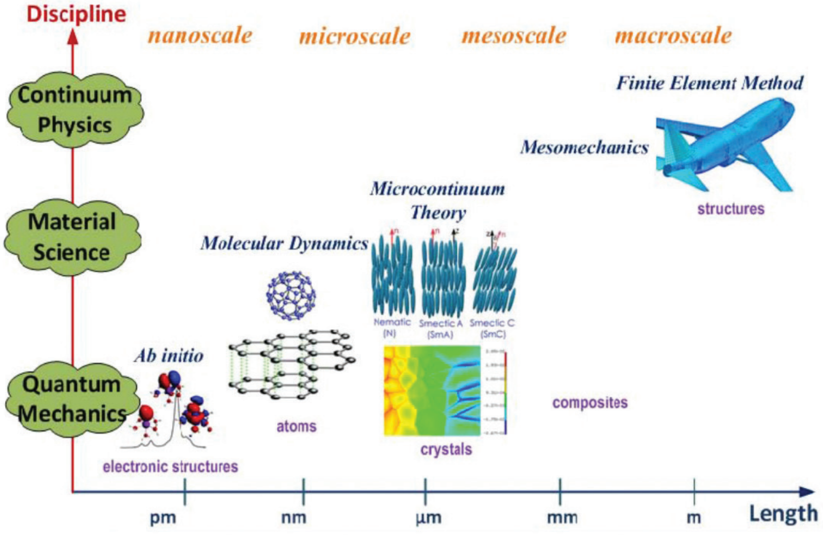

Figure 10. Examples of sequential or hierarchical modeling.

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[2] A deterministic method used in molecular dynamics to keep the temperature around an average.

[3] A set of partial differential equations that describe how electric and magnetic fields are generated and altered by each other and by charges and currents.

[4] The combination of electric and magnetic force on a point charge due to electromagnetic fields.

Multiscale Characterization, Modeling and Simulation of Stone-Based Infrastructure Materials

Linbing Wang
Virginia Polytechnic Institute and State University

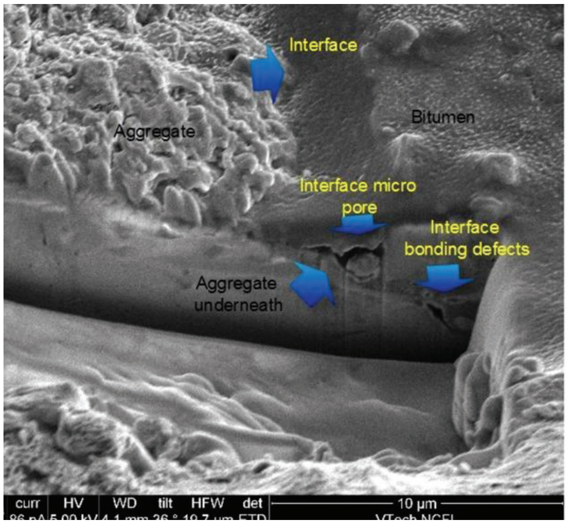


Figure 11. A focused ion beam shows the micro-pore located at the asphalt phase along the asphalt-rock interface.

© Virginia Polytechnic Institute and State University

Linbing Wang, at Virginia Polytechnic Institute and State University's (Virginia Tech) Department of Civil and Environmental Engineering, began by addressing the motivation for multiscale characterization, modeling, and simulation of stone-based infrastructure materials. Wang discussed the importance of infrastructure materials in civil engineering, heterogeneity, constituent properties and configurations, representative volume elements, and a unified modeling and computational simulation framework.

Wang provided an overview of some of the multiscale characterization tools used at the quantitative imaging and computational simulation laboratory at Virginia Tech. Tools at the laboratory include an atomic force microscope, a laser scanner, a thermal imager, a gas gun and high-speed imaging system, and a biomedical imaging laboratory. Wang explained that by using a focused ion beam (FIB) it is possible to view a micro-pore located at the asphalt phase along the asphalt-rock interface, as shown in figure 11. Additional tools presented to workshop participants included the environmental scanning electron microscope and transmission electron microscope.

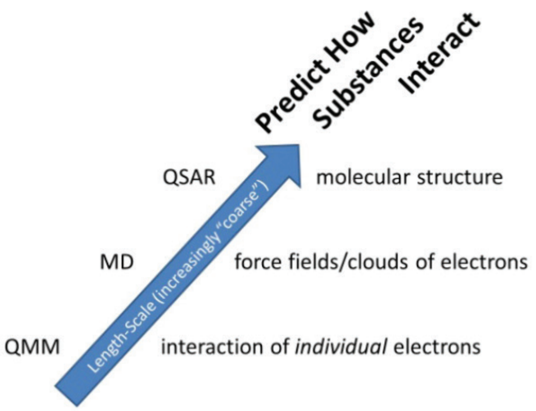
Wang moved on to explain meso, microscale, and molecular dynamics and provided an overview of a molecular dynamics simulation. He also discussed meso- and microscale digital specimen testing. Wang informed participants that a digital specimen is the digital representation of the real 3D microstructure of a physical specimen. A digital test involves the computational simulation of a mechanical test, based on digital specimens, and considers every detail of a microstructure and its evolution. Wang provided examples of simulations capable of testing high-velocity penetration of concrete and explained how individual particle reconstruction can be used to reconstruct the volume and mass center of each particle in 3D. A digital compression test, designed to simulate micro kinematics and global and local strains and deformations, was also described by Wang. One final test featured in Wang's presentation involved direct shear and showed how a model can compare particle movement across a shear plane.

Computer Aided Molecular Design: A Course-Grained Strategy for Accelerating the Discovery of Admixtures for Improved Durability and Performance of Pavement Materials

Joseph Biernacki
Tennessee Technological University

Joseph Biernacki, at Tennessee Technological University, began his presentation with a concise definition of computer-aided molecular design. According to the International Union of Pure and Applied Chemistry, this involves “all computer-assisted techniques used to discover, design and optimize compounds with desired structure and properties.”[5]

Next, Biernacki provided an overview of the scale of approximation that predicts how substances interact, as shown in figure 12. Biernacki showed workshop participants how the increasingly coarse length scale progresses from quantum mechanical methods (QMM) and the interaction of individual electrons, to MD with force fields and clouds of electrons, to quantitative structure activity relationships (QSAR) and the molecular structure.



© Tennessee Technological University

Figure 12. The scale of approximation.

Biernacki likened finding the next admixture breakthrough to finding a needle in a haystack, a process that requires a slow and incremental approach. Participants were told there might be a better way using QSAR to correlate the behavior and molecular descriptor of compounds. Using an inverse-QSAR (I-QSAR) design strategy as a case study, Biernacki questioned whether new shrinkage reducing admixtures can be identified. Biernacki showed workshop participants the compound training set and signature molecular descriptor and then how the I-QSAR was developed and used to find and validate new compounds. This enables researchers to predict behavior and identify and test new compounds for efficacy using mix formulation, autogenerous and drying shrinkage.

Biernacki concluded that an I-QSAR-based computer aided molecular design strategy offers a predictive approach for the design of shrinkage reducing admixtures and may provide similar benefits for the admixture industry at large.

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[5] Compendium of Chemical Terminology. International Union of Pure and Applied Chemistry, 2012. Retrieved November 2013 from http://goldbook.iupac.org/CT06954.html.

Part Two: Discussions

Following the presentations, there was an opportunity for group discussion. Workshop participants and presenters discussed several topics over the 2-day workshop. Five overall themes are summarized in the following pages.

Role of Modeling

Workshop participants and presenters discussed the role of modeling and why these models are being developed and exercised. Participants suggested that there are essentially two purposes for multiscale modeling.

First, the models are used to support engineering tools that will allow the construction of better roads, as shown in figure 13. For example, an admixture company might want to understand the effect on a concrete mixture of adding 20-percent fly ash. A team preparing to lay pavement could use a model-based engineering tool to compute suggested parameters for the paving process. The second purpose is to develop an improved understanding of the physics of the materials processes involved. Participants noted modeling can be used for hypothesis testing when experimentation is infeasible.

Motivation for Materials Research

The group noted the importance for researchers to be aware of the end goal of materials research is better roads. The group noted several traditional performance goals during discussion, including friction, rideability, durability, sustainability, and reduced construction time and cost. The group also noted the potential for new material functions or smart materials. One question put forward was how do computational material models help establish or support quantitative performance targets for the materials being studied and developed?

Measurement and Modeling Feedback

The group went on to discuss the essential relationship between materials modeling and

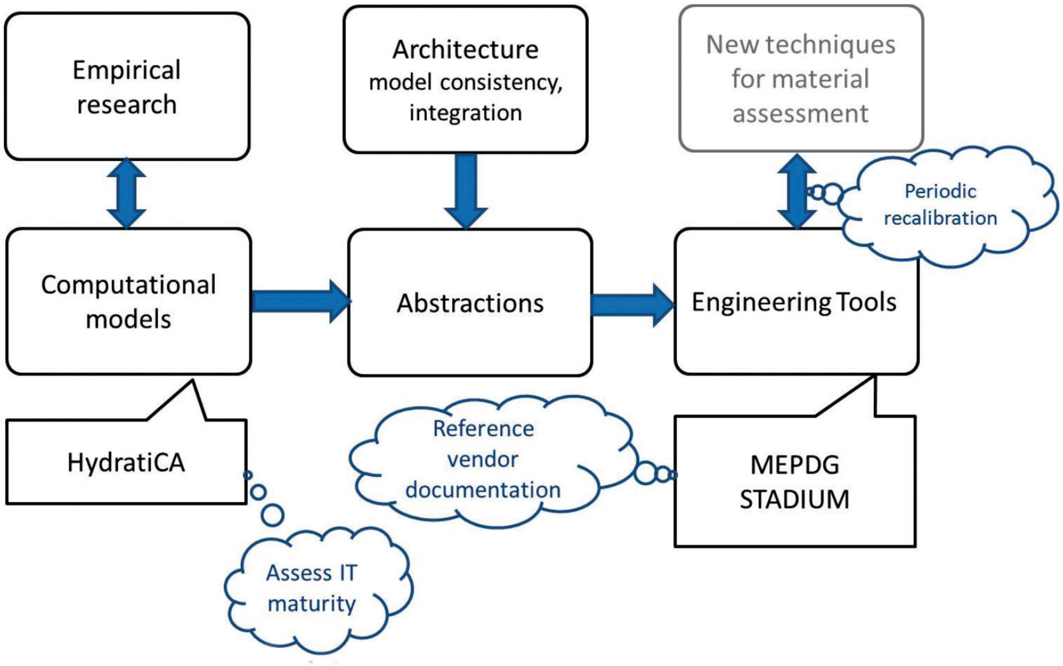

Figure 13. The relationship between computational models and engineering tools.

measurements. For example, modeling can assist in the interpretation of measurements by providing insights into dynamics at scales below that at which measurements were taken.

Addressing the following two specific needs could improve the relationship between materials modeling and measurements. First, for modeling to advance, new experimental data are required. Current models have been built on measurements that were designed and in some cases conducted years or decades ago. As understanding of material dynamics has evolved, so too must the experiments that validate that understanding so we can go beyond current frontiers. Second, to predict the long-term performance of materials, there must be a tighter coupling between tests and modeling.

Participants noted the point where admixture design parameters could be entered into a model-based engineering tool to reliably predict durability is far away; however, it is possible to do a much better job of predicting long-term performance with interim performance data. If a sample of material was aged and tested and then modeling conducted on the basis of those test results, it would enable researchers to look much farther into the future.

Questions put forward by workshop participants included asking what experiments will provide critical improvements to existing computational models of material performance? Additionally, what new methods of material measurement would allow for new or expanded material modeling capabilities? Another question was what aging and testing protocols would best position modelers to make long-term performance predictions?

Finally, the group discussed development and maintenance of a set of reference materials and problems as a means of comparing models and thereby advancing the state of the art.

Grand Model Versus Focused Models

Workshop participants discussed the state of the practice in modeling. They determined there may be value in developing a grand model that stitches dynamics across the length scales, although participants questioned the feasibility of developing a useful grand model.

Participants noted a grand model could possibly be constructed by marrying the models from the workshop that work at the micron level and below with the NIST effort, which works at larger length scales. This might work well as a modular system but participants noted not all analyses would necessarily be best accomplished with a grand model. Accordingly, focused computational models or tools that deal with a particular mechanism or problem would continue to have a place. Participants also noted that many questions can be answered without considering multiple scales.

Participants went on to discuss how models can be used to improve understanding of many properties. The following properties were discussed:

- Control of supplementary cementitious materials.
- Curing strength and fracture.
- Heat propagation.
- Shrinkage and surface tension.
- Explaining mix failures.
- Long-term durability for environmental and loading damage.

Several questions were raised as a result of this discussion. Participants questioned whether focused models are extendable and, if so, which ones are. Moreover, they asked what it is about a model that most influences its extendibility. Additional questions asked if it is conceivable that a grand model could work for any combination of aggregates and cement, and what elements a grand model needs to operate concurrently or sequentially. During discussion, it was noted that to understand cracking, model elements must run concurrently. Participants questioned if existing models allow for integration—they asked if there is a need for common or coordinated approaches for integration or a need to improve the ability to abstract computation models for improving engineering tools. Participants also queried how engineering tools have used computation model improvements. One final question asked if the grand model is an integration of focused models or if it requires an entirely separate approach.

Gaps and Opportunities for Advancing the State of the Practice

The final discussion theme examined some of the challenges ahead. Participants considered the various scales at which the models operate and concluded the most challenging length scale is the upper end of the mesoscale, near 50 nanometers (nm). Participants questioned whether anyone was focusing modeling efforts at scales near 50 nm and attempted to identify the key challenges in that modeling. Additionally, participants queried whether anyone is developing computational models for the interface between aggregates and binders.

Discussion proceeded to address the topic of applying microscale modeling to engineering problems. A critical question identified here is how and when to abstract heterogeneous materials. For example, finite element models need homogeneous cells to predict deformation. Variability was a feature identified as an essential part of asphaltic and cementitious material engineering and analysis; however, stochastic modeling was put forward as one method that could be used to manage the uncertainty associated with that variability.

Next Steps

Following discussion, workshop participants identified a couple of follow-on activities as next steps following the workshop.

These activities included: (1) characterization of existing computational material model research; and (2) additional discussion to gain feedback from people developing engineering tools.

Appendices

Appendix A—Agenda

MULTISCALE MATERIALS MODELING WORKSHOP

Turner-Fairbank Highway Research Center, McLean, VA

Tuesday, April 23, 2013

9 a.m.	**Welcome and Introductions** • Michael Trentacoste*, Director, Turner-Fairbank Highway Research Center* • David Kuehn, *Federal Highway Administration* • John Brewer, *USDOT Volpe Center*
9:30 a.m.–12 p.m.	**Degradation Mechanisms and Feedback Across the Size Scales (Atomistic, Nano-, Micro-, Meso-, and Macro-)** • Professor Gaurav Sant, *University of California, Los Angeles* • Professor Hamlin Jennings, *Massachusetts Institute of Technology* • Professor Franz-Josef Ulm, *Massachusetts Institute of Technology*
	Break • Professor Florence Sanchez, Vanderbilt University
	Discussion
12–1 p.m.	**Lunch**
1 p.m.–2:30 p.m.	**Panel Discussion: Why Would Engineers Want to Use Multiscale Modeling?** • Dr. Edward Garboczi, *National Institute of Standards and Technology* • Larry Roberts, *Roberts Consulting Group* • Professor Konstantin Sobolev, *University of Wisconsin–Milwaukee*
	Discussion
	Break
2:30–4 p.m.	**Computational Modeling and Analyses for Correlation Across Size Scales** • Professor David Allen, P*avement Scientific International (formerly of University of Texas–Pan American)* • Dr. Bob Welch, *U.S. Army Corps of Engineers* • Dr. Grace Hsuan, *National Science Foundation*
	Discussion
4–4:30 p.m.	**Review of the Day**

Wednesday, April 24, 2013

9–9:10 a.m.	**Review and Objectives**
9:10–9:30 a.m.	**Context from Other Conferences and Workshops** • Richard Meininger, Federal Highway Administration
9:30–11 a.m.	**Strength, Failure, and Durability of Pavement Materials** • Professor James Lee, *George Washington University* • Professor Linbing Wang, *Virginia Polytechnic Institute and State University* • Professor Joseph Biernacki, *Tennessee Technological University*
	Discussion
	Break
11 a.m.–12 p.m.	**General Discussion: Research Opportunities and Their Potential to Generate Improvements in Structural and Civil Applications** • What is the potential from current research to generate improvements in structural and civil engineering applications for highway transportation? • Which scientific questions will have the greatest impact on the use of Multi-Scale Modeling in highway engineering applications?
12–12:30 p.m.	**Summary and Adjourn**

Appendix B—Workshop Participants

David	Allen	Pavement Scientific International (formerly of University of Texas–Pan American)
Joseph	Biernacki	Tennessee Technological University
John	Brewer	USDOT/Volpe Center
Walairat	Bumrongjaroen	Catholic University of America
Edward	Garboczi	National Institute of Standards and Technology
Zachary	Grasley	Virginia Polytechnic Institute and State University
Terry	Halkyard	Federal Highway Administration
Grace	Hsuan	National Science Foundation
Hamlin	Jennings	Massachusetts Institute of Technology
Franz-Josef	Ulm	Massachusetts Institute of Technology
David	Kuehn	Federal Highway Administration
James	Lee	George Washington University
Kunik	Lee	Federal Highway Administration
Tyler	Ley	Oklahoma State University
Jiaoyan	Li	George Washington University
Dick	Livingston	University of Maryland
Yang	Lu	National Institute of Standards and Technology
Richard	Meininger	Federal Highway Administration
Roland	Pellenq	Massachusetts Institute of Technology
Jonathan	Porter	Federal Highway Administration
Cheryl	Richter	Federal Highway Administration
Larry	Roberts	Roberts Consulting Group
Florence	Sanchez	Vanderbilt University
Gaurav	Sant	University of California, Los Angeles
R. Panneer	Selvam	University of Arkansas
Roberto	Soares	Pavement Science International
Konstantin	Sobolev	University of Wisconsin–Milwaukee
Michael	Trentacoste	Federal Highway Administration
Linbing	Wang	Virginia Polytechnic Institute and State University
Charles	Weiss	U.S. Army Engineer Research and Development Center
Bob	Welch	U.S. Army Engineer Research and Development Center
Jack	Youtcheff	Federal Highway Administration

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