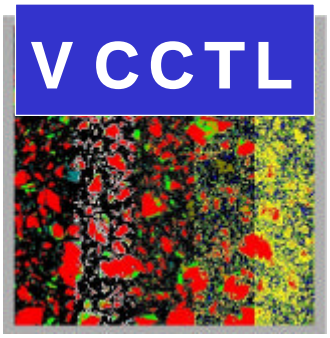

VCCTL Newsletter

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INTRODUCTION

The Virtual Cement and Concrete Testing Laboratory (VCCTL) is a web-based computer software package for simulating the microstructure and predicting the performance of cement-based materials. First installed in the winter of 2000, the system is available at the WWW address provided below.

To further advance the goals and research of the VCCTL, the VCCTL consortium was formed in January 2001. The consortium is an ongoing collaboration between three NIST laboratories (BFRL, ITL, and MSEL) and eight industrial members. Current topics of research in the consortium include cement hydration and microstructure development, experimental measurement and computer simulation of rheological properties, and computation of elastic properties of cement-based materials. Standardization activities, such as developing a standard test method for particle size distribution measurement, are coordinated with the ASTM C01 committee on Cement.

Consortium Industrial Members for 2002:

Cemex
Degussa Construction Chemicals
Dyckerhoff Zement GmbH
Holcim Inc.
Int'l. Center for Aggregate Research
Portland Cement Association
Verein Deutscher Zementwerke e. V.
W.R. Grace & Co. – Conn.

VCCTL Web Sites:

http://vcctl.cbt.nist.gov/
http://bfrl.nist.gov/862/vcctl/

VCCTL USAGE TIP

While the VCCTL web-based software can be used to generate a wide variety of plots of predicted performance (including comparison with experimental data) via menu selection 17, users occasionally want to graph some of the predicted values using their own graphical analysis package. Any of the VCCTL output files may be directly loaded into the local web browser (and then saved to the local computer) by directly providing the filename as a link to be retrieved. Specifically, with each hydration run, a set of datafiles are created and stored on the system as described in the online VCCTL User's Manual. These files have the general name image.dft.nnnn.tt.xyz where image is the name of the image file being hydrated, dft is the datafile type (pha for phase counts, chs for chemical shrinkage, heat for heat release data, adi for adiabatic heat signature, etc.), nnnn is the number of hydration cycles, tt is the starting hydration temperature in degrees Celsius, x is the conversion of primary C-S-H to pozzolanic C-S-H (prohibited=0, allowed=1), y is the thermal curing selected (isothermal=0, adiabatic=1, temperature-defined=2), and z is the initial saturation for curing (saturated=0, sealed=1). When the user submits a hydration run, the VCCTL returns a detailed listing of these files that will be created by the VCCTL (the user could print out this page through a web browser for later reference). The user may view (and download) this file through their web browser by specifying http://vcctl.cbt.nist.gov/~vcctl/data/image.dft.nnnn.tt.xyz with the appropriately substituted values for image, dft, nnnn, tt, and xyz. Once viewed, the file may be saved using the Save as option on the web browser File pulldown menu.

VCCTL APPLICATION SPOTLIGHT

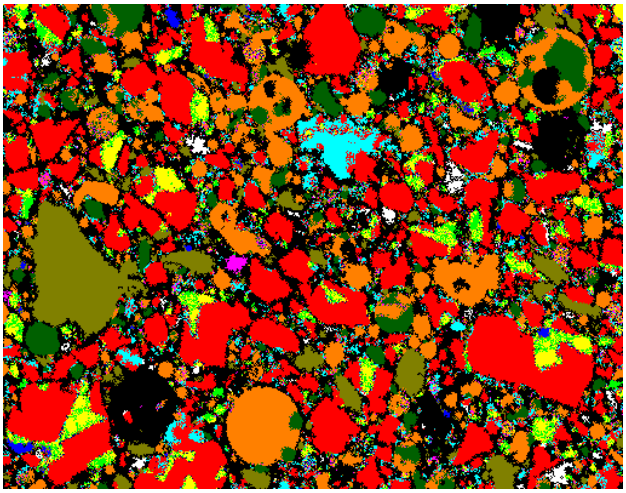
This issue of the VCCTL newsletter spotlights the usage of the system by a team of researchers led by Dr. Takashi Horiguchi at Hokkaido University, Japan in a project entitled “Application of Percolation Theory and Computer Simulation for Study of Concrete Durability and Transport Properties”. The following paragraphs were supplied by Petia Staneva, a team member.

In the first phase of this research, the VCCTL was used in order to create simulated digital images of two different cements (lunar-like and portland) that were objects of our investigation. The VCCTL menu selections for distribution of all phases amongst the cement particles and hydration of the 3-D microstructures were extensively applied. We found the capability to plot the predicted properties against the experimental results to be very convenient. Some of the results of our project were recently reported at the 9th International Conference on the Durability of Building Materials and Components, held in Brisbane in March of 2002. An evaluation of carbonation and its relationship with the percolation state of the concrete will soon be performed, based on the results obtained to date by the NIST team.

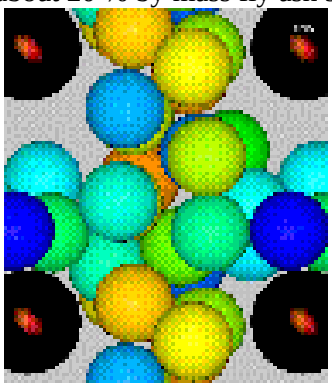
We are currently modifying some portions of the present programs and algorithms to reflect the curing conditions and some other specifics of the dry mix/ steam injection method. In such a way, it should be possible to identify the optimum mixtures and curing conditions to achieve desired mechanical and durability properties, and then validate these experimentally. This approach is useful not only from an economic point of view, but also for materials intended to be produced or used in new environments (like space, lunar, aggressive medium, etc.) where there are obvious constraints to conducting numerous experiments.

We would also like to express our gratitude to the NIST team and researchers for the great efforts and achievements with the creation of the VCCTL and for all of their support in our research.

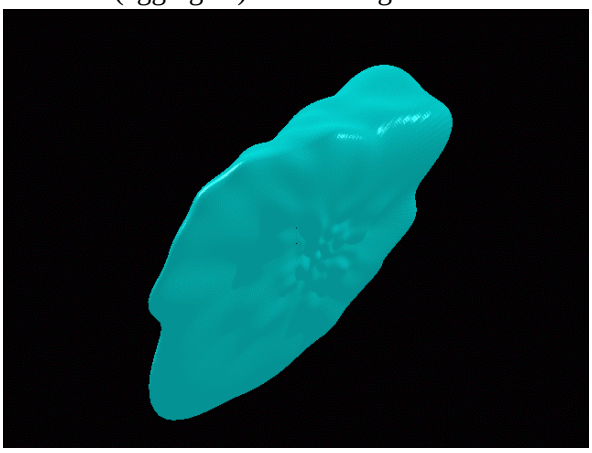
VCCTL IMAGE GALLERY



SEM/X-ray composite image of a blended cement containing about 20 % by mass fly ash substitution.



Dissipivative particle dynamics-based simulation of concrete (aggregate) flow through a set of rebars.



3-D aggregate simulated based on spherical harmonic analysis of real coarse aggregates.

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