

HIPERPAV III—An Enhanced FHWA Software for Simulating Early-Age Concrete Pavement Behaviors

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Synopsis—This paper describes the enhancements made to the FHWA’s HIPERPAV software program for simulating early-age concrete pavement behavior. It gives a brief background describing the software, discusses the modeling improvements that have been made, and suggests future work for additional improvements. An enhanced moisture transport model has been developed and incorporated into the HIPERPAV software, and results show that the moisture distribution and associated stress/strength developments are significantly affected by the model parameters, environmental, and construction conditions. New inputs were included in the software to define the experimentally determined hydration curve parameters to improve predictions of degree of hydration and portland cement concrete (PCC) temperature development. A batch mode was added for analysis of multiple strategies at once, and a comparison module was created that allow users to compare simulation results from multiple strategies and run sensitivity analysis for multiple variables.

Keywords: heat evolution; HIPERPAV; moisture model; sensitivity analysis.

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INTRODUCTION

Originally created in the mid 1990s, HIPERPAV is a software program that allows users to predict early-age concrete pavement behavior based on user-defined inputs for environmental, design, and construction conditions [1]. The user inputs variables such as ambient weather conditions, thickness of pavement, mix design, time of placement, and type of curing. Mathematical models calculate the progression of the concrete's strength gain and developing stresses for the first 72 hours after placement. If the stresses are greater than the strength for any given point of time within the first 72 hours, the concrete has an increased potential for early-age cracking. HIPERPAV alerts the user to this potential for jointed plain concrete pavement (JPCP) and continuously reinforced concrete pavement (CRCP).

While a very useful tool in its original version, it was realized that the HIPERPAV software could be improved to better fit the needs of its users. As user's needs have evolved, upgrades to the software have resulted in newer versions such as HIPERPAV II and now HIPERPAV III.

HIPERPAV III includes several features that improve it over its predecessors. Listed below, each feature is further described in subsequent sections:

- An improved interface allows users to navigate through the software with more ease;
- The incorporation of an enhanced moisture model improves the accuracy of the software's predictions;
- The ability to characterize heat evolution of a particular cement paste also improves precision of temperature predictions;
- A batch mode allows the user to analyze several strategies at once; and
- A Comparisons Module includes sensitivity analysis tools that offer the user an opportunity to quickly discern differences in the effects of environmental, design, and construction variables on strength gain, stress development, and early-age strength-to-stress relationships.

IMPROVED INTERFACE

It has always been a goal for HIPERPAV to be as user friendly as possible. However, not all users have the same level of concrete knowledge or expertise. As a result, what may be intuitive to one user may not be understood at all by another. To help the less experienced user understand what inputs are required and why, previous versions of HIPERPAV included a help icon that linked the user to more information. It soon became apparent that a link was not enough to help the most inexperienced user navigate through the software easily or intuitively. Therefore, HIPERPAV III offers two levels for use: a Simple View for the novice users and an Advanced View for those with more experience. The user can choose which level best suits their needs by selecting accordingly from the drop-down menu that appears under the View icon within the Strategies screen (see Fig. 1).

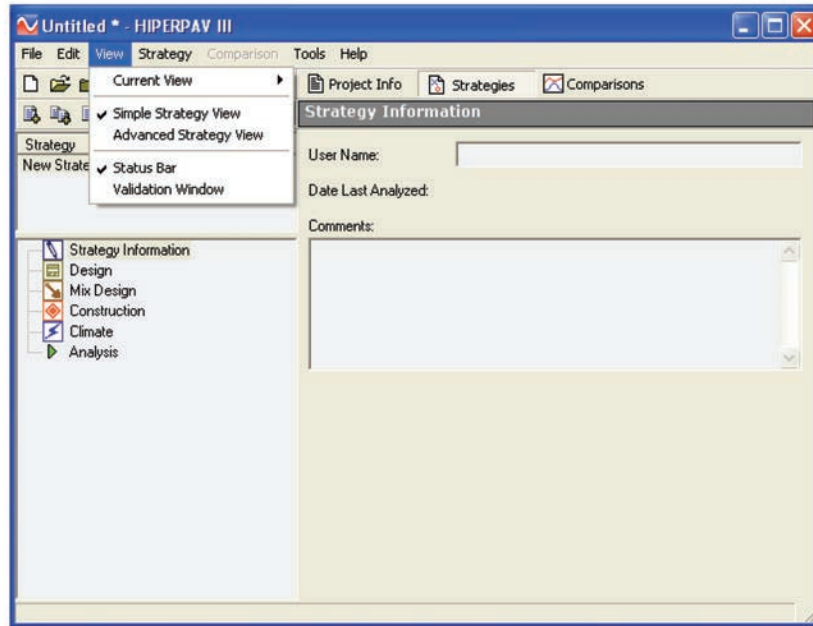


Fig. 1—Screen shot of the Simple Strategy View within HIPERPAV.

The Simple View requires limited input data and estimates variables that are otherwise inputs for the advanced level user. As a result, the user navigates through fewer screens that are arranged in tree view on the left side of the screen. The analysis screen is the final screen in the list and clues the user to initiate evaluation of the inputs.

Like the Simple View, the Advanced View lists screens in tree view. However, as seen in Fig. 2, the user is required to supply more information for the advanced level HIPERPAV application. Default values are supplied in the Advanced View for various inputs, but the user is encouraged to supply job specific information for the most accuracy.

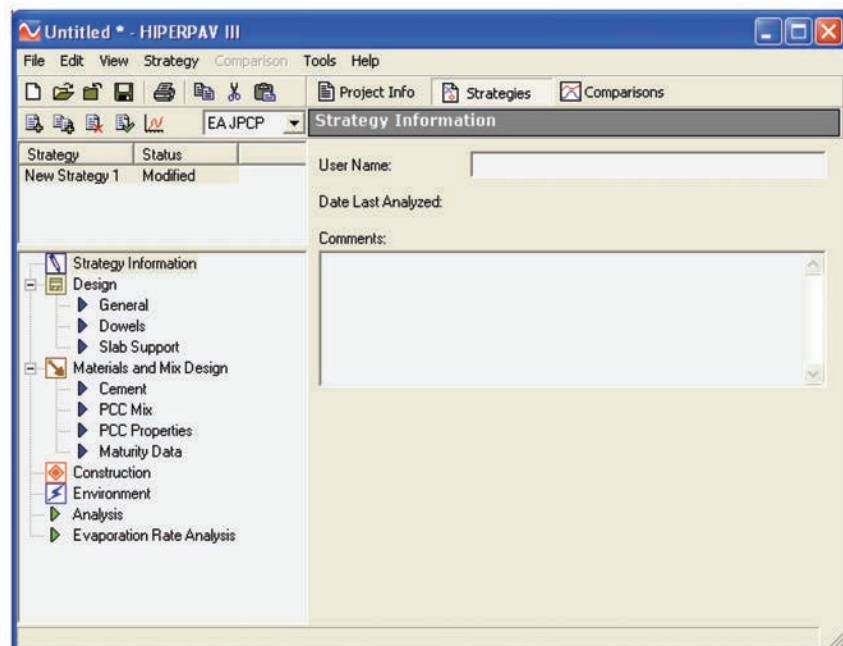


Fig. 2—Screen shot of Advanced View within Strategies of HIPERPAV. The Advanced Strategy View allows the user to enter more detailed input.

Both the Simple and Advanced Strategy Views within HIPERPAV predict early-age behavior of Hydraulic Cement Concrete Pavement. The Simple Strategy View requires fewer inputs and estimates some variables based on built-in default values. However, the Advanced Strategy View can give more accurate predictions of PCCP early-age behavior as long as some default values are replaced with job specific values.

For simplicity, both, the evaporation rate analysis during the plastic state and the analysis results for tensile stress and strength during the first 72 hours after construction are presented in one single screen in the Simple Strategy View (Fig. 3).

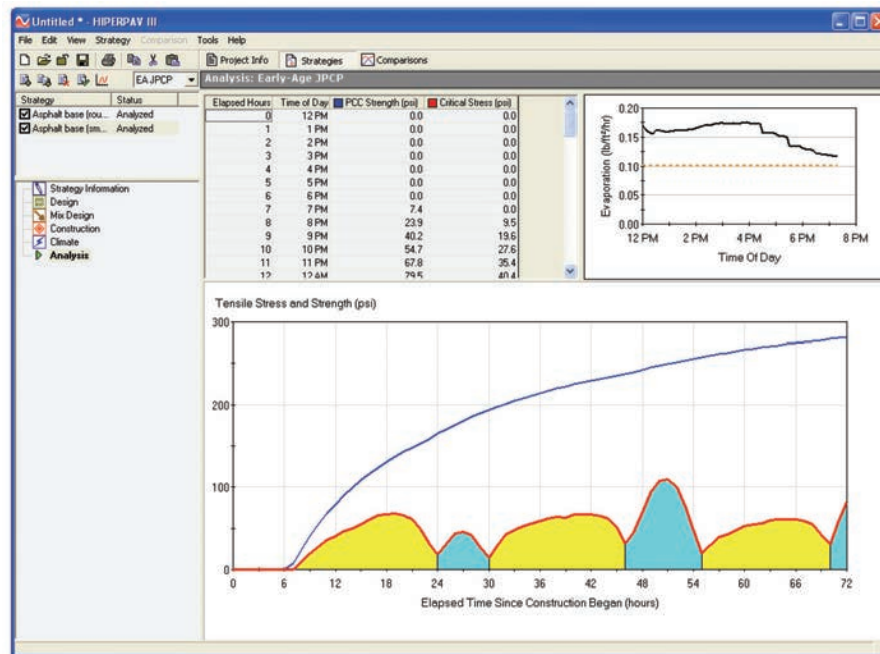


Fig. 3—Screen shot of Simple Strategy View Analysis results.

ENHANCED MOISTURE MODEL

An enhanced moisture model was developed and incorporated into HIPERPAV III to increase accuracy of early-age behavior predictions. In previous versions of HIPERPAV, mathematical models used to calculate early-age behavior focused primarily on temperature effects. However, moisture in PCC and its migration through concrete's pore structure has a great influence on PCCP early-age behavior and needs to be accounted for.

Moisture content in concrete is influenced by factors such as type of base, water-cementitious materials ratio, type of cement, admixtures, SCMs, aggregates, temperature, wind speed, relative humidity, and type of curing. Changes in moisture content are the result of drying due to hydration, evaporation, or moisture transport into the base oftentimes resulting in non linear gradients. As the concrete dries, it shrinks. This shrinkage coupled with temperature gradients cause axial, curling, and warping movements creating tensile stresses in the concrete and ultimately the potential for early-age cracking.

The potential for early-age cracking due to moisture content is calculated in HIPERPAV III by a one-dimensional finite-difference model that relates materials, environmental effects, and curing procedures for PCCP. The model is based on Fick's second Law, a self-desiccation empirical model, and moisture profiling. It is incorporated into HIPERPAV software using FORTRAN and Microsoft Excel's Visual Basic Application coding.

Model Expression

Moisture transport in the pore structure of concrete—This enhanced moisture model has accounted for the moisture transport in the pore structures of concrete, as well as moisture losses due to self-desiccation. Fick's second law is used to describe the moisture transport in the pore structures of concrete due to drying/wetting as follows:

$$\frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left(D(H) \frac{\partial H}{\partial x} \right) \quad (1)$$

where:

H = moisture content (or relative humidity in the pore structure, $0 \leq H \leq 1$);

D = diffusivity coefficient, and it is dependent on moisture content, material properties and pore structure;

x = depth of pavement slab from top to bottom; and t = time.

The diffusivity coefficient is determined by Bažant and Najjar's model which has accounted for the influence of moisture content and degree of hydration as follows [2]:

$$D(H) = D_r \left[\alpha_0 + \frac{1 - \alpha_0}{1 + \left(\frac{1 - H}{1 - H_c} \right)^n} \right] \quad (2)$$

where:

D_r = maximum diffusivity coefficient;

α_0 = a constant (0.05);

H = moisture content;

H_c = moisture at ultimate degree of hydration;

n = an integer constant.

Moisture loss due to self-desiccation—With regards to the moisture loss due to self-desiccation effect, Oh and Cha's model [3] regards moisture loss as a function of degree of hydration, which is considered to better represent the physical mechanism than some other models. Meanwhile, it is relatively a simple model with less input parameters (e.g. compared to Mjörnell's model [4]), which more appropriately fits the requirements of the present research for application with limited access to experimental test data. Therefore, Oh and Cha's model [3] was adopted in this research to capture moisture loss due to self-desiccation as follows:

$$\frac{H_s - 1}{H_{s,max} - 1} = \left(\frac{\alpha}{\alpha_{max}} \right)^S \quad (3)$$

where:

H_s = moisture content at self-desiccation;

$H_{s,max}$ = the maximum moisture content due to self-desiccation;

α = degree of hydration of cement;

α_{max} = the ultimate degree of hydration of concrete;

S = a material parameter, which is dependent on w/c ratio.

Accordingly, moisture loss can be determined in the following equation:

$$H_L = 1 - H_s = - \left(H_{s,max} - 1 \right) \left(\frac{\alpha}{\alpha_{max}} \right)^S \quad (4)$$

Moisture loss to the environment due to evaporation—The new moisture model work currently focuses on characterizing the effect of moisture on drying shrinkage and warping stresses as well as its effect on strength gain. The evaporation rate analysis in HIPERPAV takes into account environmental conditions and concrete temperature to estimate evaporation loss from the surface of the concrete based on Menzel's equation (PCA nomograph) [5]. The new moisture model does not impact the evaporation rate analysis and the goal of the work in this project was not focused on developing the required models to properly characterize this effect. Future work could be conducted to achieve this goal. The moisture has been verified using the laboratory measured data of other researchers [6].

Sensitivity analysis

The moisture distribution, and associated material stress and strength development are affected by the moisture model parameters (e.g. diffusivity and surface emissivity), environmental conditions (temperature, wind speed, etc.), and construction conditions (e.g. concrete cast time, base moisture, curing methods). As examples, the effects of diffusivity coefficient, base moisture, and curing methods on the moisture distribution and stress and strength developments are presented below.

Effects of diffusivity coefficient on moisture distribution—Figure 4 shows that moisture contents decrease with increasing diffusivity especially at the positions close to slab center. However, the slab surface and bottom have minor changes since those areas are primarily affected by the relative humidity of ambient air and base layer, respectively.

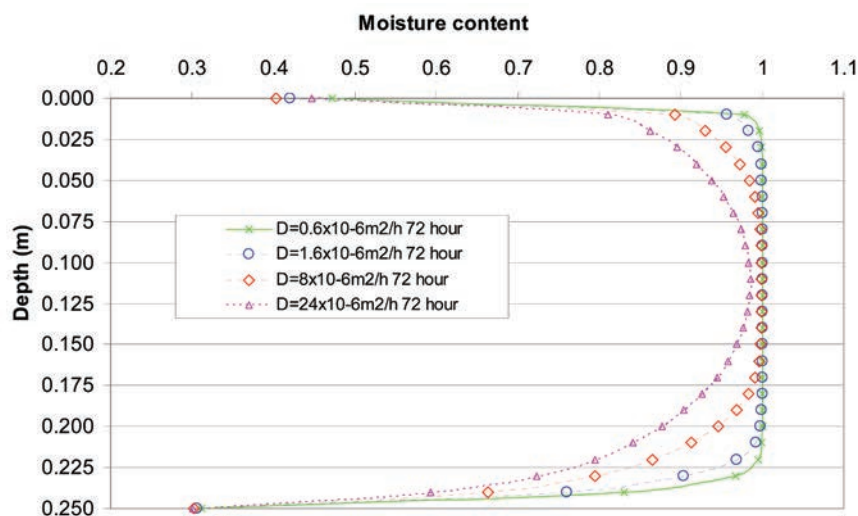


Fig. 4—Moisture profiles at the center of PCCP for different diffusivities. (Note: 1 m = 3.281 ft.)

Effect of base moisture—A large effect on stresses as a function of the base moisture was identified during the development of the moisture model. It is observed that a higher moisture content in the base layer results in higher stress/strength ratios (cracking risks) as displayed in Fig. 5 (note: the test is based on a Texas weather and material condition). Therefore, it is recommended to maintain a moist base during construction.

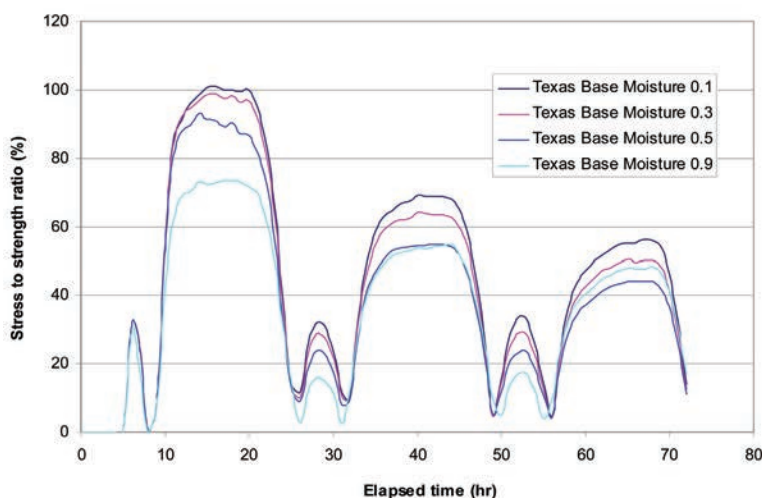


Fig. 5—Stress to strength ratios for different base moistures.

The effect of moisture loss depends on how permeable the base is. This effect would be more critical for a permeable base and will also depend on the slab thickness. For simplicity, the base moisture conditions for user inputs in HIPERPAV represent only the two extremes: critical moisture loss to the base (dry permeable base) and low moisture loss (moist non-permeable base), as shown in Fig. 6. Although the selection of base moisture in HIPERPAV is rather subjective, if the user believes there is a potential for excess moisture loss from the slab to the base, an analysis for the dry base condition should be run to evaluate the cracking risk.

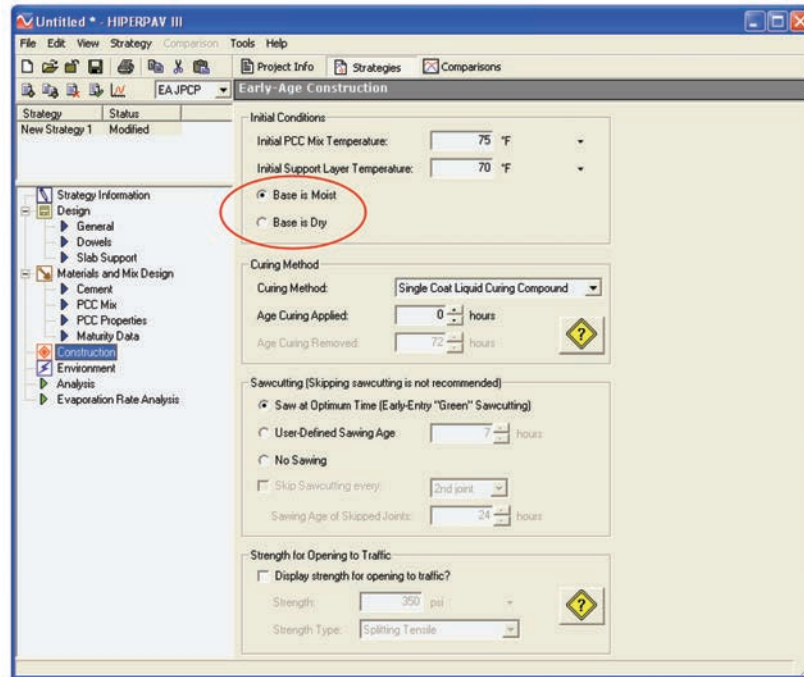


Fig. 6—Construction input for base moisture.

Effect of curing—Figure 7 shows that the stress to strength ratio (cracking risk) has pronouncedly reduced after applying curing on concrete pavement (e.g. the curing of polyethylene sheet and cotton mat has reduced the cracking risk by 48.13% and 41.23% at the peak hours of 19 and 42, respectively). These results indicate how HIPERPAV predicts that adequate curing will effectively prevent cracking risk.

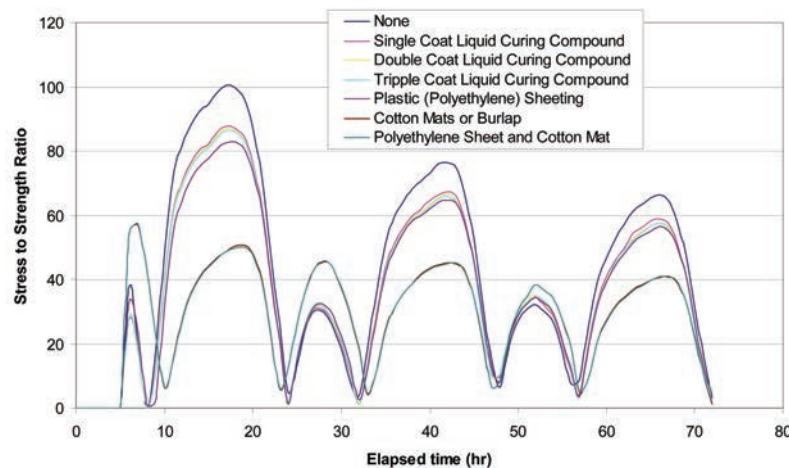


Fig. 7—Strength-to-stress ratios under different curing conditions. (WA, July 25th, 2007, 10:00 am.)

HEAT EVOLUTION CHARACTERIZATION

Heat evolution (heat of hydration) influences thermal gradients and affects tensile stresses in early-age concrete. The ability to characterize heat evolution of cement paste from semi-adiabatic calorimetry testing improves precision of the software's mathematical models in predicting how these stresses relate to strength.

Consequently, the well-known formula for degree of hydration at equivalent age t_e is applied [7-8]:

$$\alpha(t_e) = \alpha_u \cdot \exp\left(-\left[\frac{\tau}{t_e}\right]^\beta\right) \quad (5)$$

where:

$\alpha(t_e)$ = degree of hydration at equivalent age, t_e ;

t_e = equivalent age at reference temperature (21.1°C [70 °F]), (hrs);

α_u = ultimate degree of hydration;

τ = hydration time parameter (hrs); and

β = hydration shape parameter.

Hydration curve parameters can also be determined using semi-adiabatic test data. Firstly, the rate of heat generation is calculated as follows [8]:

$$P(t_e) = H_u \cdot C_p \left[\frac{\tau}{t_e}\right]^\beta \left[\frac{\beta}{t_e}\right] \alpha(t_e) \cdot \exp\left(\frac{E_a}{R} \left(\frac{1}{273.15 + T_r} - \frac{1}{273.15 + T_c}\right)\right) \quad (6)$$

where:

$P(t_e)$ = rate of heat generation at equivalent age, t_e , (W/m³);

H_u = Total heat of hydration (J/kg);

C_p = The specific heat of cement/concrete;

E_a = activation energy (J/mol);

R = universal gas constant (8.3144 J/mol/°C).

Consequently, the generated heat at a time step (from time t_i to time t_{i+1}) can be determined as follows:

$$\Delta H(t) = \int_{t_i}^{t_{i+1}} P(t_e) \quad (7)$$

Herein, the temperature rise at the semi-adiabatic condition can be determined as follows:

$$\Delta T = \frac{\Delta H(t)}{C_c} \quad (8)$$

where:

C_c = specific heat of cementitious material.

Thus, temperatures can be determined by integrating Eq. (8).

The hydration curve parameters are then back-calculated by minimizing the errors (differences) at every time step from the actual hydration curve to the theoretical hydration curve. For example, Fig. 8 shows the actual semi-adiabatic temperatures versus theoretical results for the materials used in three highway sites: Alma Center of Wisconsin, Atlantic of Iowa, and Ottumwa of Iowa [9].

Previous versions of HIPERPAV modeled heat evolution based on linear regression models relating cement and supplementary cementitious materials (SCM) chemistry to heat of hydration. However, semi-adiabatic testing of cements provides values that characterize heat evolution with more accuracy. When available, these values can be entered directly into HIPERPAV III under the Advanced Strategy View. Figure 9 shows where in HIPERPAV III heat evolution data can be entered. Figure 10 shows what information is required by the software to calculate heat of hydration based on calorimetric test data.

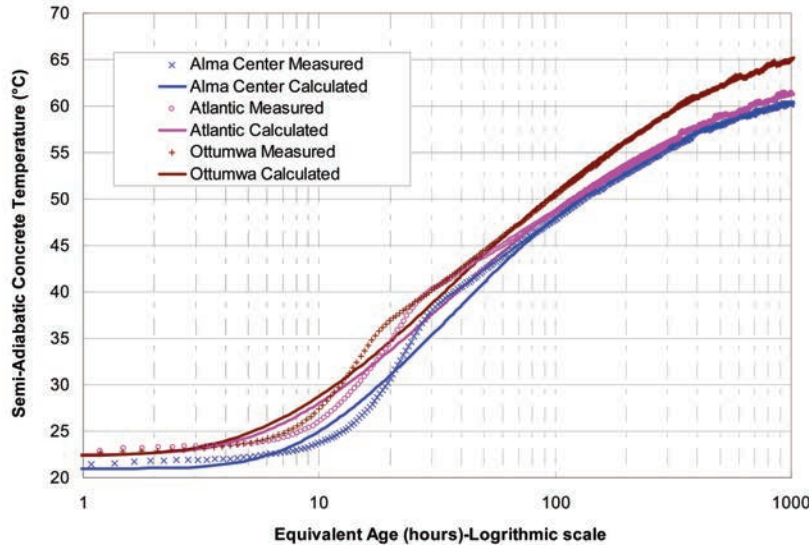


Fig. 8—Ottumwa field concrete. (Note: °F = 5/9 × °C.)

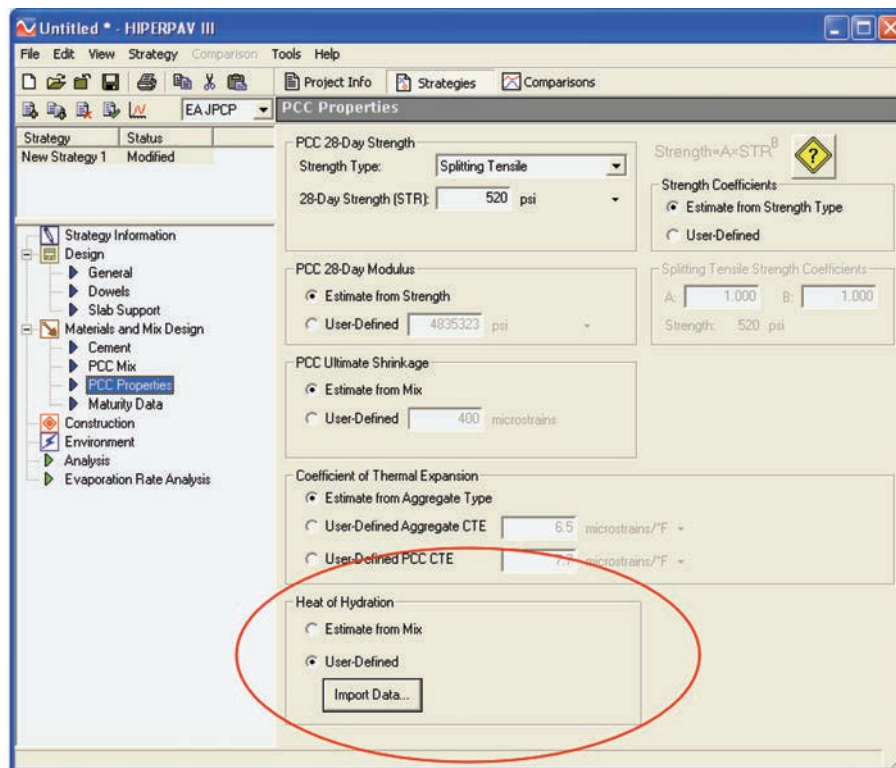


Fig. 9—Snapshot identifying where to input heat evolution characterization data. The user can input specific heat of hydration data from semi-adiabatic testing to improve accuracy.

The user inputs of hydration parameters have improved the temperature predictions verified by in-situ measurements of three highway sites [10].

BATCH MODE ANALYSIS

A batch mode for analyzing multiple strategies at once was also included in this version. If the user has multiple strategies that require to be analyzed, all the strategies can be run at once by selecting “batch mode” from the

Calorimetry Test Data

Total Heat of Hydration (J/kg)
☒ Estimate from Mix
☐ User-Defined

Activation Energy (J/mole)
☐ Estimate from Mix
☐ User-Defined

Time, tau (hours)
 Shape, beta
 Ultimate Degree of Hydration, alpha

$$\alpha(t_e) = \alpha_u \cdot \exp\left(-\left[\frac{\tau}{t_e}\right]^\beta\right)$$

where, $\alpha(t_e)$ = degree of hydration at equivalent age, t_e
 t_e = equivalent age at reference temperature (21.1°C), (hrs),
 α_u = ultimate degree of hydration,
 τ = hydration time parameter (hrs), and
 β = hydration shape parameter.

OK

Fig. 10—Snapshot of input data required for heat of hydration calculations.

Strategy Dropdown Menu (see Fig. 11). A check box will appear to the left of each strategy. Then the user checks only the strategies to be analyzed and after clicking on the Run Analysis icon, all strategies are automatically analyzed instead of having to run one by one.

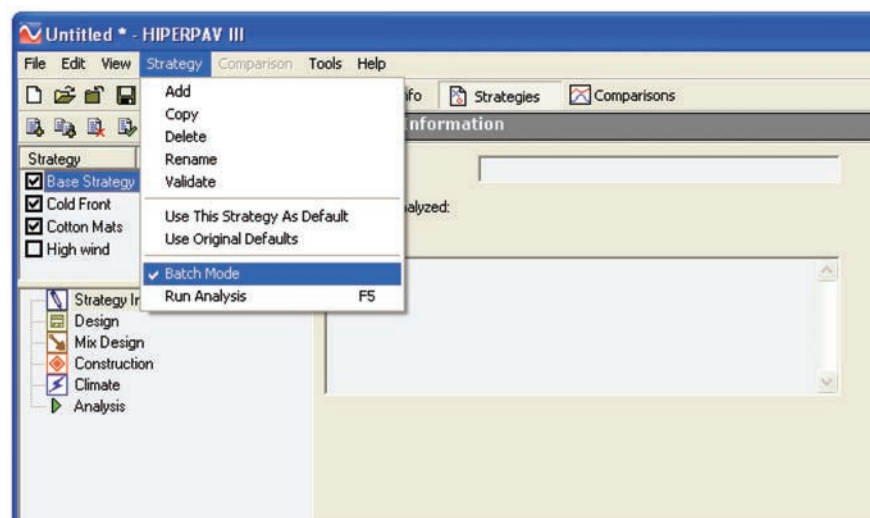


Fig. 11—Snapshot of batch mode analysis under strategy dropdown menu.

COMPARISONS MODULE

New sensitivity analysis tools can be found under the Comparisons tab located next to the Strategies tab (see Fig. 12). There are two tools: Quick Compare and Sensitivity Comparisons.

The Quick Compare screen offers the user a chance to quickly discern differences between strategies in terms of environmental, design, and construction inputs and the resulting differences on strength gain, stress development, and early-age strength-to-stress relationships. The differences are presented in a side-by-side comparison. Previous versions of HIPERPAV did not offer a side-by-side strategy comparison. Instead, the user would have to toggle back and forth between analysis screens of individual strategies to try and make any comparisons.

Quick Compare allows the user to quickly identify the differences between strategies. The advantage of this tool is the ability to compare up to ten individual strategies and how their differences affect concrete properties in a side-by-side comparison for each property. The user checks which strategies are of interest (limit of 10) in comparing and clicks the Compare button. A chart that lists the date and any input differences is generated. The user can toggle between the chart and graphs that provide a visual comparison between strategies and their

properties including strength, critical stresses, strength-to-stress differences, and stress-to-strength ratios for each of the chosen strategies.

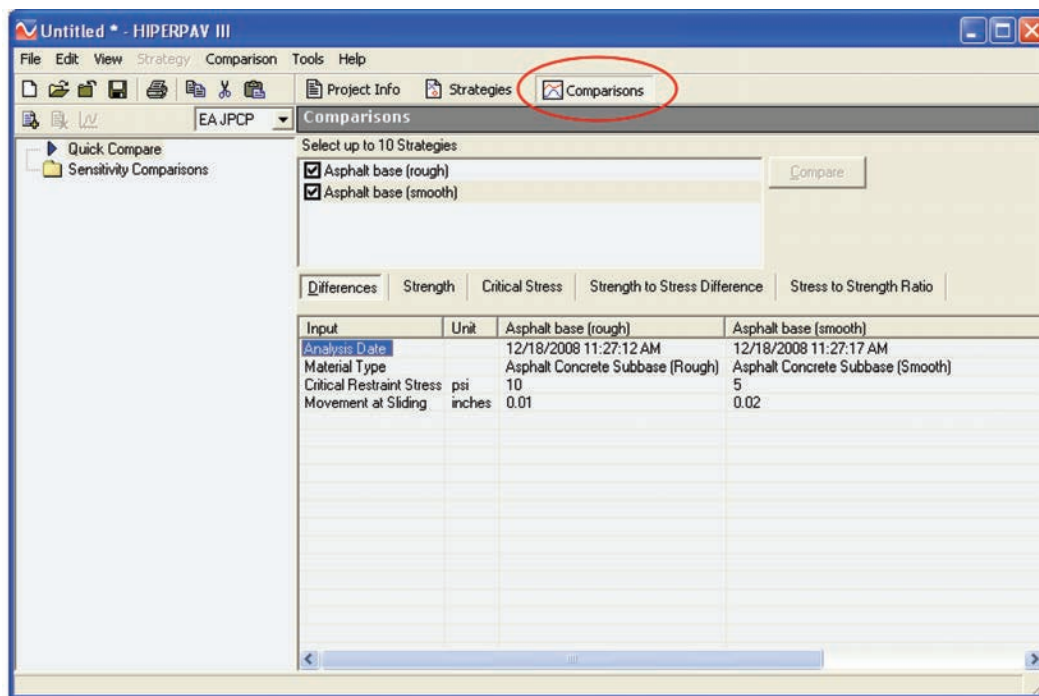


Fig. 12—Snapshot of the quick compare chart of differences.

Like Quick Compare, Sensitivity Comparisons also generates a chart and graphs through which the user can toggle to compare. However, the user is not comparing strategies. Instead, this tool compares the effects of changing input variables within one strategy. The advantage of the Sensitivity Comparisons tool is the ability to evaluate for a single strategy the effect of any input variable on concrete properties and to see that effect in a side-by-side comparison for each property.

To use this tool, the user clicks on the Sensitivity Comparisons and Adds a comparison with Add button  on the upper left corner of the screen. A Sensitivity Comparison Wizard screen pops up asking the user to select the strategy of interest. The user then proceeds to select the input variable to evaluate, and chooses a range for that variable (if applicable) and analysis interval. **Figure 13** shows a sensitivity comparison for “Initial Mix Temperature”. For this example, a range from 50 °F (10 °C) to 90 °F (32.2 °C) is used. Also, an interval of 10 °F (12.2 °C) is selected so that the wizard runs an analysis with an initial mix temperature from 50 °F (10 °C) to 90 °F (32.2 °C) at every 10 °F (12.2 °C) for a total of 5 runs.

HIPERPAV then calculates the following properties: strength, critical stresses, strength-to-stress differences, and stress-to-strength ratios for the range of the input variable.

Figure 14 presents the results from this sensitivity analysis in terms of Stress-to-Strength ratio. A summary tab is also available in this analysis to show the maximum stress-to-strength ratio for each analysis run in a bar plot as seen in **Fig. 15**. The bars are plotted in a color gradient from green to red to show the proximity to the critical stress-to-strength ratio of 100%.

Most often, users of previous HIPERPAV versions requested the ability to compare the effect of different times of construction without having to do individual strategies for each interval of time. The Sensitivity Comparisons tool gives the user that ability. The user identifies a base strategy, selects Construction Time as the variable to evaluate, and chooses a range from 1 to 6 hours.

For this sensitivity analysis, the user also has the option to use custom initial PCC mix and support layer temperatures for each analysis interval. If this information is not readily available, HIPERPAV can estimate these temperatures based on current environmental conditions for each construction time by leaving the check boxes

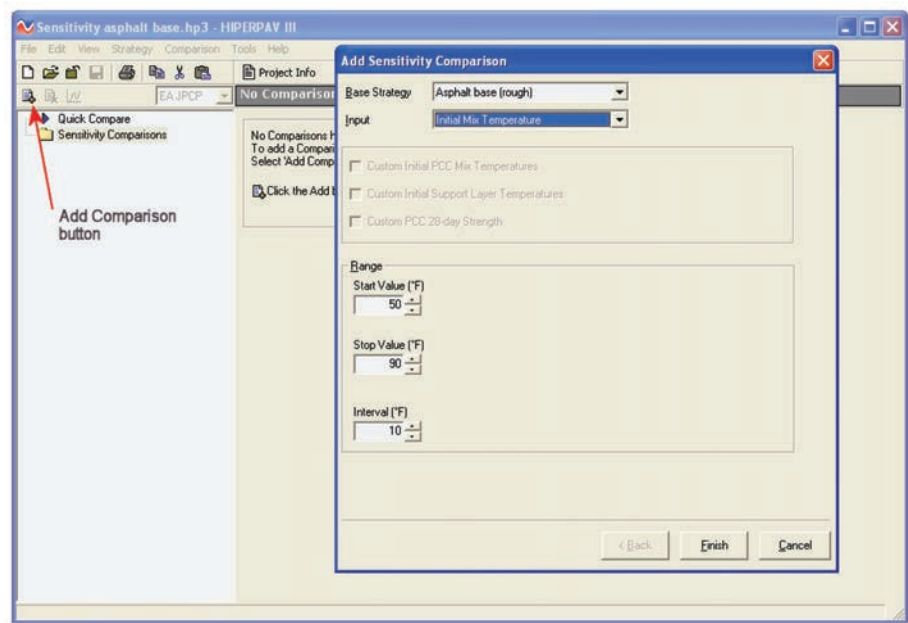


Fig. 13—Snapshot of the sensitivity comparison wizard.

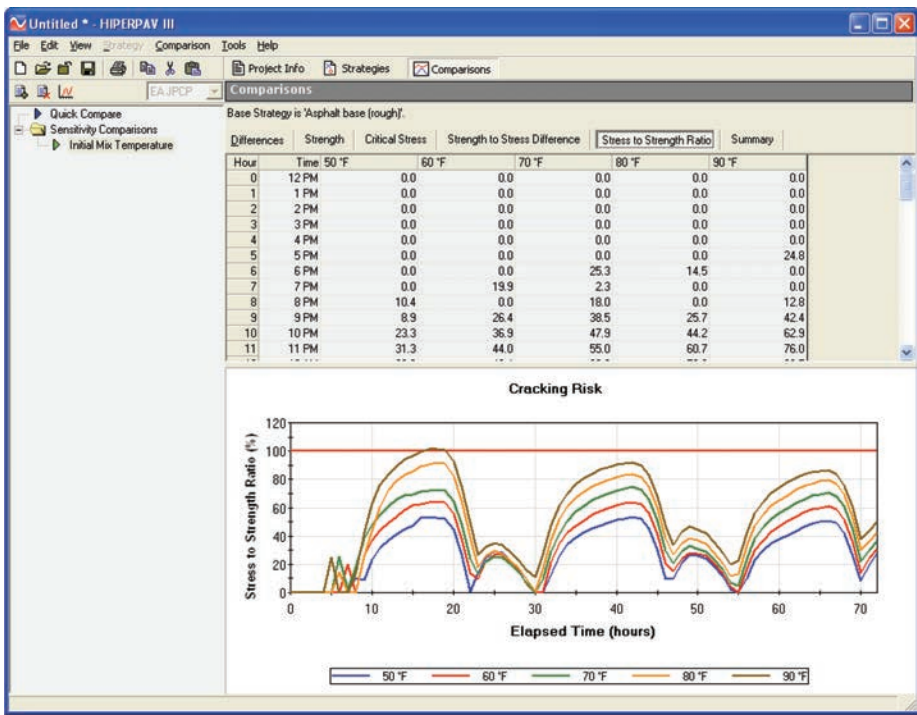


Fig. 14—Snapshot of sensitivity comparisons’ stress-to-strength screen.

under each of these inputs unchecked. HIPERPAV calculates and generates charts and graphs accordingly. Similar to the previous example, the user can see in one snapshot the effect that time of construction has on stress-to-strength ratio. Figure 16 shows a summary of the Stress-to-Strength Ratio for a time of construction sensitivity analysis. The user can quickly see that some hours in the morning there is a higher probability of exceeding the Cracking Risk line.

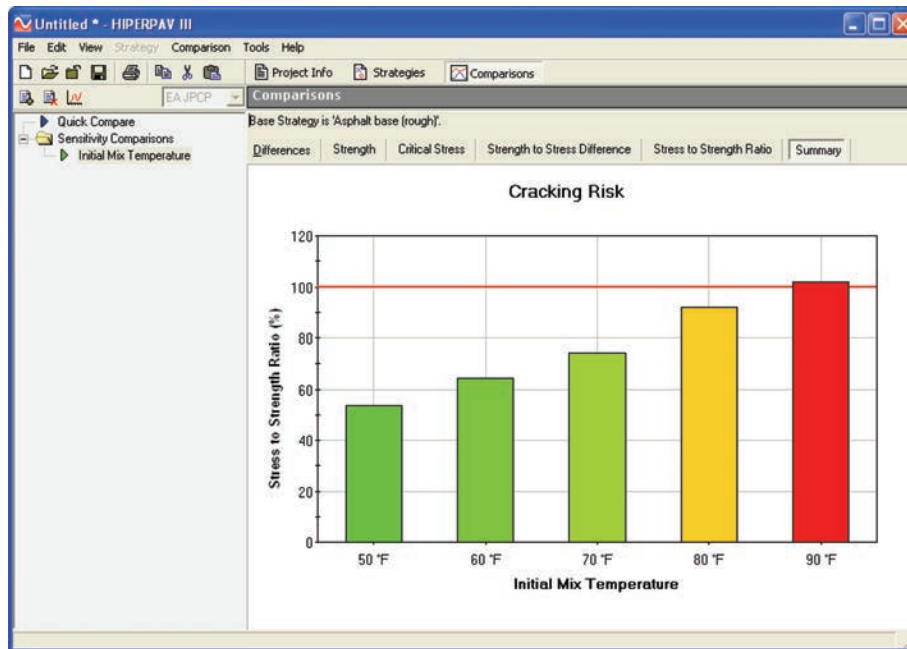


Fig. 15—Snapshot of the sensitivity summary screen for PCC mix temperature.

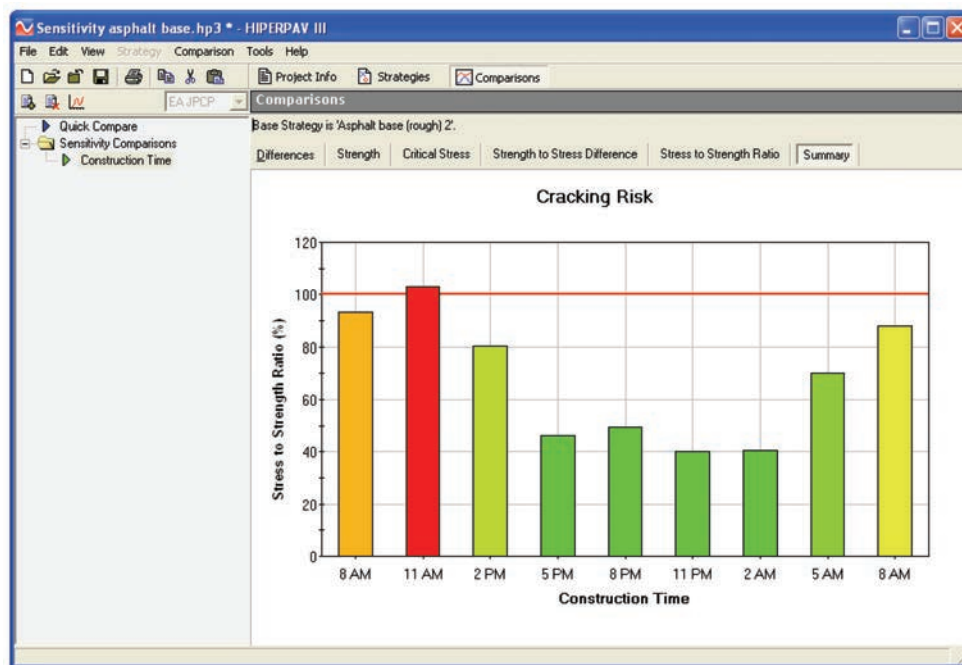


Fig. 16—Snapshot of the sensitivity summary screen for PCC mix temperature.

SUMMARY AND CONCLUSION

New features to FHWA's HIPERPAV software have resulted in an upgraded version: HIPERPAV III. Upgrade features include an improved interface that allows users to opt between a Simple or Advanced Strategy View. The Simple Strategy View is easy to use and more intuitive while the Advanced Strategy View gives the user an option to enter additional information on each of the input categories to get more accurate predictions of early-age behavior. An improved moisture model captures the interaction between pavement design, materials, environ-

mental, and construction inputs, as well as provides a more realistic characterization of moisture transport in the slab and its effect on early-age drying shrinkage, warping stresses, and strength development in the slab. The ability to input calorimetric data for the purpose of characterizing more precise heat evolution is included. A new batch mode feature speeds up the analysis process for multiple strategies at once. Finally, the “Comparisons” module gives the user the ability to see side-by-side comparisons of how strategies or their variables affect early-age pavement behavior.

Although this work has taken the HIPERPAV software to a new level, there is still potential for HIPERPAV to be even better. Future work needs to focus on topics such as cold weather and real time applications, as well as incorporating a wireless version of SmartCure. The reason for focusing on cold weather is a result of the interest of northern states in improving the accuracy of early-age behavior prediction for cold weather conditions with use of cold weather admixtures.

A real time HIPERPAV application has been highly supported by the Technical Working Group for this project where the user can initially enter the zip code and download via Internet local weather data from NOAA. In addition, this version would incorporate a wireless adaptation of SmartCure to obtain data on site-specific climatic conditions and PCC surface temperatures. This information would provide for enhanced HIPERPAV predictions in real time.

These topics for future work close the gaps in making HIPERPAV a truly intelligent system that would improve the industry as a whole.

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Virtual Testing of Concrete Transport Properties

by D.P. Bentz, E.J. Garboczi, N.S. Martys, K.A. Snyder,
W.S. Guthrie, K. Kyritsis, and N. Neithalath

Synopsis: The transport properties of concrete are critical to its field performance. Commonly encountered degradation mechanisms are dependent on ionic diffusivity, sorptivity, and permeability. In this paper, virtual testing of two of these concrete transport properties, diffusivity and permeability, will be reviewed. Virtual evaluations of ionic diffusion (and equivalently conductivity) will be presented as one example that spans the full range of applications, from computations on cement paste with micrometer resolution to a virtual rapid chloride permeability test (RCPT) that simulates the standard ASTM test method for conductivity of concrete cylinders. At the concrete scale, a hard core/soft shell (HCSS) microstructural model may be employed to estimate diffusion coefficients, while finite difference solutions of Fick's laws that incorporate sorption/reaction may be employed to evaluate remediation strategies for real world bridge decks. Virtual evaluations of permeability are dependent on a sufficient resolution of the pore sizes that are critical for flow under pressure. Two recent successful evaluations will be presented in this paper: the permeability of cement pastes (hydroceramics) cured at elevated temperatures, where transport is controlled by micrometer-sized pores, and the permeability of pervious concrete that is dominated by its coarse porosity (scale of mm). Many of the presented computational (virtual) tools are freely available over the Internet, either for direct access (remote computation) or for downloading.

Keywords: building technology; diffusion; durability; microstructure; permeability; transport; virtual testing.

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INTRODUCTION

To engineer durable concrete structures that will provide an acceptable service life, appropriate mechanical and transport properties are equally critical.¹ All common concrete degradation processes including corrosion of steel reinforcement, sulfate attack, alkali-silica reaction, and damage due to freezing/thawing (scaling) are strongly influenced by one or more of the following three major transport mechanisms: diffusion, permeability, and sorptivity. Thus, a viable approach to increase concrete service life is to reduce the values of these transport coefficients. Understanding the relationships between microstructure and transport can accelerate the achievement of such reductions. In this paper, approaches for obtaining an increased understanding of diffusion and permeability of cement-based materials based on computational materials science will be presented. This virtual testing of concrete properties can provide deeper insights into microstructure-property relationships and can also reduce expensive, laborious experimental testing.²

RESEARCH SIGNIFICANCE

While computational materials science has been applied to cement-based materials for well over 20 years, it generally has focused more on fundamental scientific issues rather than real world practical scenarios. This

paper will present results that bridge this gap between computational materials science and real world applications. In addition to having immediate application to the real world problems, these results will demonstrate the powerful (and real) potential of a computational materials-science-based approach and hopefully aid in demystifying the modeling of concrete materials and performance.

MODELING TECHNIQUES

Microstructural Models

While the focus of this paper is on transport, a brief introduction into three different microstructural models that will be employed to provide inputs to algorithms for computing transport will be presented. The first, CEMHYD3D, is a computer model for the hydration and microstructure development of cement paste that is founded on a digital-image-based approach in which a three-dimensional computational volume is divided up into a cubic grid of voxels, where each voxel contains a single cementitious phase (starting material, water, or hydration product).^{3,4} The hydration process is simulated by iteratively applying a set of rules to mimic dissolution, diffusion, and precipitation throughout the three-dimensional set of voxels. A typical CEMHYD3D microstructure is 100 elements on a side (or 1 million voxels in total) with a voxel dimension of 1 μm (3.94×10^{-5} in). Because the model microstructure is available as a three-dimensional digital image, it can be easily utilized as input to finite element or finite difference algorithms for computing mechanical or transport properties. At this voxel size, the CEMHYD3D model exhibits a percolation/depercolation transition for the capillary porosity at a value of about 20 %, in general agreement with experimental data for ordinary portland cement pastes.⁵ In a percolated system, there is a continuous pathway across the microstructure within the capillary porosity. In a depercolated system, there is no such pathway within the porosity from one side of the microstructure to the opposite one.

The second microstructural model is the so-called hard core/soft shell (HCSS) model, one documented version of which is readily available from NIST.⁶ As opposed to CEMHYD3D, HCSSModel is a continuum-based model consisting of hard impenetrable (spherical) particles, optionally surrounded by a soft shell. Originally developed to represent concrete aggregates and their surrounding interfacial transition zones (ITZ),⁶ the model has been extended and adapted for numerous concrete applications including the mitigation of spalling of high-performance concretes via the addition of polymeric fibers,⁷ the adaptation of the protected paste volume concept to internal curing,⁸ and most recently the documentation of the influence of water-cement ratio (w/c) and cement particle size distribution on particle spacing in fresh cement paste.⁹ The model represents a three-dimensional cube of concrete (mortar or paste) and the particle size distribution for the particles is chosen to match that of the real materials. For example, models as large as a 50 mm x 50 mm x 50 mm (2 in. x 2 in. x 2 in.) cube of concrete have been created, requiring well over 1 million individual particles to adequately represent a realistic concrete aggregate size distribution. For the HCSSModel, the percolation/depercolation transition for the “bulk” phase (not contained in the hard cores or the soft shells) occurs at a volume fraction of 3 % to 4 %, as it is more difficult to disconnect the bulk phase by concentric spherical shells than it is by the random growth processes employed in the CEMHYD3D model.^{10,11}

The third microstructural model is a general image-based reconstruction algorithm for creating a three-dimensional microstructural representation based on a two-dimensional image, as obtained using scanning electron microscopy, for example.¹² Assuming an isotropic material, the autocorrelation function measured on the porosity phase in the two-dimensional image is utilized to reconstruct a “representative” three-dimensional microstructure with the same porosity, surface area, and correlation as the original material. While first developed by Joshi¹³ and then extended by Quiblier¹⁴ many years ago, very recently these algorithms have found renewed applications to cement-based materials, including pervious concrete¹¹ and hydroceramics¹⁵ (high temperature cements for oil and geothermal well applications) as will be demonstrated in the results to follow. For the reconstruction-based model, the percolation threshold for the “porosity” phase has been observed to be on the order of 10%, a value intermediate between the CEMHYD3D and HCSSModel values.¹²

Diffusivity/Conductivity

Based on the Nernst-Einstein equation shown in equation (1), diffusion and conduction in porous microstructures containing a conductive solution can be solved using the same basic computational procedures.¹⁶

$$\frac{\sigma}{\sigma_0} = \frac{D}{D_0} \quad (1)$$

where σ is the conductivity of the microstructure, σ_o is the conductivity of the pore solution, D is the diffusivity of a specific ion in the microstructure, and D_o is the corresponding diffusion coefficient for the ion in bulk solution of identical composition. Based on this equation, an electrical analogy can be used to estimate the diffusivity of a three-dimensional cement paste microstructure such as that produced by CEMHYD3D, as shown in the top portion of Fig. 1. Adjacent voxels in the microstructure are simply connected together by resistors, where the resistance level indicates the relative conductivity (diffusivity) of the phases of the two voxels being connected. Specifically, resistors connecting together two capillary pore voxels are assigned a value of 1, while those connecting two voxels of the calcium silicate hydrate gel (C-S-H) are typically assigned a value of 250 to 400.^{16,17} The resultant electrical network can then be solved by finite element or finite difference techniques to obtain the conductivity (diffusivity) of the complete microstructure.¹⁸ Such an approach was used in the past to develop an equation for the diffusivity of tricalcium silicate pastes as a function of capillary porosity,¹⁶ an approach that was later extended to cement pastes, including those with silica fume additions.¹⁷

For a continuum-based microstructure, such as one generated by the HCSSModel, applying the electrical analogy is difficult. Instead, a continuum random walker (blind ant) approach is commonly employed for estimating diffusivities (conductivities) as indicated in the middle portion of Fig. 1.^{6,19,20} In these simulations, each blind ant carries his own watch and global positioning system (GPS) and steps randomly (and blindly) through the microstructure, with steps in a more porous ITZ taking less time than equivalent steps in the bulk cement paste, for example. After a large number (hundreds of thousands to millions) of steps, the diffusivity of the microstructure can be estimated from the mean distance squared per unit time achieved by all of the ants (Fig. 1). For a typical simulation, 10 000 ants are used. The HCSSModel provides an extremely flexible format for simulating real world variations, such as a concrete with internal curing, where the lightweight aggregates are not surrounded by the ITZs that are present around their normal weight counterparts, producing a significant reduction in the diffusion of chloride ions.²¹

Based on computations performed on virtual cement paste and concrete,^{17,20} the next logical step is to proceed to virtual test procedures, such as simulating the response of a field concrete to a standard ASTM or American Association of State Highway and Transportation Officials (AASHTO) rapid chloride permeability test (RCPT) as indicated in the bottom portion of Fig. 1.²² Such a virtual test has been developed by NIST and is available at <http://ciks.cbt.nist.gov/VirtualRCPT.html>. The interactive application allows the user to select their mixture proportions and testing conditions and provides predictions of the pore solution composition, its conductivity,²³ and ultimately the RCPT response. Features include the ability to reduce the testing time from the standard 6 h to just a few minutes, to avoid temperature effects, as suggested by Snyder et al.²⁴ in 2000 and more recently advocated by Riding et al.²⁵ An example of the predictive ability of the virtual RCPT test is provided in Fig. 2, which contrasts the experimental and virtual RCPT values²² for a variety of concretes from one particular study.²⁶

The final step in the modeling of diffusion is the prediction of chloride ion profiles obtained under realistic field exposure conditions. NIST has developed a web-based application (Computer Integrated Knowledge System-CIKS) for providing such predictions (<http://ciks.cbt.nist.gov/~bentz/millandfill/clpenmillandfill.html>).²⁷ The model is based on a one-dimensional finite difference solution for diffusion that includes chloride ion binding by the cementitious hydration products and reaction with the aluminate phases to form Friedel's salt. The user specifies the average exposure temperature and chloride loading for each month of the year, as well as a variety of mixture proportioning parameters.²⁷ Working with Brigham Young University, NIST has recently extended this application to consider real world remediation strategies such as surface treatments²⁸ and scarification and overlays (SO),²⁹ as will be presented further in the results section to follow.

Permeability

The basic goal in computing the permeability of a material is to apply a pressure gradient across the three-dimensional microstructure and compute the resultant flow. NIST has developed and recently distributed a three-dimensional linear Stokes solver for performing this calculation for a three-dimensional microstructure consisting of pores and solids.³⁰ A finite difference solution of the linear Stokes equations for slow, incompressible, steady-state flow is utilized to determine the x, y, and z components of the fluid velocity in each porosity voxel. Once this finite difference solution converges sufficiently, the intrinsic permeability, k , of the composite three-dimensional microstructure is calculated by volume averaging the local fluid velocity (in the direction of the flow) and applying the Darcy equation:

$$u = -\frac{k}{\eta} \frac{\Delta P}{L} \quad (2)$$

where u is the average fluid velocity in the direction of the flow (x-direction) for the microstructure obtained via the Stokes solver program, η is the fluid viscosity, and L is the length of the sample microstructure across which an applied pressure difference of ΔP exists.³¹ For a given microstructure, three separate runs of the computer codes may be conducted to determine the (different) permeabilities for pressure-driven flow in the x, y, and z directions. Obviously, for permeability predictions to be accurate, the three-dimensional microstructure used as input must adequately represent the pores (sizes, connectivity, and tortuosity) that are dominating the flow paths through the material.

RESULTS AND DISCUSSION

Diffusivity/conductivity

Many state departments of transportation (DOTs) are concerned with the penetration of chlorides (from de-icing salts, for example) into bridge deck concretes and the resultant corrosion problems and concrete degradation. Two approaches that are often considered for remediation of existing bridge decks are the application of impermeable surface treatments to prevent ingress of future chlorides and the scarification (milling) of the existing bridge deck followed by the application of an overlay (filling), to remove the most chloride-laden portion of the concrete and replace it by a (thicker) high-performance concrete.^{28,29} As mentioned above, the CIKS-Chloride computer model has been recently modified to simulate the effects of both of these remediation strategies.

The application of these computer models has been demonstrated in a project that considered differences in predicted performance for various cover depths for bridge decks with and without stay-in-place metal forms (SIPMFs).^{28,29} Relevant chloride ion diffusion coefficients were determined from chloride-ion profile measurements obtained on specimens from 12 existing concrete bridge decks (six without SIPMFs and six with SIPMFs). The CIKS system was then employed to simulate chloride concentrations at the (variable) depth of cover as a function of the exposure age and the time of application of a given remediation strategy. Example results are shown in [Figures 3 and 4](#) for the case of a 50 mm (2 in.) concrete cover. When SIPMFs are employed, higher diffusion coefficients are measured, due to the increased saturation level of the concrete. This requires the remediation strategies to be employed at earlier times to provide the same performance. [Table 1](#) summarizes the latest time at which successful remediation can be achieved with the performance criteria that the chloride concentration at the level of the top layer of reinforcement (cover depth) does not exceed 1.18 kg/m³ (2 lb/yd³). Because the scarification and overlay treatment actually removes a portion of the chlorides (in the removed top layer of the concrete), treatment can be slightly delayed when this more severe (and expensive) remediation strategy is employed. However, the differences between treatments are far outweighed by the differences in deck type due to the increase in chloride ion diffusion coefficients for decks with SIPMFs compared to those without SIPMF. This study thus emphasizes the criticality of producing a concrete with a low chloride ion diffusivity.

Permeability

Originally, the permeability computation codes were developed with the hopes of computing permeabilities as a function of degree of hydration for cement paste microstructures. While the predictions for fresh cement pastes were reasonable, experimental permeabilities fell dramatically as the capillary pores depercolated during hydration and the digital-image-based cement paste microstructural model was not able to adequately resolve a wide enough range of pores sizes to provide reasonable permeability predictions. The permeability codes then remained dormant for a number of years until recently when two new applications were found: cement pastes cured at elevated temperatures (hydroceramics) and pervious concrete.

In deep oil and geothermal well cementing applications, hydration occurs at vastly elevated temperatures, as the wells have typical working temperatures in the range of 200 to 350 °C (392 to 662 °F).¹⁵ This requires the utilization of special cements and leads to the formation of a variety of hydration products not typically encountered for room temperature hydration.¹⁵ In addition, the porosities of these materials are generally higher and the pore sizes larger than those in a well hydrated ordinary portland cement. Thus, application of the permeability computation procedures to these hydroceramic materials was of interest. The general procedure employed in reference 15 is summarized in [Fig. 5](#). Starting from a two-dimensional scanning electron microscopy (SEM) image, a binary (pore/solid) image is obtained and analyzed by determining the two-dimensional correlation function for the porosity phase. This correlation function and the experimentally measured porosity for the material (values in the range of 25% to 40%) are then used to reconstruct a three-dimensional representation of the microstructure based on the procedures described above. The permeability computation code is then employed to compute a fluid permeability for the reconstructed microstructure.

Experimental and computational results are compared in [Figure 6](#) for hydroceramics cured at 200°C (392°F) and containing either alumina or silica additions. While the alumina creates a more porous and permeable microstructure, the silica produces a denser microstructure with a dramatically reduced permeability. For both silica and alumina additions, the experimental trends are well captured by the estimates provided by the computational procedures. Further, the predictions are observed to be reasonably accurate for permeabilities spanning four orders of magnitude.

A second application where permeability is controlled by pores in a very limited size range is that of pervious concrete. Pervious concrete is basically produced by removing the fine aggregate fraction from a concrete mixture, producing a concrete with enhanced porosity and a set of connected pores that are up to several millimeters in size. In this case, an optical microscope can be utilized to capture a two-dimensional image of the porosity of the pervious concrete. The same two-dimensional image to three-dimensional microstructure algorithms can then be employed as shown in [Figure 5](#). [Figure 7](#) provides an overview of the process for a pervious concrete, along with a graph comparing previously obtained experimental and model permeability values. Once again, the predictions provided by the reconstruction/computation algorithms are in reasonable agreement with the experimental values compiled from three different sources.³²⁻³⁴ Conversely, as shown in the graph in [Figure 7](#), model predictions generated based on a version of the HCSSModel produced permeabilities that were well above those measured experimentally, most likely due to that models much lower percolation threshold as mentioned earlier. In addition to permeability, the reconstructed three-dimensional microstructures of the pervious concrete can also be analyzed to assess other issues such as the potentials for clogging and freezing/thawing damage.¹¹

SUMMARY AND PROSPECTUS

Successful applications of virtual testing of transport properties have been demonstrated for both diffusion and permeability. In the case of diffusion, a multi-scale approach allows modeling of transport from the nanoscale (C-S-H) to the macroscale (bridge decks). Finite difference, finite element, and random walk computational methods are valuable techniques for transforming microstructural representations into quantitative diffusion coefficients. Such an approach can be further extended to consider changes in transport properties due to material damage including leaching³⁵ and tensile cracking.³⁶ In the case of permeability, a 3-D microstructure reconstruction method has been paired with a Stokes solver to provide a quantitative virtual permeability test. Predictions for porous hydroceramics and pervious concrete agree well with experimental measurements. In both of these cases, pore structures of materials with nominally 20% to 30% porosity are well captured by the reconstruction method, whose inherent percolation threshold of around 10% can sometimes limit the accuracy of predictions at lower porosity values.¹²

Virtual testing of concrete transport properties aids in the development of fundamental microstructure/property relationships, such as those between transport coefficients and porosity ([Fig. 7](#)) or other microstructural characteristics. Additionally, virtual testing has the potential to be applied to a wide variety of “what if” field scenarios to optimize mitigation and remediation strategies, as demonstrated for remediation of chloride-contaminated bridge deck concretes ([Fig. 3](#) and [4](#)). The various models described in this paper and their locations on the Internet are summarized in [Table 2](#). All are freely available for execution and/or downloading; documentation in the form of user manuals or accompanying technical articles is also provided.

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Table 1—Latest treatment times versus bridge deck type and remediation strategy

Bridge deck type	Treatment type	Latest treatment time
SIPMF	Surface	1 year
No SIPMF	Surface	5 years
SIPMF	Scarification and overlay	2 years
No SIPMF	Scarification and overlay	6 years

Table 2—NIST models for virtual testing (available for remote execution or downloading)

Model	Description/Purpose	Download location or web page address
CEMHYD3D	Cement hydration (version 3.0)	ftp://ftp.nist.gov/pub/bfrl/bentz/CEMHYD3D/version30
HCSSModel	Hard core/soft shell 3-D microstructural model	http://ciks.cbt.nist.gov/cmml.html
3-D Reconstruction	Correlation-based transformation from 2-D image to 3-D microstructure	ftp://ftp.nist.gov/pub/bfrl/bentz/permsolver/
VirtualRCPT	Virtual RCPT test	http://ciks.cbt.nist.gov/VirtualRCPT.html
CIKS-Chloride	Chloride penetration simulation including surface treatment and/or scarification and overlay	http://ciks.cbt.nist.gov/~bentz/millandfill/clpenmillandfill.html
Permsolver	3-D Stokes solver for permeability	ftp://ftp.nist.gov/pub/bfrl/bentz/permsolver/

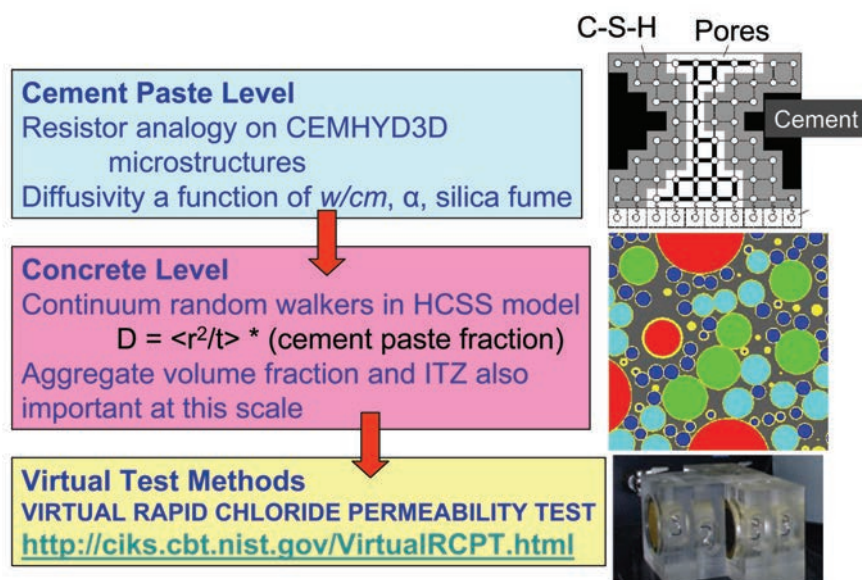


Fig. 1—Summary of multi-scale modeling of conductivity/diffusivity in cement-based materials.

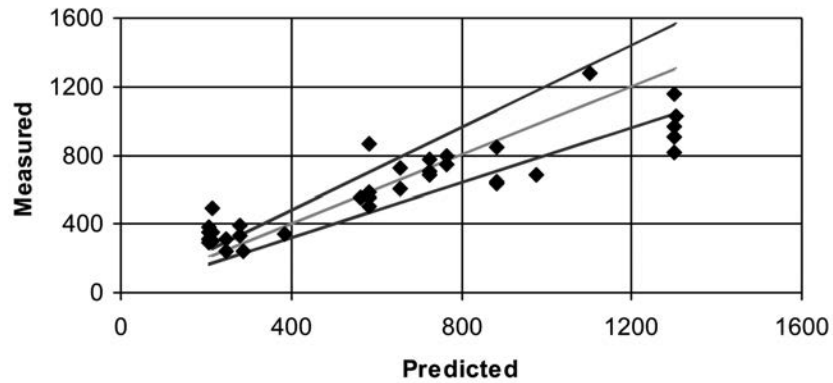


Fig. 2—Measured versus predicted (virtual) RCPT test results.²² Experimental data taken from Reference 26. Gray line indicates line of equality, and dark lines indicate $\pm 20\%$ of the measured values.

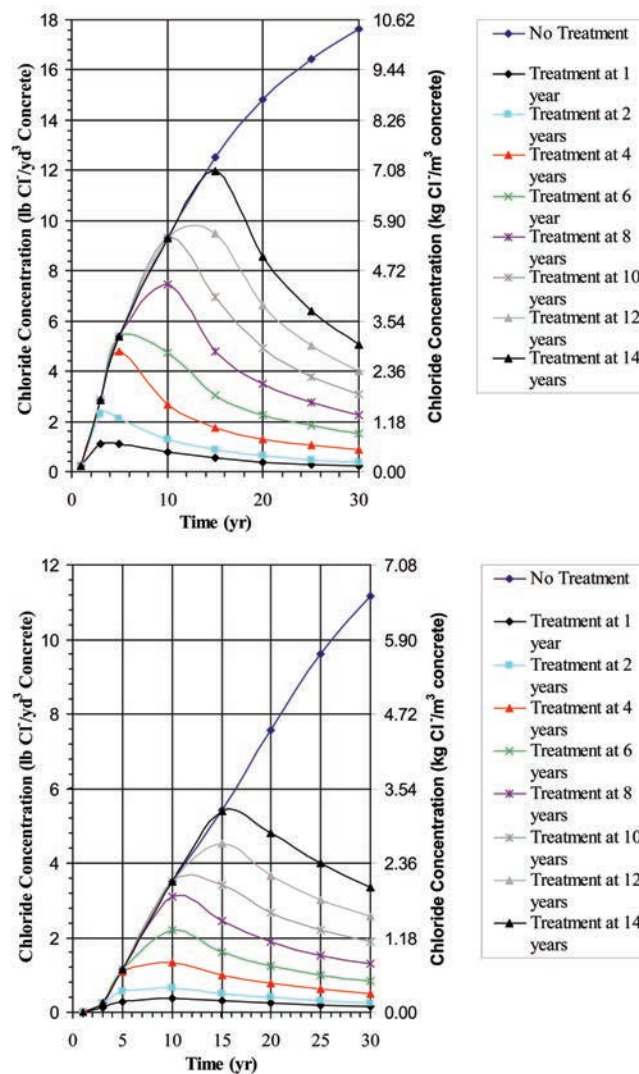


Fig. 3—Comparison of simulated chloride concentrations of decks with (top) and without (bottom) SIPMFs at 50 mm (2 in.) cover depth as a function of time of application of surface treatment.²⁸

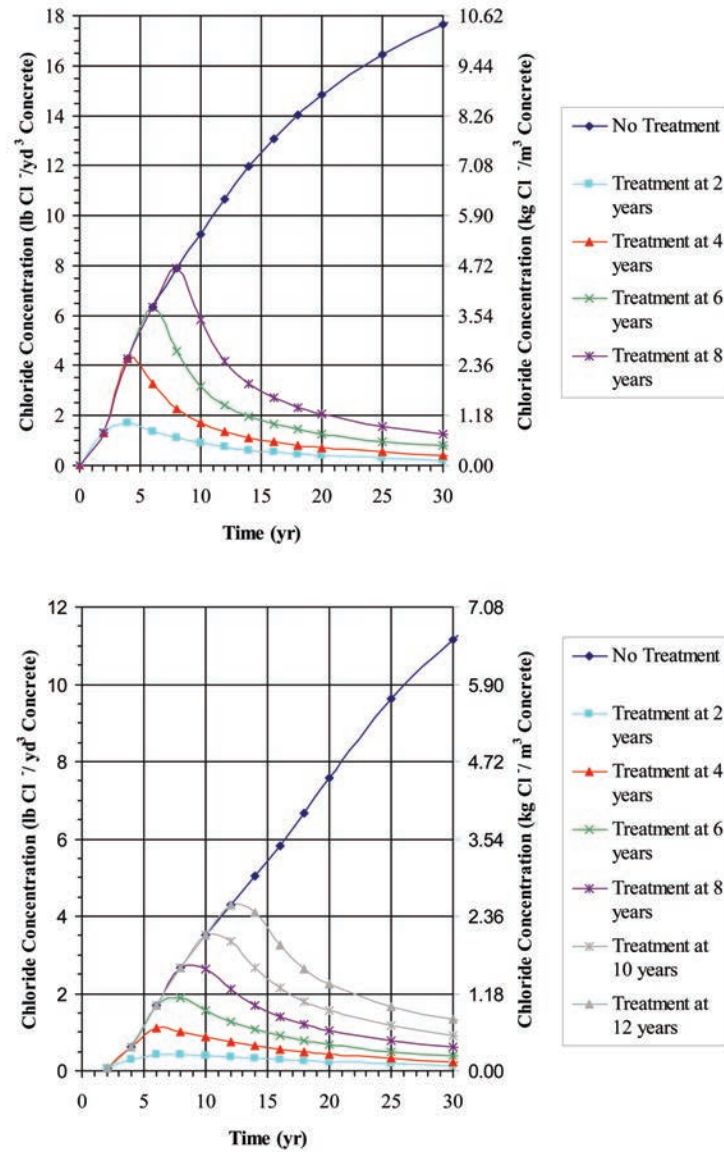


Fig. 4—Comparison of simulated chloride concentrations of decks with (top) and without (bottom) SIPMFs at 50 mm (2 in.) cover depth as a function of timing of a 12.7 mm (0.5 in.) scarification and 38 mm (1.5 in.) overlay treatment.²⁹

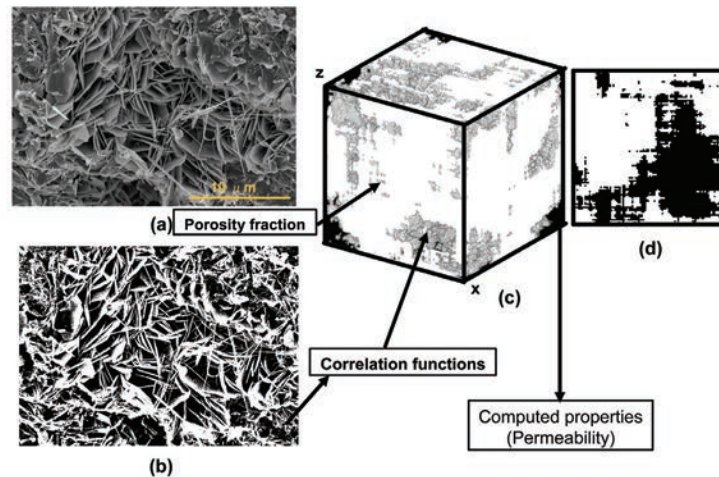


Fig. 5—Illustration of the process of creating a three-dimensional microstructure for subsequent computation of permeability¹⁵: (a) SEM image showing hexagonal crystals of truscottite. The needle shaped crystals are of xonotlite. Sample cured at 350°C (662°F) containing 40% by mass of silica flour; (b) binary image used to extract the correlation functions for the 3-D reconstruction; (c) reconstructed three-dimensional microstructure (100 pixels x 100 pixels x 100 pixels) for which permeability is computed; and (d) slice of the reconstructed three-dimensional microstructure.

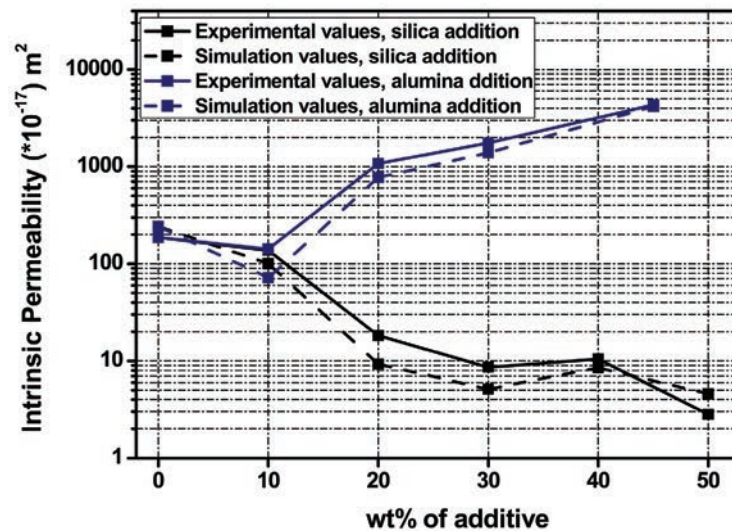


Fig. 6—Comparison of experimental and simulation values of intrinsic permeability with silica or alumina additions in hydroceramic samples.¹⁵ (Note: 1 m^2 = 10.76 ft^2 .)

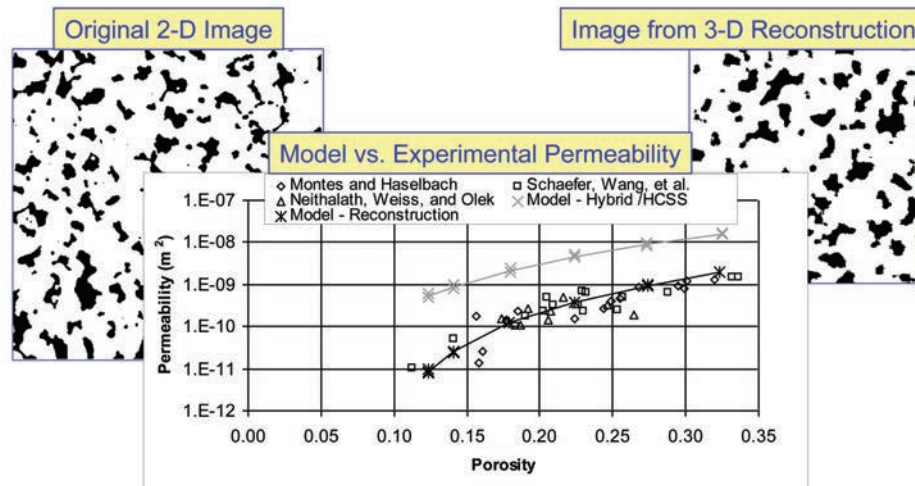


Fig. 7—Comparison of experimental and simulation values for intrinsic permeability for pervious concretes.¹¹ Original image is 63 by 63 mm (2.5 by 2.5 in.). Experimental values were extracted from the references listed in the legend.³²⁻³⁴ (Note: $1 \text{ m}^2 = 10.76 \text{ ft}^2$.)

Virtual Cement and Concrete Testing Laboratory for Quality Testing and Sustainability of Concrete

by J.W. Bullard, P.E. Stutzman, L.M. Ordoñez Belloc,
E.J. Garboczi, and D.P. Bentz

Synopsis: The NIST-Industry Virtual Cement and Concrete Testing Laboratory (VCCTL) Consortium has developed an integrated software package for performing simulations of a number of engineering test measurements, including isothermal calorimetry, adiabatic temperature change, chemical shrinkage, elastic moduli, and compressive strength. In the last two years, the software interface has been redesigned to be easier to navigate, with online tutorials and documentation for easy reference. As a result, VCCTL is now ready to be integrated in industrial settings as a supplemental tool to accelerate research on mix designs and to streamline routine quality testing procedures. This paper will demonstrate the software interface, and two applications will be described to illustrate the utility of the software to help solve practical problems. In the first application, we address sustainability issues by investigating the replacement of coarse clinker particles with limestone and its effect on elastic moduli and compressive strength. In the second application, we illustrate VCCTL's potential for screening the quality of incoming cement clinkers by providing rapid estimates of compressive strength development in mortar specimens.

Keywords: building technology; hydration; microstructure; strength; sustainability; virtual testing.

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INTRODUCTION

Design, optimization, and quality testing of concrete typically are accomplished by intensive physical testing procedures that consume large amounts of labor and materials. This task is becoming increasingly difficult as requirements for sustainability and performance begin to necessitate the use of blended cements and chemical admixture cocktails that may have significant interactions affecting durability and service life. As a result of this complexity, the performance of concrete over its intended service life is difficult to predict without extensive physical testing, since simple empirical relations cannot be universally applied with confidence. A promising alternative is to use scientifically based computer models to guide testing and development efforts. Properly validated computer models can supplant much of the current empirical design and testing procedures with computer simulations that are relatively quick and inexpensive. This paper describes an integrated package of computer-modeling software, called the Virtual Cement and Concrete Testing Laboratory (VCCTL), the goal of which is to enable a rapid exploration of concrete design space at significantly reduced cost. This software has been developed for the last eight years through a consortium led by the National Institute of Standards and Technology (NIST) and with a membership that has included cement manufacturers, chemical admixture suppliers, aggregate suppliers, and industry associations. The computer models in VCCTL continue to be refined to include a wider range of materials and curing conditions. Nevertheless, the models—and the user interface that ties them together—have advanced to a point where they can provide immediate benefits to industry in a number of ways. Features of the VCCTL software will be described in this paper, and then two case studies will be presented to demonstrate how the software can assist in mixture design and quality testing.

RESEARCH SIGNIFICANCE

Scientifically based computer models of concrete materials have existed for several decades but, so far, they have not been widely adopted in industry. To gain better acceptance in concrete research and testing environments, computer models must (1) be supported by adequate characterization of the materials that are being

used, (2) provide the materials engineer with reliable guidance about the likely effects of different material characteristics and realistic curing conditions on concrete performance, and (3) be accessible through an intuitive, easy-to-use software interface. VCCTL software has been designed and developed with these objectives in mind. By adopting such modeling software, the concrete industry can streamline mixture design and testing activities.

DESCRIPTION OF VCCTL MODELING SOFTWARE

Materials Characterization

To be as accurate as possible, VCCTL models have been built upon principles of chemistry, physics, and materials science. As a result, these models require accurate input about the materials that are being simulated, including the cement powder as well as the physical properties of the fine and coarse aggregates. Therefore, we begin this section with a cursory description of the materials characterization that is required for VCCTL use.

The VCCTL module for cement hydration is based on the CEMHYD3D model developed at NIST¹. This module simulates microstructure development at the micrometer scale and, as such, requires knowledge of the cement particle size distribution (PSD) and spatial distribution of solid phases at this length scale. The PSD of cement powder, which typically ranges from less than 1 μm to more than 50 μm , can be characterized by a number of techniques, although no universally recognized standard test method currently exists.^{2,3} By far the most common method employed in industry is laser diffraction.^{2,3} Ideally, for blended cements, the PSD of each component (cement, limestone, fly ash, etc.) should be measured separately, although if these components are interground then the overall PSD of the final composite powder may be the only feasible measurement. Regarding the spatial distribution of solid phases in cements, the most accurate procedure is a combination of backscattered scanning electron microscopy (SEM), X-ray microprobe analysis, and quantitative X-ray powder diffraction (QXRD) using Rietveld refinement.⁴ QXRD provides an accurate measurement of the mass fraction of most of the solid phases, while SEM gives an indication of the spatial distribution of those phases in the microstructure, which can be quantified for isotropic powders by using two-dimensional (2-D) autocorrelation functions. From this information, a three-dimensional (3-D) digital-image representation of the microstructure can be generated and used as input to the VCCTL microstructure model⁵ (see Fig. 1). In recent years, the SEM/QXRD procedure has been simplified considerably by using modern image processing software. Even so, proper specimen preparation for SEM imaging can be time consuming and requires considerable experience. We have gathered evidence that QXRD alone, which is a widely available and simple technique, combined with reasonable assumptions about the surface area fraction of each component phase, is typically sufficient to make accurate predictions with VCCTL software.

For the fine and coarse aggregates, the density, size distribution, and shape of the individual aggregate particles must be measured. The density and size distribution are easily measured using standard methods. The particle shapes can be accurately quantified using X-ray computed microtomography (μCT) and the shape data can be stored efficiently for thousands of particles as spherical harmonic coefficients.⁶ μCT also can be used to characterize the shapes of cement particles.⁷

Computer Models and User Interface

The VCCTL software is a web server application, which means that it can be installed on a web server and then accessed through a web browser on any client computer with internet access to the server. The user interface has been designed to represent different parts of a cement and concrete testing laboratory, with modules for storing and accessing materials, mixing concrete, curing concrete, and performing tests of mechanical and transport properties. Figure 2 shows the basic work flow for virtual testing with VCCTL. Figure 3 shows a portion of the Lab Materials module, from which the user can browse the characteristics of available cements and supplementary cementitious materials (SCMs). Existing materials can be edited in place to change their properties, and newly characterized materials can be easily uploaded to the database. These features make it easy to customize the VCCTL to a particular organization's material inventory.

The Mix Preparation module, a portion of which is shown in Figure 4, enables the user to select the cement, aggregate sources, and any SCMs that are to be included. The proportions of these materials, water, and entrained air volume can be entered in text fields. The entered data are sent to a program that generates a 3-D digital image of the virtual cement paste microstructure and of the larger-scale virtual mortar or concrete aggregate packing.

The user can perform virtual curing on the resulting virtual cement paste microstructure, by entering the curing conditions in the Curing module (also shown in Figure 4). The thermal conditions (isothermal, adiabatic, or semi-adiabatic) and initial temperatures of the paste and aggregate can be specified, together with the moisture

conditions provided for curing (saturated or sealed). The time scale of the curing simulation can be calibrated either to an empirical parameter or, more realistically, to isothermal calorimetry or chemical shrinkage data that can be conveniently uploaded in the Lab Materials module. The input data are sent to a program that simulates the 3-D microstructure development and tracks the value of several properties such as heat release, temperature, chemical shrinkage, and Powers' gel-space ratio.

Once curing is completed, an online graphing package in the Measurements module enables the user to plot the hydration properties (temperature, chemical shrinkage, degree of hydration, etc.) as a function of time or any other independent variable. The Measurements module can also be used to calculate several mechanical properties of the cement paste, mortar, or concrete, such as the linear elastic moduli and the compressive strength. A finite element program⁸ is used to calculate the effective linear elastic moduli of the hydrated cement paste, and these computed data are then used in a second C program, based on differential effective medium theory, to compute the elastic properties and to estimate the compressive strength of the mortar or concrete.⁹

VCCTL APPLICATIONS

As the VCCTL software has matured, members of the VCCTL consortium have used the models in short-term quality testing and troubleshooting efforts, and have reported significant savings in materials and labor costs for each project. In each case, the VCCTL models were used to identify *likely* (not guaranteed) results or troubleshooting solutions, which were then validated using a small set of physical tests. In this section, we describe two applications of VCCTL software that illustrate the types of practical problems that the models can address.

Application 1: Limestone additions for increased sustainability

In concretes made with cement binders having a low water-cement mass ratio (w/c), the coarsest cement particles often remain largely unhydrated for the life of the material because of insufficient water in the mix and/or insufficient space in which the hydration products can form. Permanently unhydrated clinker particles are generally undesirable (except in cases where autogenous healing of cracks is an issue) because their contribution to the strength of the concrete is the same as a less expensive inert filler material, such as limestone. In addition, a filler such as limestone can be used with zero CO_2 emission, while the manufacture of cement clinker releases about 1 metric ton of CO_2 for every metric ton of clinker produced. If one were to replace the coarsest fraction of a cement powder with coarse limestone particles, then nearly the same mechanical properties should be obtainable with a less expensive, more sustainable binder. In fact, the concept of limestone replacement has been demonstrated previously with both experiments¹⁰ and computer modeling studies with CEMHYD3D.¹¹

Figure 5 shows 2-D slices through 3-D virtual cement pastes made with and without coarse limestone replacement. In both cement pastes, the cement used was Proficiency Sample Cement 152 issued by the Cement and Concrete Reference Laboratory (CCRL). Both pastes were generated with $w/c = 0.35$. In the microstructure with limestone replacement, all cement particles with equivalent spherical diameter exceeding $40\text{ }\mu\text{m}$ were replaced with limestone particles (green in the images) of the same equivalent spherical diameter. This amounts to a replacement of 12.5% by mass on a total solids basis. Also shown in Figure 5 are the simulated microstructures after isothermal hydration at 20°C (68°F) under saturated conditions for 28 d. These microstructures demonstrate that the coarse limestone particles, which are relatively inert during hydration, take the place of the unhydrated cores of large clinker particles, since there are fewer unhydrated clinker particle cores in the microstructure with limestone replacement after 28 days. The mechanical properties are also predicted to not be adversely affected by the limestone replacement. In Figure 6, the predicted Young's modulus and compressive strength are plotted at 2, 7, and 28 days. At all three ages, both the Young's modulus and the compressive strength are predicted to be modestly greater for the material with 12.5% replacement with coarse limestone. These results are qualitatively consistent with previous numerical and experimental studies on the effects of coarse limestone replacement,^{10,11} although those earlier studies predicted a slight decrease in strength, instead of a slight increase, upon limestone replacement. The strength increase predicted in the current simulations are largely due to a decrease in capillary porosity that must accompany mass-based replacement of a higher-density material (cement powder) with a lower-density material (limestone). In any case, the VCCTL predicts, and experiments confirm, that for low w/c ratios, partial replacement of coarse clinker particles with coarse limestone particles can yield a less expensive and more sustainable concrete binder without significantly diminishing the mechanical properties. Further work using the VCCTL and supporting experiments could seek to find optimum replacement levels as a function of w/c ratio and of the particle size distribution of the original cement powder.

Application 2: Screening clinker quality based on 28-day compressive strength

The concrete industry uses cement that is produced in numerous regions, such as North America, Western Europe, China, and India. The available raw materials for clinker production can be highly variable from region to region. Therefore, it would be desirable to find a rapid test method for screening the quality of incoming clinkers, based on some convenient metric, so that potential problems can be rapidly identified without using excessive amounts of labor and materials. As a first step toward this goal, we report on a simple test procedure that can be used in conjunction with VCCTL simulations to directly compare different clinkers according to the 28-day compressive strength.

The following simple screening procedure is proposed here. As already described, each clinker powder is characterized using either SEM/X-ray image processing or QXRD to obtain the mass fractions of each mineral in the clinker. If SEM/X-ray imaging is used, then the surface area fractions and autocorrelation functions can be obtained directly from a sampling of segmented images. If QXRD alone is used, then reasonable assumptions, based on research on many different cements, can be made about the proportionality of the surface fraction to the volume fraction of each clinker mineral. The PSD of the clinker also must be measured. Once characterized, each clinker is blended with 5% replacement of gypsum from a fixed consistent source with a well-defined PSD. A small volume of paste is produced for obtaining isothermal calorimetry data up to 2 days of hydration. With these calorimetry data on pastes for calibration, the VCCTL models can simulate the microstructure development and mechanical properties of virtual mortars of the same materials mixed with a standard sand (ASTM C778-02 or EN 196-1, for example) out to 28 d or later.

In this case study, this test procedure was used to predict the mechanical properties of mortars made from a coarse clinker originating in China. Isothermal calorimetry on a cement paste formed from this clinker ($w/c = 0.4$) was performed at 20°C (68°F) for 48 h. A representative phase-segmented SEM image of the clinker is shown in [Figure 7](#), and the mass fractions of clinker minerals are given in [Table 1](#). Although not shown here due to space limitations, the PSDs of both the clinker and the gypsum were measured. The median particle diameters of the clinker and the gypsum are 18.7 μm and 20.7 μm , respectively. The European EN 196-1 sand was used to make virtual mortars with a mass ratio of sand:cement:water equal to 3:1:0.5. The specimens were assumed to include 4% entrained air by volume. Hydration of the mortar specimens was simulated at 20°C (68°F) under saturated conditions for 28 d. For comparison, actual mortar specimens were prepared using the EN 196-1:2005 test method,¹² which uses the same mixture proportions and curing conditions as employed in the VCCTL simulations. [Figure 8](#) compares the predicted and measured compressive strengths at 2, 7, 14, and 28 days. The specimen-to-specimen variability in the experimental measurements is about ± 1 MPa (145 psi), and the uncertainty in the VCCTL prediction, due to assumptions about the entrained air volume fraction and statistical sampling from the particle size distribution, is about the same. Therefore, the differences between measured and predicted strengths at intermediate ages are probably significant. Similar differences have been observed for several other cements over the last several years, although application of the VCCTL to most Type I Portland cements has yielded better agreement to experiment than that shown in [Fig 8](#). Further research needs to be conducted to determine the source of these differences and to determine whether the VCCTL strength predictions for other clinkers show a comparable agreement with experimental measurements.

SUMMARY AND PROSPECTUS

The VCCTL modeling package has been developed and refined over the last 10 years. It now enables users to quickly simulate the hydration and to calculate a number of important engineering properties of cement paste, mortar, and concrete. Improvements in the graphical user interface now make it possible for knowledgeable materials engineers to obtain useful data with only a modest amount of training. In this paper, we have demonstrated two potential applications—exploring new and more sustainable concrete mixture designs, and quality testing of clinker sources—that could begin producing immediate dividends in several sectors of the concrete industry. Other features of the software not described here, such as the ability to specify initial aggregate temperature and monitor heat evolution in hydrating cements, have immediate application for predicting and controlling the maximum temperature excursions at a job site. Research for improving the computer models that comprise the VCCTL is ongoing and should enable even more practical utility. Short-term improvements planned for the software include the addition of component costs to the mixture proportioning modules and more flexibility in mixing different clinker sources to customize a mixture. Longer-term research is already underway to improve the predictions of mechanical and transport properties, and to integrate new models of early-age hydration and the rheological behavior of fresh cement paste, mortar and concrete.

ACKNOWLEDGMENTS

Technical input, research directions, and partial financial support for the VCCTL project has been provided by the Virtual Cement and Concrete Testing Laboratory Consortium led by NIST. The current industry members of the consortium are BASF, Mapei, the Ready-Mixed Concrete Research and Education Foundation, Sika AG, the U.S. Federal Highway Administration, and W.R. Grace & Co.-Conn.

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Table 1—Mass fraction of clinker phases determined by QXRD using Rietveld refinement

Phase	Mass Fraction
C_3S	0.543
C_2S	0.259
C_3A (Cubic)	0.067
C_3A (Orthorhombic)	0.011
C_4AF	0.106
KS	0.011

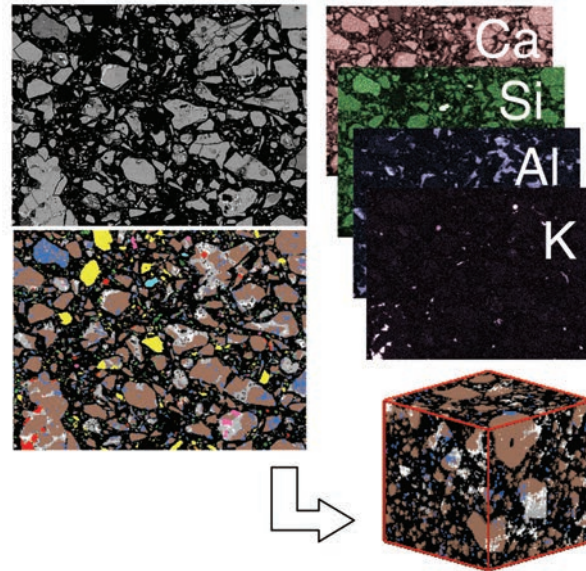


Fig. 1—SEM/X-ray microprobe characterization of 2-D cement microstructure images. A backscattered electron image (gray scale upper left) is filtered through element maps (upper right) to produce a phase segmented 2-D image (lower left). Autocorrelation functions measured on this image can be used to generate the final microstructure as a 3-D digital image (lower right). In the color images, alite is brown, belite is blue, tricalcium aluminate is gray, ferrite is white, potassium sulfate is red, periclase is pink, and calcium sulfate is yellow.

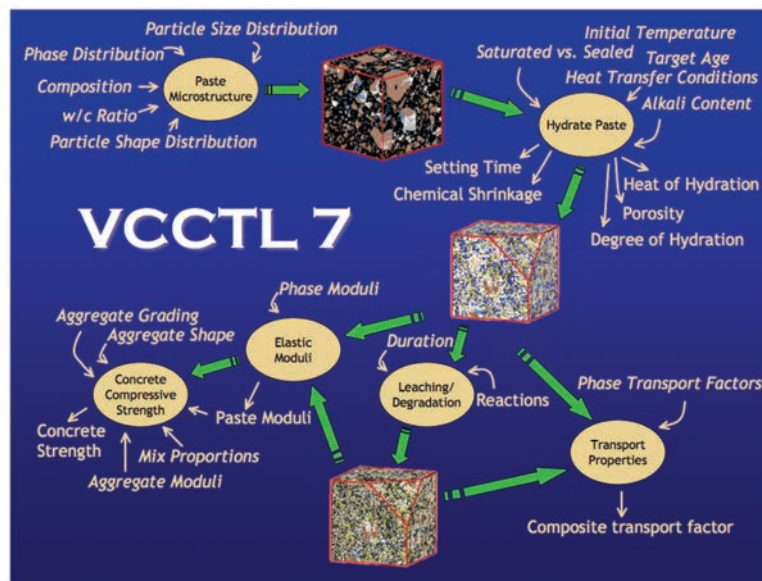


Fig. 2—Pictorial representation of the VCCTL software work flow, showing the various steps of virtual testing and the inputs (in *italics*) and outputs.

Material Inventory

▼ Edit or create a cement

Name: cement140

Upload data from a ZIP file for the cement:

► Cement data

Mass fractions of sulfates

Dihydrate 0.0039 Hemihydrate 0.022 Anhydrite 0.016

► Edit or create a fly ash

Fig. 3—Laboratory materials module in the VCCTL software interface can be used to view or edit the properties of cements or SCMs in the database, or to upload newly characterized materials.

Step 1: Prepare mix

Binder

Choose a cement: cement140

► Modify phase distribution in the *clinker*

► Modify calcium sulfate amounts in the *cement*

► Add SCM to the *binder*

Mix

	Mass fraction	Volume fraction
Binder	0.1724	0.1307
Water	0.0776	0.1897
Water/Binder ratio	0.45	
☒ Add Coarse Aggregate	0.30	0.2658
► Change properties		
☒ Add Fine Aggregate	0.45	0.4138
Change properties		
Air		0.04

Curing Conditions

Thermal

Conditions:

☒ isothermal

☐ semi-adiabatic

☐ adiabatic

Initial temperature: 25.0 °C

► Aggregate

Aging

Hydrate for 28.0 days

... Or stop at degree of hydration:

☒ Use time conversion

Time conversion factor 3.5E-4 h/cycle²

☐ Use a calorimetry file

☐ Use a chemical shrinkage file

Saturation conditions

☒ saturated

☐ sealed

Fig. 4—A portion of the VCCTL Mix Preparation module (left) and Curing module (right). The Mix Preparation module enables the user to select cement, SCMs, and aggregate sources from the database, choose the gradings and proportions of these components with water, and entrained air volume. The Curing module enables the user to choose the thermal and moisture conditions of the fresh concrete, in addition to the duration and more detailed parameters, such as the hydration activation energy, heat transfer coefficients, and aggregate temperature.

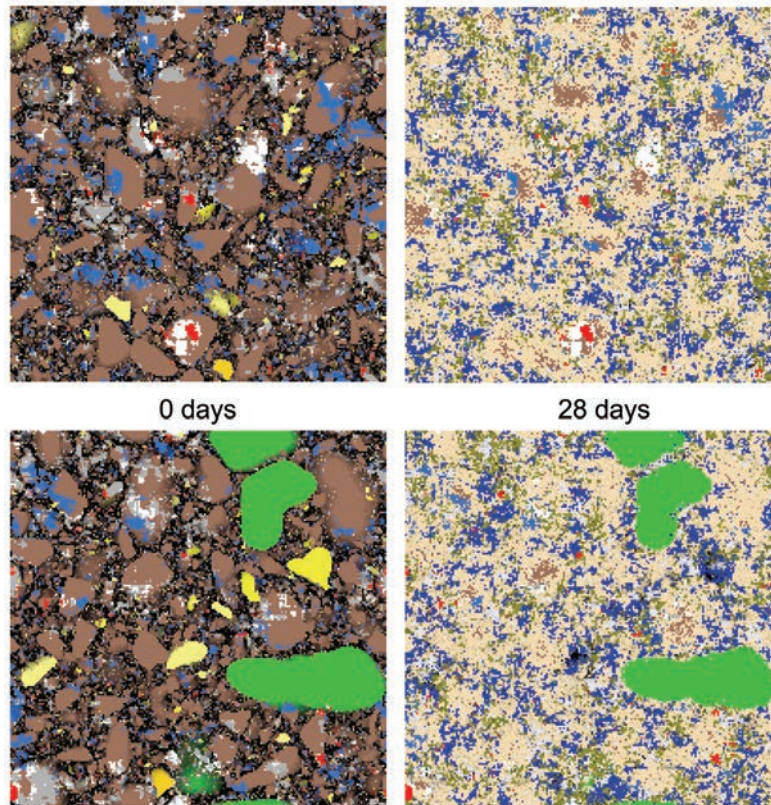


Fig. 5—Virtual mortar microstructures of CCRL Cement 152 at 0 days and 28 days of hydration without limestone (top) and with 12.5 % limestone replacement by mass. The scale is 200 μm on a side. In both microstructures, $w/c = 0.35$ initially, and curing was simulated at 20°C (68°F) under saturated conditions. The phases are colored as follows: brown = C_3S , light blue = C_2S , gray = C_3A , white = C_4AF , yellow = CS , red = KS , green = limestone, light brown = C-S-H , dark blue = CH , and olive = ettringite. Here and throughout, conventional cement chemistry notation is used ($\text{C} = \text{CaO}$, $\text{S} = \text{SiO}_2$, $\text{A} = \text{Al}_2\text{O}_3$, $\text{F} = \text{Fe}_2\text{O}_3$, $\text{S} = \text{SO}_3$, $\text{K} = \text{K}_2\text{O}$, $\text{H} = \text{H}_2\text{O}$)

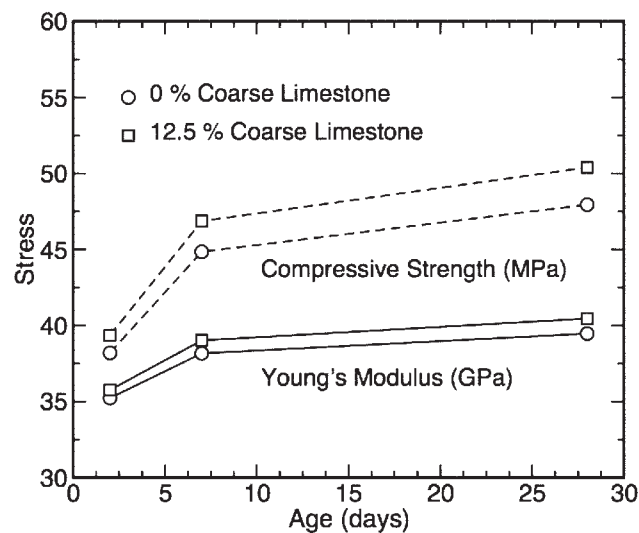


Fig. 6—Comparison of predicted Young's modulus (solid curves) and predicted compressive strength (dashed curves) for the two mortar microstructures shown in Figure 5. The variability in predictions due to both statistical sampling and uncertainty in the entrained air volume fraction (assumed $\pm 1\%$) is about the size of the symbol.

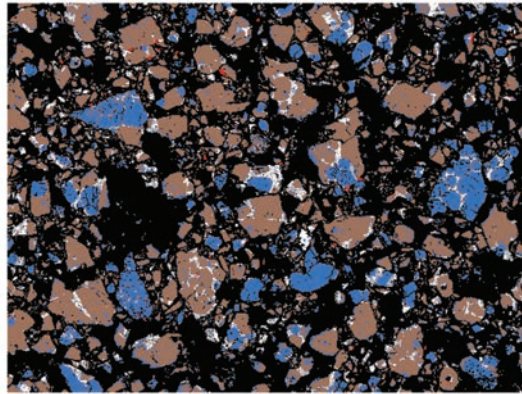


Fig. 7—Representative phase segmented SEM image of coarse clinker from China. The color scheme is the same as in Fig. 1 and 5. The image is $512\ \mu\text{m} \times 384\ \mu\text{m}$.

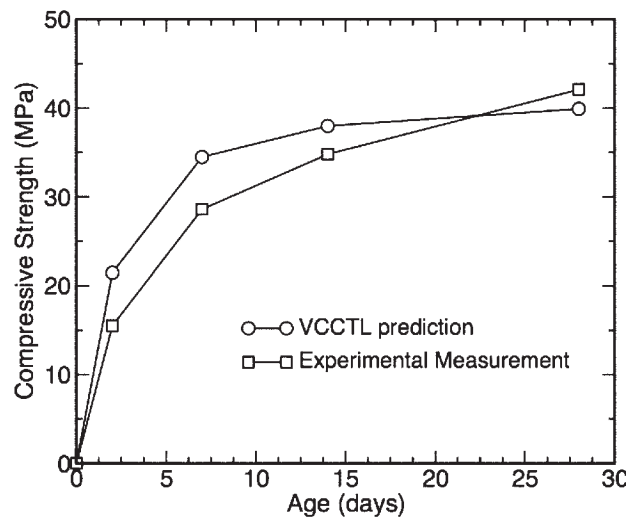


Fig. 8—Comparison of experimental and simulation values for the compressive strength of mortar specimens made according to the EN 196-1:2005 standard test method, using coarse clinker imported from China and mixed with 5% coarse gypsum by mass. The variability in predictions and experimental measurements due to both statistical sampling and uncertainty in the entrained air volume fraction (assumed $\pm 1\%$) is about $\pm 1\ \text{MPa}$ (145 psi). (Note: $1\ \text{MPa} = 145\ \text{psi}$.)

A Concept for the Development of Mathematical and Mechanical Models for the Deformations of Composites under Uniaxial Load

by S. Popovics

Synopsis: The primary purpose of this paper is to introduce and demonstrate the applicability of a statistical concept, the *average*, for the modeling of the deformations of two-phase composites under load. Concrete is modeled as a well-compacted two-phase composite, the hardened paste as the matrix, and the aggregate as the dispersed phase. Only the paste has creep. The demonstration is done by the development of novel viscoelastic models and their mathematical equivalents for the instantaneous as well as time-dependent deformations of concrete, as a two-phase composite, under load.

The underlying principle of the work is based on an extension of earlier publications by the writer in which averages of the averages of the related the phases, the *composite averages* are offered for the estimation of the modulus of elasticity of composites. Since experimental results supported the *composite average method*, CAM, quite well for this, it seemed worthwhile to investigate whether the method can be extended for the calculation of time-dependent deformations.

The extension consists of the addition of dashboard elements to the existing composite average spring models for the modulus of elasticity of concrete, for the estimation of creep. This is the combinations of two existing spring-dash models for the calculation of the creep: the Poynting-Thomson model with the Maxwell model the results of which are two CAMs that are determined by the type of combination between these two: one for normal-weight concretes when the two models are connected in a series, and the other, when they are in parallel for lightweight-aggregate concretes. Experimental data on creep with uniaxial loading taken from the literature support these composite models well. Among others, the data and the models show that during the period when the creep development is gradually decelerating: 1. creep values as a function of loading time, give straight lines, let us call them *creep lines* (compliance functions) in semi-log system as well as in log-log system of coordinates. Consequently, they can be approximated both by logarithmic as well as power functions. Such formulas are suitable for the estimation of creep at a later time from an earlier measurement; and 2. various creep lines of comparable concretes may be parallel, regardless at what age t' the loading started.

It is shown that the new models are: well supported by experimental results within reasonable time limits; they are conceptually simple and logical; they are novel; they can consider the composition of the concrete; they represent both E and creep; and they are valid both normal-weight and lightweight-aggregate concretes.

Keywords: composite average; creep; creep recovery; modulus of elasticity; optimization; spring-dashboard model.

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INTRODUCTION

There is hardly any topic in the area of concrete technology of which more has been written than the creep [Bažant 2008]. Thus, it is difficult to write about it that is novel as well as meaningful. Difficult but not impossible. Also, further work is needed because the large number of the recent related publications is a clear sign that this problem has not had yet a satisfactory solution.

The topic of this paper is restricted to modeling the deformations of concrete under uniaxial load. Several rheological models, the composite average models, CAMs, are presented. These are considered novel, conceptually simple and logical, take the concrete composition into consideration, applicable both for the calculation of the modulus of elasticity as well as creep and creep recovery, and valid both for normal-weight and lightweight-aggregate concretes. Experimental results indicate that they are suitable for the calculation of deformations of two-phase composites under uniaxial load from its composition as well as or better than other models, such as Maxwell chains. The experimental results used were published by others. Particularly useful were publications by Bažant and Neville.

The calculations have originated from the composite average concept that was published earlier, and applied successfully. This is demonstrated in Fig. 1 for the estimation of the modulus of elasticity E of concretes with various aggregates at the age of 28 days as a function of the quantities and moduli of elasticity of the aggregates [Popovics 1969].

The idea of calculation of certain characteristics of a two-phase composite as the average of the characteristics of the two phases originated probably in the nineteen twenties. Several different averages have been developed, some of these are interdependent. The most frequently used ones are the *arithmetic*, *harmonic* and *geometric* averages. Voigt, for instance, recommended the arithmetic average [Voigt 1928], and Reuss the harmonic average [Reuss 1929] for the calculation of the modulus of elasticity of composites from the phases. Since the Voigt model, arithmetic average E_a , highly over estimates the actual modulus of concrete, and the Reuss model, harmonic average E_h , highly underestimates it, the idea was offering itself that the suitability of the *average* of the two averages of these models, that is, the *composite average* should be checked out. (Fig. 2)

In this paper it is shown that the obtained composite average models are suitable not only for the calculation of the instantaneous deformation (modulus of elasticity) but also for the calculation of creep and creep recovery (relaxation) of structural concretes as a function of the moduli and quantities of the aggregate and hardening cement paste, age of concrete, and time and duration of loading. Presentation and discussion of earlier creep models can be found in the literature [Neville 1970; Bažant 1988, 2008; ACI Committee 209].

The fundamental mechanism of creep is outside the framework of this paper. Nevertheless indications are presented that the concrete creep may be considered as consisting of at least three subsequent mechanisms: at the very beginning, say $t - t' = 2$ days, the creep is accelerating, followed by a gradually decelerating mechanism, topic of this paper, ending about at the concrete age of about $t = 1000$ days (≈ 3 years), then accelerating starts again.

RESEARCH SIGNIFICANCE

The topic of this paper is restricted to providing a basis for modeling the deformations of concrete under uniaxial load. Its practical significance is that novel formulas are offered for the limited estimation of deformations of concrete under load, including creep, in terms of its composition, age, time and duration of loading. They also permit the calculation of late creep from early measurements. So, the work is significant whenever the concrete creep is meaningful.

Curve fitting is used as a tool for the establishment of some of the constants in the model, but the method is more than an exercise in curve fitting. It is based on a solid concept, the *composite average* concept which makes it possible to include the concrete composition into the modeling. Within the established limits of validity, limited experimental specific creep results support the values calculated from the presented models just as well as, or better than do other existing models, such as fitted Maxwell chains.

STARTING FORMULAS

The starting formulas are the mathematical equivalents of the composite average concept, as applied to the estimation of the modulus of elasticity of composites: applying certain assumptions, such as the Poisson's

ratios of the two phases do not differ too much, the air content is negligible or the same in all specimens, etc. the characteristic of a composite is some kind of an average of the related characteristics of the phases. [Popovics 1998]

Several types of averages have been developed, the most frequently used are the arithmetic E_a , harmonic E_h and geometric (logarithmic) E_g averages:

$$E_a = pE_1 + (1 - p)E_2 \quad (1)$$

$$1/E_h = p/E_1 + (1 - p)/E_2 \quad (2)$$

$$E_g = E_1^p E_2^{1-p} \quad (3)$$

where

p = fractional volume of the cement paste (matrix) in concrete,

E_1 and E_2 = modulus of elasticity of the hardened cement paste and that of the aggregate, respectively (Fig. 2).

The arithmetic average implies that the strains in the two phases are equal under uniaxial load, and the harmonic average implies that the stresses are equal.

Two phases can be combined in two ways:

- The matrix is the stiffer component. This is represented by the Reuss model the modulus of elasticity of which is the *harmonic* average E_h of the moduli of the two phases (e. g., lightweight-aggregate concrete). This model is called the *hard* composite; and
- The dispersed phase is stiffer which is the Voigt model and the modulus of elasticity of this is the *arithmetic* average E_a of the moduli of the two phases (e. g., normal-weight concrete). This model is called the *soft* composite.

That is, the deformability of a composite is determined not only by the quality and quantity of the two phases but also how the phases are combined. Experimental results have shown that the hard composite is stiffer, slightly, for the usual concrete compositions, than the other even when the components and the percentage compositions are identical. For instance, when a composite consists of 30% of cobalt with $E_1 = E_{co} = 30 \times 10^6$ psi (207×10^3 MPa) and 70% tungsten carbide, with $E_2 = E_{tu} = 102 \times 10^6$ psi (703×10^3 MPa), the composite is stiffer when the tungsten carbide is the matrix (the hard composite) than when the cobalt is (the soft composite), even though the components and volumetric compositions are identical. The difference is small when E_2/E_1 smaller than 10, nevertheless the composite average model can show this numerically (POPOVICS 1980). The ways to eliminate this complication are: (a) develop a model for hard composite, and another one for soft composite; or (b) when the difference between the deformabilities of the two phases are not large enough, as in the example above, the difference between the two composite models is so small that it is within the error limits of the two models, therefore both of them are applicable for the calculation of the deformabilities of either the hard or the soft composite; and (c) try some other average, such as the geometric average.

Therefore, it is expected that for hard composites the arithmetic CAM gives a suitable approximation to experimental results, and for soft composite the harmonic CAM does. That is, the following composite average model E_A is recommended for the modulus of elasticity of hard composites ($E_1 > E_2$):

$$E_A = AE_h + (1 - A)E_a = \frac{A}{\frac{p}{E_1} + (1-p)\frac{1}{E_2}} + (1 - A)(pE_1 + (1 - p)E_2) \quad (4)$$

where

E_A = the combination, specifically the arithmetic average of the Voigt and Reuss models,

A = characteristic of the model structure, in many cases $A = 0.5$,

p = fractional volume of the cement paste in the concrete,

E_1 and E_2 = modulus of elasticity of the hardened paste and that of the aggregate, respectively.

$A = 0.5$ is equivalent with the assumption that E_a and E_h have equal weight in the composite average, that is, the experimental values are located halfway between E_a and E_h .

For soft composites ($E_1 < E_2$):

$$\frac{1}{E_H} = \frac{A}{E_a} + \frac{1-A}{E_h} = \frac{A}{pE_1 + (1-p)E_2} + \frac{1-A}{\frac{p}{E_1} + \frac{1-p}{E_2}} \quad (5)$$

where E_H is the combination, the harmonic average of the Voigt and Reuss models. The other symbols are identical with the symbols of Eq. (4). These equations have also mechanical, electrical and hydraulic models [Popovics 1970].

According to these equations, not only the stresses differ in the hardened paste and the aggregate in the concrete under load but also the strains, too, and this is taken care of in the model by making the stresses equal in the paste and aggregate in A portion of the concrete, and in the remaining portion making the strains equal.

Note that the geometric average (Eq. (3)) itself is actually a composite average since it is well known that

$$E_g = (E_a E_H)^{0.5} \quad (6)$$

THE NEW VISCOELASTIC MODELS

The composite average concept has been quite successful for the estimation of the moduli of elasticity of normal- as well as lightweight-aggregate concretes from the composition, as shown, among others, in Figure 1 [Popovics 1980]. Therefore, this writer has attempted to extend the concept to the calculation of the time-dependent deformations of concrete as a two-phase composite under long-term loading. In this attempt the simplifying assumption was used that only the matrix creeps. Assuming linear viscoelasticity, these two models can also be presented in the forms of differential equations [Neville 1970; Bažant 1988]. Below, however, a mathematically simpler, semi-empirical method will be used. This is that Eqs. (4) and (5) are supplemented by the viscous characteristics of the matrix portion of the material. This is for normalweight concretes the following power function:

$$\epsilon_{total} = 0.5 \left(\frac{P}{E_1} + \frac{1-P}{E_2} + \frac{p}{\eta} (t-t')^n \right) + 0.5 \left(\frac{1}{pE_1 + (1-p)E_2} \right) \exp \left(- \frac{p \left((1-P) 2E_1 E_2 \right)}{pE_1 + (1-p)E_2 \eta} (t-t')^n \right) \quad (7)$$

where

ϵ_{total} = the sum of the instantaneous and time-dependent deformations,

η = characteristic of the viscosity of the hardened cement paste,

n = experimental parameter,

t = age of concrete, days,

t' = age of concrete when it was loaded,

$t - t'$ = duration of the loading period, days.

The rest of the symbols are the same as in the previous equations. Note that Eq. (7) does include the pertinent characteristics of the concrete composition. The specific creep is the difference between Eqs. (7) and (4).

Further analysis reveals that Eq. 7 can be simplified to the form of

$$\epsilon = K_1 (t - t')^{K_2} \quad (8)$$

where ϵ is the creep, and K_1 and K_2 are experimental constants functions of the composition. Indeed, the goodness of fit is still good, the various creep lines formed by the pertinent experimental results are parallel in the log-log system within the range of the experimental data, thus justifying Eq. (8).

The mechanical, spring-and-dashboard models of the latest of this attempt are shown in Fig. 3. Readers will recognize that one of the two new models is formed by the connection of two earlier published models, the Poynting-Thomson and the Maxwell models connected in *series*; and in Fig. 3(b) the same two models in *parallel*.

The other promising compliance function is a logarithmic function of the loading time:

$$\epsilon = K_3 \ln(t - t') + K_4 \quad (9)$$

where K_3 and K_4 are again experimental constants, and $\ln$ is the natural log. The examined experimental creep values form straight lines within reasonable limits with good approximation not only in the log-log system, meaning parabolic decreasing deceleration, but also in semilog system of coordinates, meaning linearly decreasing deceleration. The mathematical relationship between the power function and log function can be shown by an expansion into series.

COMPARISON TO EXPERIMENTAL CREEP RESULTS

The acceptability and flexibility of the presented CAMs are demonstrated below where concrete creep values, calculated from the two new models, are compared to experimental values taken from the literature. Each line represents a specific testing and/or treatment of the concrete specimen.

The numerical values of certain constants in the equations were obtained from the composition of the concrete. Where certain needed data were not published, reasonable estimates were used [Popovics 1998]. Other needed constants were obtained from the optimization process for which commercially available software programs are available.

Plenty of pertinent data were found in the literature and analyzed but since all of them support the composite average model in the same way, only six examples are presented below to illustrate how the CAM can handle various aspects of concrete creep. *Specific creep* is defined as the creep divided by the stress.

The same information is presented both in linear, semi-log and log-log systems of coordinates because they provide different insights of the goodness of fit between the calculated and experimental data.

Example 1: the effects of concrete composition as well as the loading age and duration on creep

The creep experiments in this example were performed by L'Hermite and his coworkers [L'Hermite, 1965]. The compressive strength of concrete at the age of 28 days was 370 kg/cm² (5250 psi) and the applied stress for creep was one fourth of the strength. The specimens were 7 x 7 x 28 cm (2.5 x 2.5 x 10 in.) prisms. The composition was: 350 kg/m³ (590 lb/yd³) cement and 171 kg/m³ (290 lb/yd³) water. The aggregate was sand and gravel from the river Seine. Thus, $p = 0.17$ by absolute volume, and $w/c = 0.49$ by mass. E_a assumed to be 7×10^6 psi (492×10^3 kg/cm²), E_c at the age of 28 days to be 3.78×10^6 psi (268×10^3 kg/cm²) and the cement Type I.

After the substitution of these values into Eq. (5) and (7), for $t' = 7$ days, the optimization produced (Fig. 5 and 6)

$$\varepsilon/\sigma = 0.295(t - t')^{0.0653} \quad (10)$$

or

$$\varepsilon/\sigma = 0.0254 \ln(t - t') + 0.288 \quad (11)$$

where ε/σ is the specific creep in 10^{-6} /psi and $\ln$ is the natural log.

Example 2: the effects of loading age and duration on creep

The same experimental data by L'Hermite are used here as in Example 1 but the CAM is simplified, first in the form of Eq. (9), then in Eq. (10).

For *power function relationship* the specific creep lines ε/σ (solid lines), best fitting to selected experimental results (points), are shown in Fig. 4(a) in linear system of coordinates, in Fig. 4(b) in semi-log system, and in Fig. 4(c) in log-log system. Details are the following:

$$\text{For } t' = 7 \text{ d. } \varepsilon/\sigma = 0.295(t - t')^{0.0653} \quad R^2 = 0.96 \quad (12a)$$

$$\text{For } t' = 21 \text{ d. } \varepsilon/\sigma = 0.222(t - t')^{0.0768} \quad R^2 = 0.88 \quad (12b)$$

$$\text{For } t' = 28 \text{ d. } \varepsilon/\sigma = 0.204(t - t')^{0.0753} \quad R^2 = 0.97 \quad (12c)$$

$$\text{For } t' = 90 \text{ d. } \varepsilon/\sigma = 0.186(t - t')^{0.0667} \quad R^2 = 0.84 \quad (12d)$$

$$\text{For } t' = 365 \text{ d. } \varepsilon/\sigma = 0.165(t - t')^{0.0629} \quad R^2 = 0.91 \quad (12e)$$

These equations and Fig. 5 suggest that these five equations can be condensed for every t with further

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approximation to the form

$$\varepsilon/\sigma \approx 0.351(t')^{-0.137}(t-t')^{0.0694} \quad (13)$$

Eq.13 is also shown in Fig. 4 with dotted lines.

For logarithmic relationship the results of creep lines ε/σ , fitting to selected experimental results are shown in Figures 5a in linear system of coordinates, in 5b in semi-log system, and in 5c in log-log system. Details are the following:

$$\text{For } t' = 7 \text{ d. } \varepsilon/\sigma = 0.0252(\ln(t-t')) + 0.2880 \quad R^2 = 0.94 \quad (14a)$$

$$\text{For } t' = 21 \text{ d. } \varepsilon/\sigma = 0.0254(\ln(t-t')) + 0.2001 \quad R^2 = 0.87 \quad (14b)$$

$$\text{For } t' = 28 \text{ d. } \varepsilon/\sigma = 0.0209(\ln(t-t')) + 0.1966 \quad R^2 = 0.93 \quad (14c)$$

$$\text{For } t' = 90 \text{ d. } \varepsilon/\sigma = 0.0167(\ln(t-t')) + 0.1798 \quad R^2 = 0.78 \quad (14d)$$

$$\text{For } t' = 365 \text{ d. } \varepsilon/\sigma = 0.0144(\ln(t-t')) + 0.159 \quad R^2 = 0.83 \quad (14e)$$

where ε/σ = the specific creep, in 10^{-6} /psi, and R^2 = coefficient of correlation.
ln is the natural logarithm.

These equations and Fig. 5a suggest that these five equations can be condensed for every t to the form

$$3/\sigma \approx 0.020(\ln(t-t')) - 0.029\ln(t') + 0.34 \quad (15)$$

Equation (15) is also shown in Fig. 5 with dotted lines. It is obvious that Eq. (10) and (11) are practically identical with Eq. (13a) and (14a), respectively.

Example 3: the effects of loading age and duration on creep

The data in this example were obtained originally from a test series performed for Ross-Dam and quoted by Bazant again in the same publication [Bazant 1975]. 150 x 400 mm (6 x 16 in.) cylinders were used that were cured in sealed condition at 70°F (21°C). Type II cement was used with $w/c = 0.56$ by mass. The maximum particle size was 375 mm (1.5 in.). The 28-day compressive strength was 4970 psi (350 kg/cm²) and the applied stress was not more than one-third of the strength. Cement content is not given but one can infer from the higher value of the w/c that it was somewhat less than in the previous example. For this reason $p = 0.15$ was used in the model. E_c is again 7×10^6 psi (492,000 kg/cm²), and except for the new water-cement ratio, Eq. (5) and (7) were used in the same way as in the previous example because similar equations have not been developed for Type II cements at that time.

Here again these values were substituted into Eq. (5) and (7), resulting in two hard composite average models for the Ross Dam experiments: one with power function approximation, the other using logarithmic functions.

For power function relationship, the results for the creep lines best fitting to selected experimental results (points) are shown in Fig. 6(a) to 6(c) with linear, semi-log and log-log systems, respectively. Details are the following:

$$\text{For } t' = 7 \text{ d. } \varepsilon/\sigma = 0.359(t-t')^{0.1013} \quad R^2 = 0.93 \quad (16a)$$

$$\text{For } t' = 28 \text{ d. } \varepsilon/\sigma = 0.238(t-t')^{0.1084} \quad R^2 = 0.97 \quad (16b)$$

$$\text{For } t' = 90 \text{ d. } \varepsilon/\sigma = 0.179(t-t')^{0.127} \quad R^2 = 0.98 \quad (16c)$$

$$\text{For } t' = 365 \text{ d. } \varepsilon/\sigma = 0.150(t-t')^{0.131} \quad R^2 = 0.93 \quad (16d)$$

For log relationship the creep lines ε/σ are shown with solid lines, best fitting to selected experimental results (points), in Fig. 7(a) through 7(c) in three different systems of coordinates. Details are the following:

$$\text{For } t' = 7 \text{ d. } \varepsilon/\sigma = 0.0556 \ln(t-t') + 0.320 \quad R^2 = 0.94 \quad (17a)$$