## COMPUTER SIMULATION OF THE INTERFACIAL TRANSITION ZONE MICROSTRUCTURE

Using computer models, the researchers at the National Institute of Standards and Technology (NIST) have been conducting interesting simulations of the cement and concrete microstructure. The references at the end of this hyperlink provide a good starting point for those interested in obtaining further information in this growing research area. Computer simulations can be used to study the microstructure of the interfacial transition zone and how to modify it by using very small particles of mineral admixtures such as silica fume.

Figure 1 shows a simplified geometry where the aggregate is modeled by a small flat plate. This geometry also demonstrates the so-called "wall effect" caused by large aggregates in concrete. The Portland cement is segmented by color into the six phases: tricalcium silicate (red), dicalcium silicate (aqua), tricalcium aluminate (green), tetracalcium aluminoferrite (yellow), gypsum (gray), and water-filled porosity (black). Chapter 6 describes in detail the hydration reaction of the cement compounds. The computer simulation specifies a set of cellular automata rules that control the events that occur with each pixel during the hydration reaction. Hydration products, calcium hydroxide (blue) and calcium silicate hydrate (orange), start to form as the unhydrated materials are exposed to water. Figure 3 shows the porosity distribution as a function of distance from the aggregate surface. As discussed in the main text, the gradient in porosity existing in the interfacial transition zone will impact the strength and durability of mortar or concrete.

Figure 2 shows a similar type of computer modeling of the interfacial transition zone when fine particles of silica fume (pale blue) are used in the cement paste. This mineral admixture effectively reduces the porosity near the aggregate surface, as indicated in Figure 3. Silica fume particles are less than 1/100th of the size of the anhydrous cement grain; therefore, their introduction affects significantly the physical arrangement of the system, particularly near the aggregate surface where a higher porosity exists. Because it is a pozzolanic material, silica fume further densifies the system as it reacts with calcium hydroxide to form calcium silicate hydrate (designated pink, to differentiate it from the calcium silicate hydrate formed by the cement hydration).

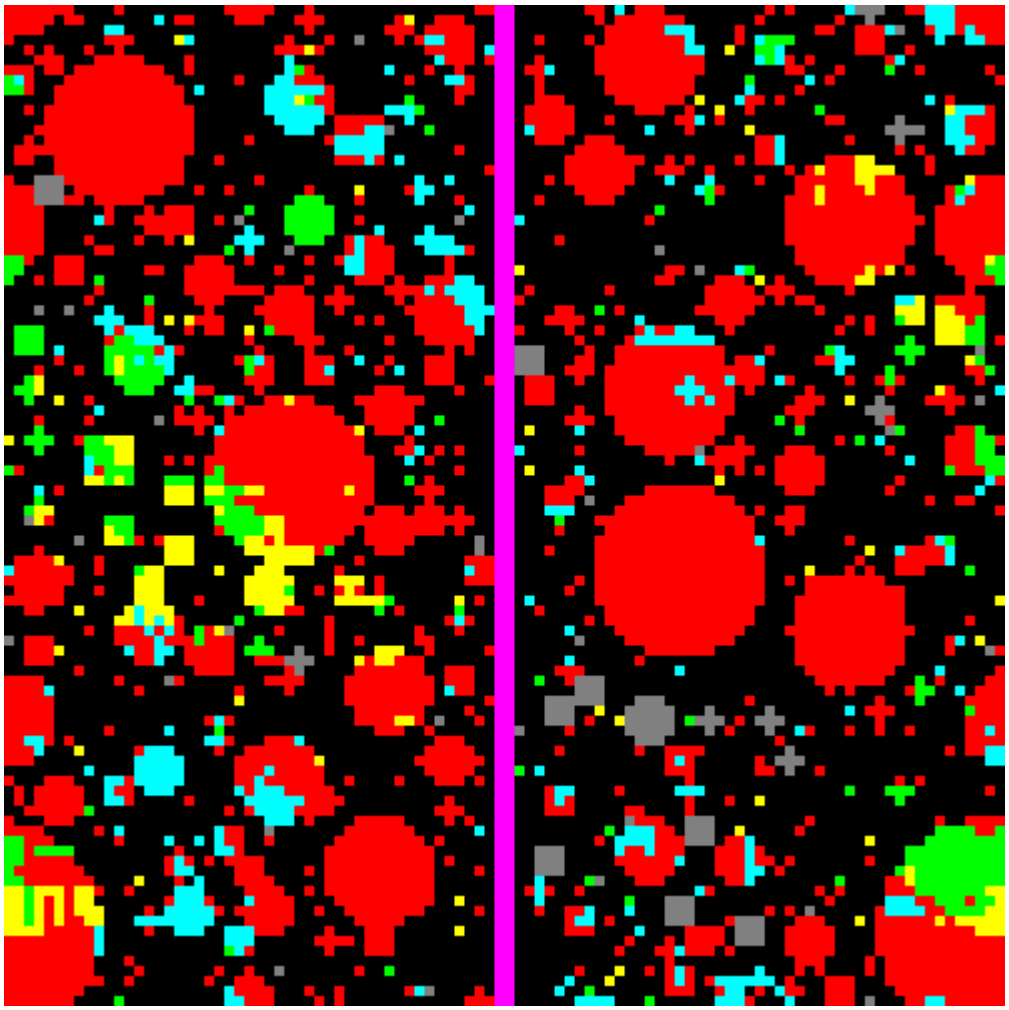

Figure 1. Initial 2-D slice from a 3-D microstructure of a cement paste with a 0.45 water to cement ratio and no silica fume. Run the file paulom~1.gif for the animation (courtesy D. Bentz, NIST).

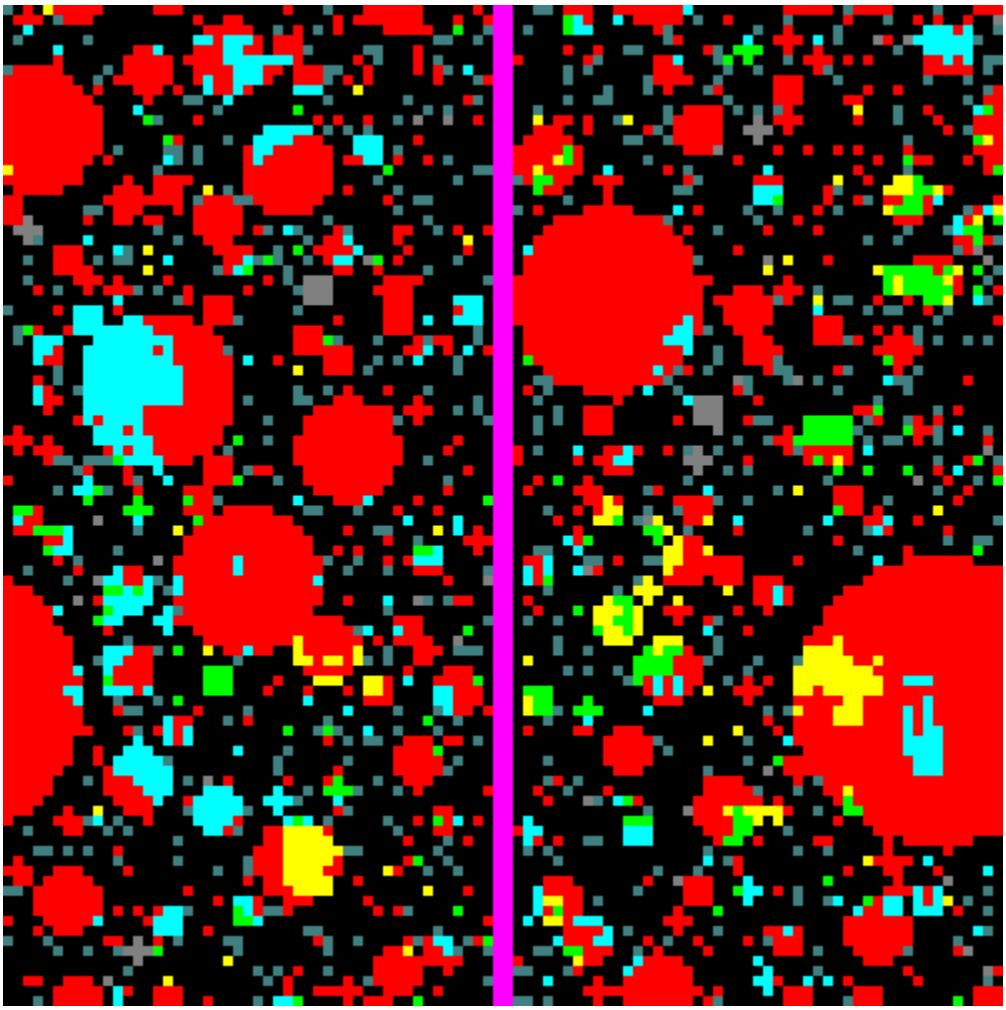

Figure 2. Initial 2-D slice from a 3-D microstructure of a cement paste with a 0.45 water to cement ratio and 10% silica fume. Run the file paulom~2.gif for the animation (courtesy D. Bentz, NIST).

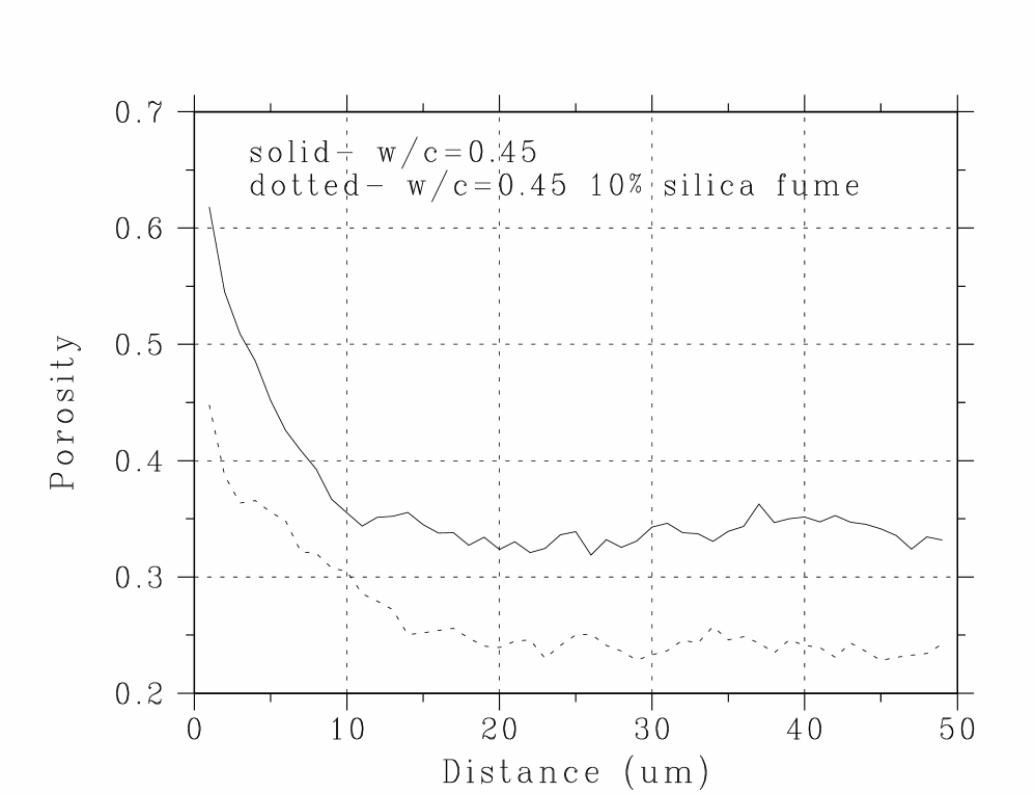


Figure 3. Porosity distribution as a function of distance from the aggregate after 3650 cycles of hydration at roughly 180 days.

**References:**

Virtual Cement and Concrete Testing Laboratory, http://ciks.cbt.nist.gov/vcctl/.

Bentz, D.P.; Schlangen, E.; Garboczi, E.J., Computer Simulation of Interfacial Zone Microstructure and Its Effect on the Properties of Cement-Based Composites. American Ceramic Society. Materials Science of Concrete. Volume 6. 1995, Westerville, OH, Skalny, J. P.; Mindess, S., Editors, pp. 155-199, 1995. http://fire.nist.gov/bfrlpubs/build95/art013.html

Bentz, D.P.; Garboczi, E.J., Computer Modelling of the Interfacial Transition Zone Microstructure and Properties. In Engineering and Transport Properties of the Interfacial Transition Zone in Cementitious Composites, RILEM ETC Report, pp. 349-385, 1999. http://ciks.cbt.nist.gov/monograph/rilemreport/report.html.

Bentz, D.P. , Guide to Using CEMHYD3D: A Three-Dimensional Cement Hydration and Microstructure Development Modeling Package. NISTIR 5977; 146 p. February 1997. http://ciks.cbt.nist.gov/monograph/monograph/appendix2.html

Bentz, D.P.; Hwang, J.T.G.; Hagwood, C.; Garboczi, E. J.; Snyder, K.A.; Buenfeld, N.; Scrivener, K.L, Interfacial Zone Percolation in Concrete: Effects of Interfacial Zone Thickness and Aggregate Shape. Materials Research Society. Microstructure of Cement-Based Systems/Bonding and Interfaces in Cemetitious Materials. Materials Research Society Symposium Proceedings, Volume 370. November 28-December 1, 1994, Boston, MA, Materials Research Society, Pittsburgh, PA. Diamond, S.; Mindess, S.; Glasser, F.P.; Roberts, L.W., Editors, pp. 437-442, 1995. http://ciks.cbt.nist.gov/monograph/paper72/paper72.html