Using Characterization Data to Model Microstructure and Properties

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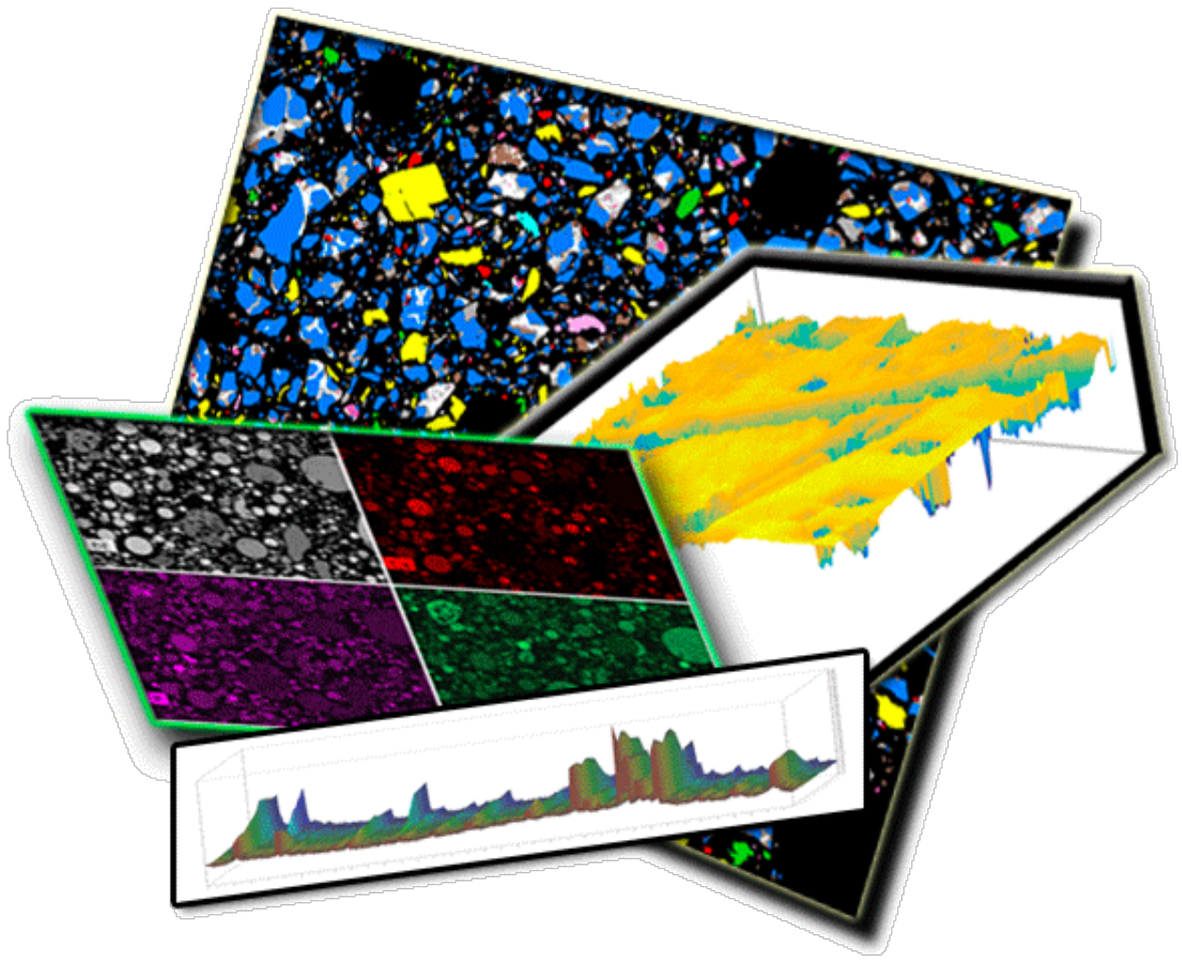

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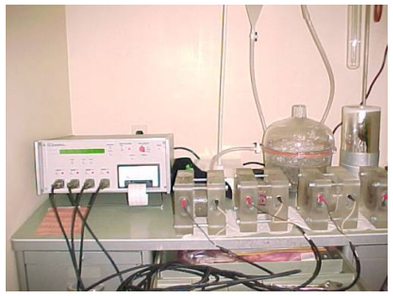
Hydration

Mixing

Transport Properties



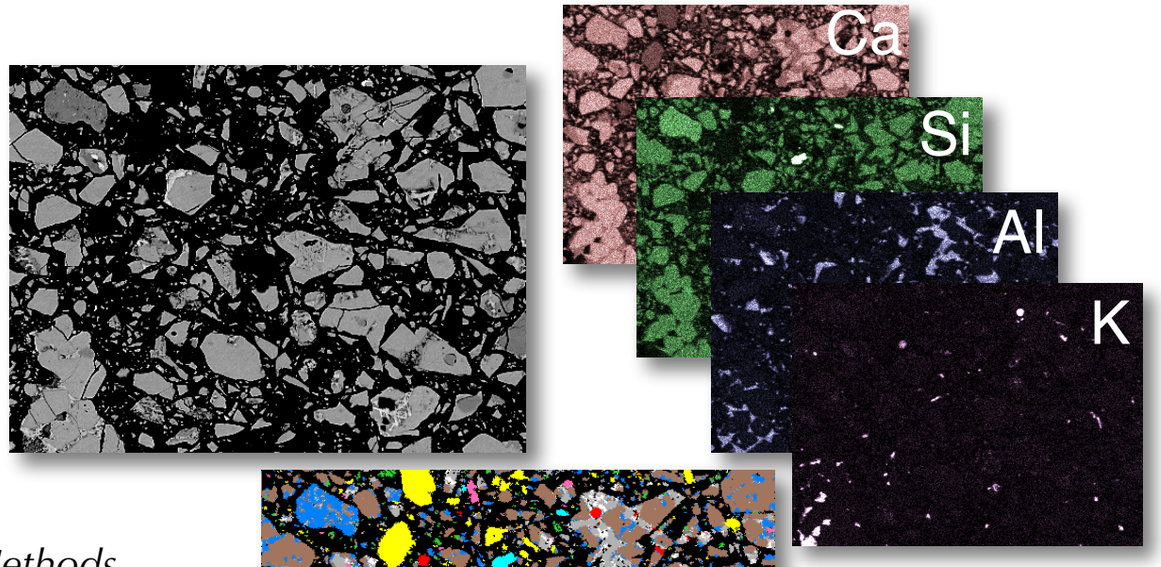
Software Interface

Mechanical Properties

Materials

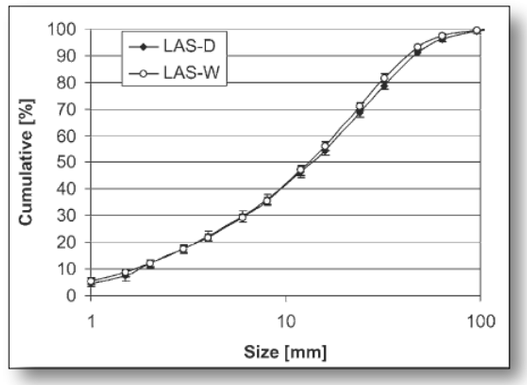
(Database)

SEM/BSE Image and QXRD...

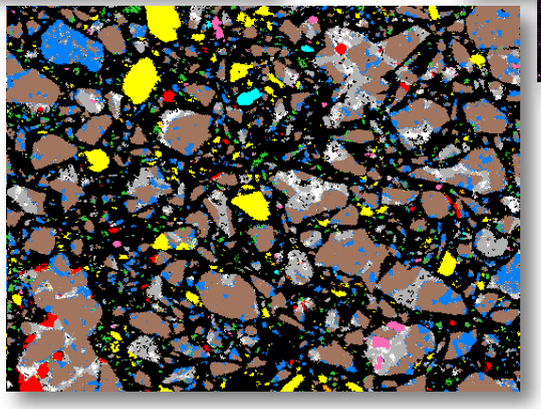


Methods developed by Dale Bentz & Paul Stutzman (NIST)

...X-ray element maps ...

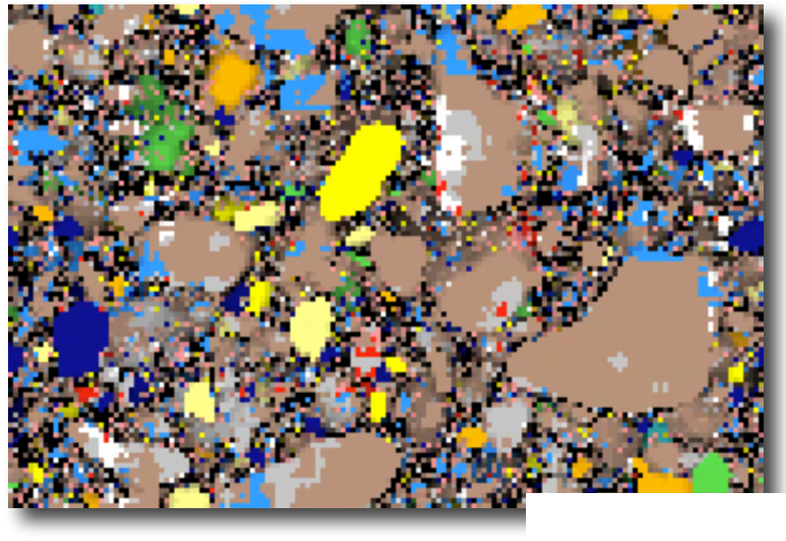


Particle Size Distribution



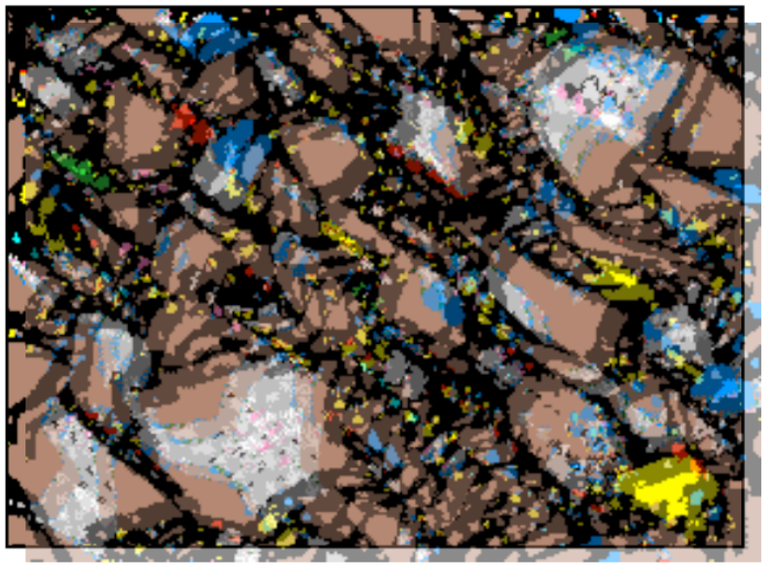
... segmented image ...

... measure autocorrelation fns on majority phases



We want to distribute the clinker phases among particles in a spatially realistic way, at least statistically.

To do so, first measure two-point correlation functions on different phases or collections of phases in segmented SEM image:



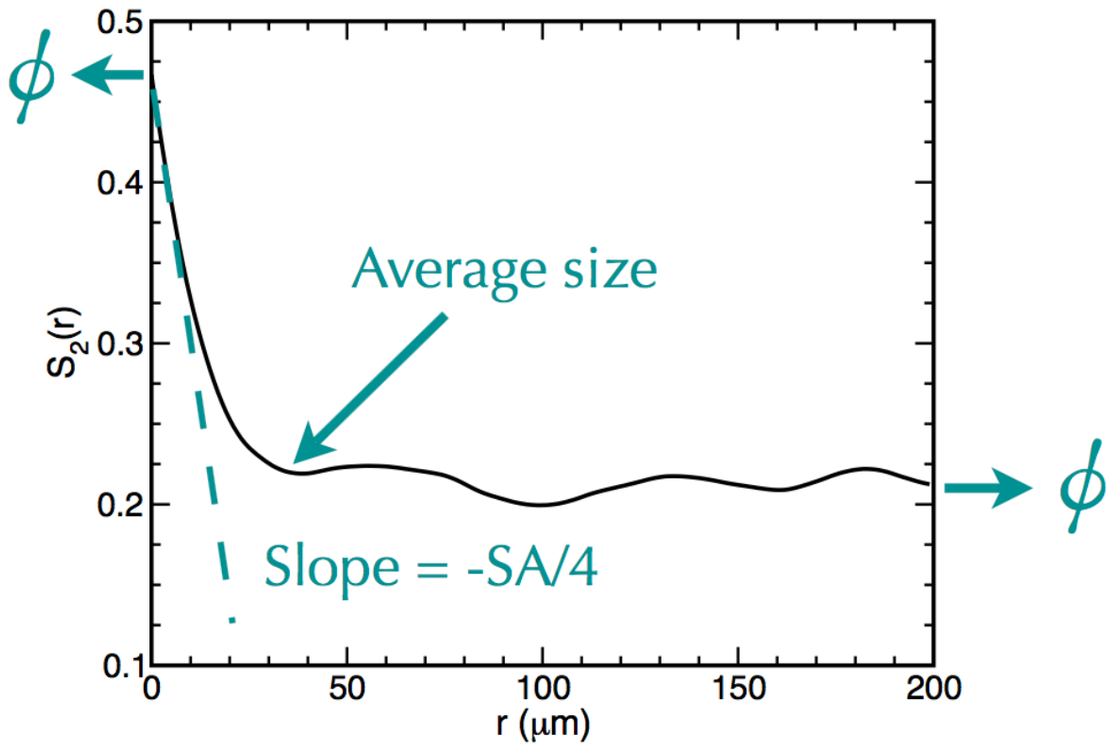
$$S_{2,i}(r) = \int_{-\infty}^{\infty} f_i(x+r) f_i(x)\,\mathrm{d}x$$

where $f_i(x) = 1$ if phase i is located at x, and $f_i(x) = 0$ otherwise.

Equivalent to overlaying a displaced image on an original and measuring the overlapping areas of the same phase for different displacements.

Features of S2:

- $S_2(0)$ = vol frac
- $S_2(\infty)$ = (vol frac)^2
- Slope at r = 0 is -1/4 of the specific surface area
- First minimum is average domain size
- Is the same in 2D and 3D for homogeneous, isotropic structures!



J.G. Berryman and S.C. Blair, *J. Appl. Phys.* **60** [6] 1930-1938 (1986)

→ We can use S_2 measured on 2D images to construct 3D images with the same statistical features

Material Inventory

▼ Edit or create a cement

Name: cement140

Upload data from a ZIP file for the cement: Browse...

▶ Cement data

Mass fractions of sulfates

Dihydrate 0.0039 Hemihydrate 0.022 Anhydrite 0.016

Cancel Save Save as... Delete

▶ Edit or create a fly ash

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

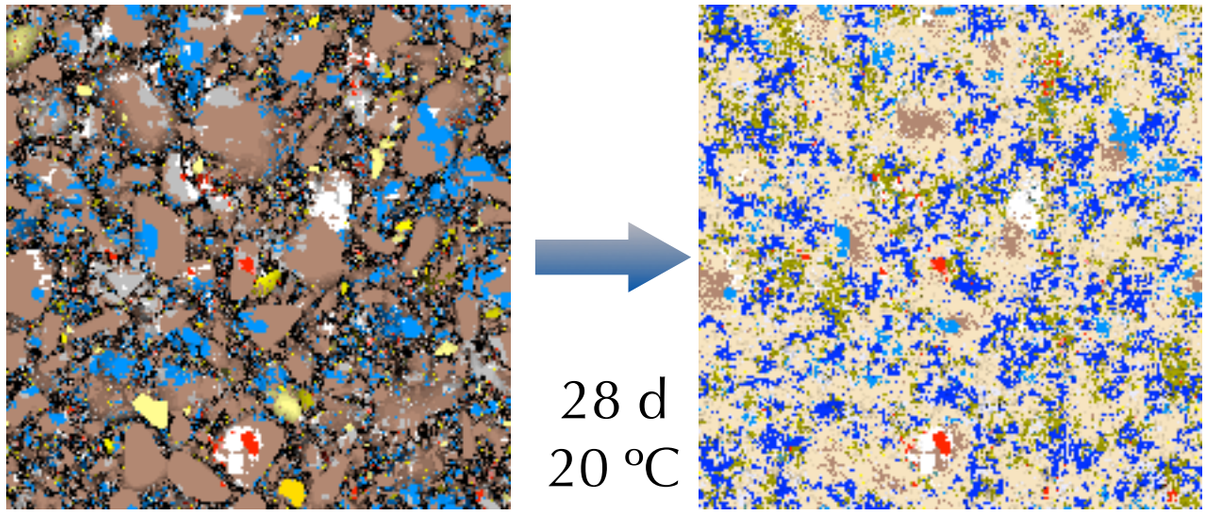
... Or stop at degree of hydration: 1.0

- (•) Use time conversion
  - Time conversion factor 3.5E-4 $h/cycle^2$
- ( ) Use a calorimetry file
- ( ) Use a chemical shrinkage file

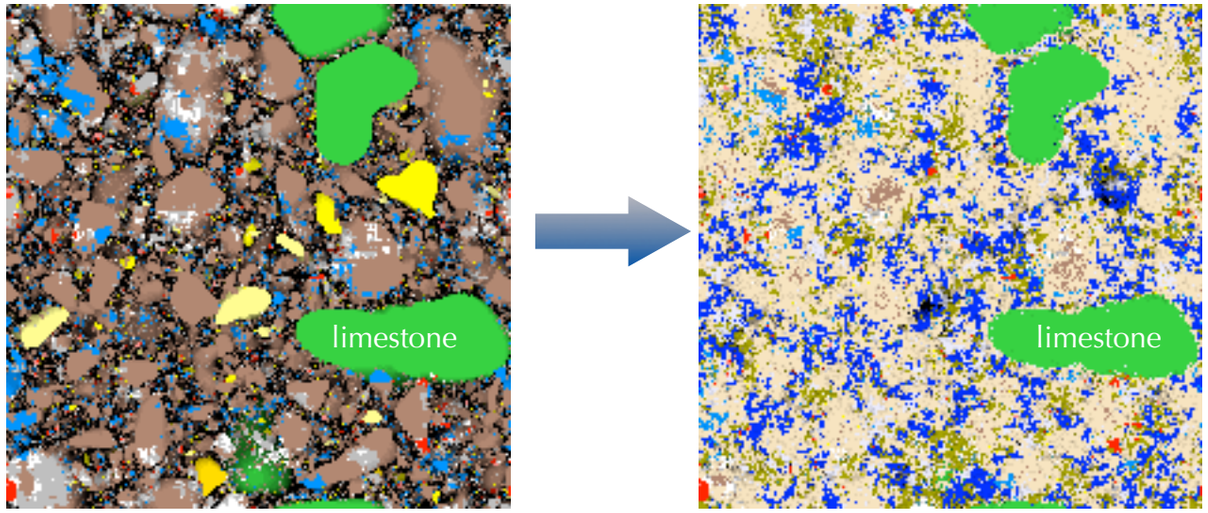
Saturation conditions

- (•) saturated
- ( ) sealed

OPC, w/s = 0.35

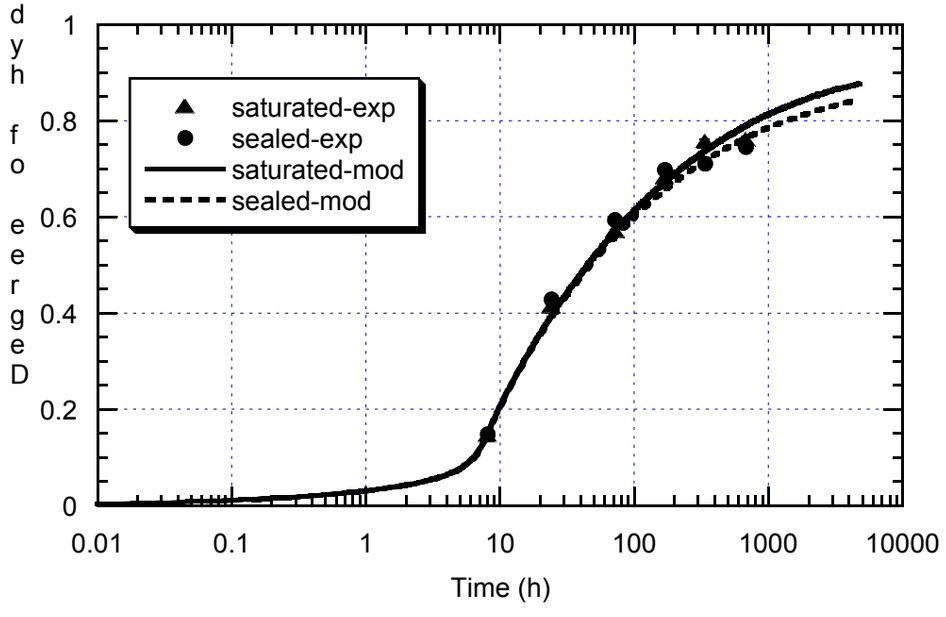


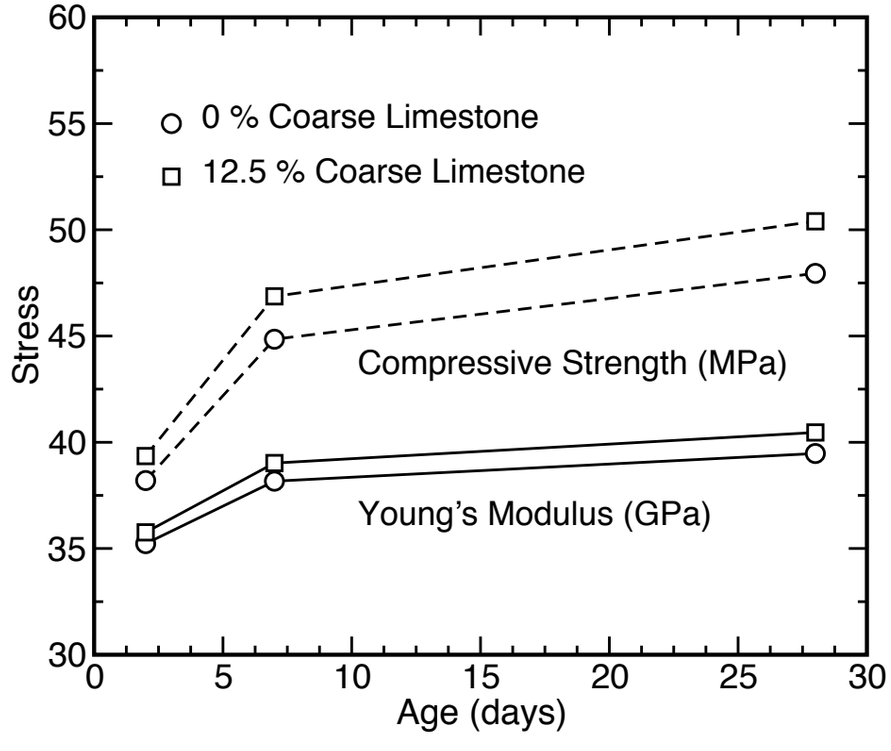
OPC, w/s = 0.35 with 12.5 % replacement by limestone



Linking Microstructure to Properties

- Some properties of hydrating pastes can be tracked directly as the structure evolves
- Mechanical properties of paste (linear elastic moduli, thermal expansion) is calculated directly on the microstructure image using finite element model
- For mortar and concrete, these paste properties are coarse grained and then effective medium theory is used to compute the properties of the material

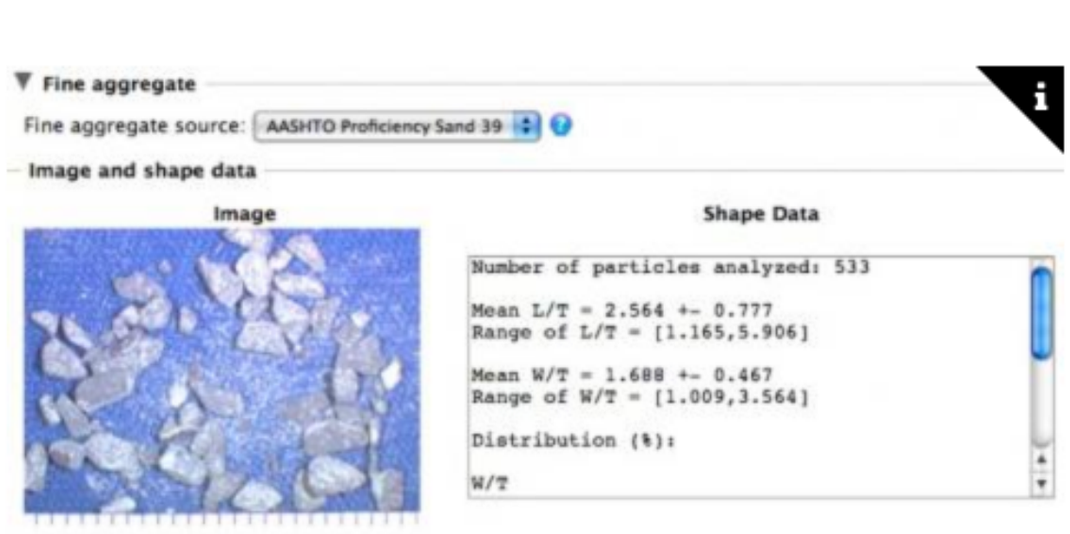




SOFTWARE

VCCTL Software

(Return to Cement Hydration and Degradation Modeling Software)



The Virtual Cement and Concrete Testing Laboratory (VCCTL) software provides a virtual testing laboratory environment that can be used by concrete scientists, engineers, and technologists for virtual testing of cement paste and concrete materials. With this software the user can

- create *virtual materials*, using carefully characterized cement powders, supplementary cementitious materials, fillers, and aggregates;
- simulate the curing of these materials under a wide range of conditions; and

Version
9.5

Type of Software
virtual testing of cement and concrete materials

Last Updated
May 20, 2014

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