A REPRESENTATIVE VOLUME ELEMENT BASED MODELING OF CEMENTITIOUS MATERIALS WITH VARIOUS ADDITIVES

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A suite of special purpose computational codes were employed to estimate the elastic properties of heterogeneous C-S-H based multi-phase cementitious materials. The primary focus here is on predicting homogenized macro mechanics properties using micro mechanics based models. The micro-structure of heterogeneous cementitious material consisting of typical volume fractions of various constituent phases is numerically generated using CEMHYD3D [1-2] for various microstructure resolutions. The microstructure is modeled as micro-scale representative volume element (RVE) using continuum hexahedral elements in commercial general purpose ABAQUS finite element code [3] to generate a cube of 100x100x100 microns. The RVE is subjected to various prescribed idealized simple tension and shear deformation modes in order to generate the effective elastic tensor of the cementitious material. In addition, the effects of RVE size (1M and 4M), particle size distribution, volume fraction of various constituents, and statistical variation on elastic properties were also considered in the modeling and simulation. Computational simulations using ABAQUS were performed with both kinematic and periodic boundary conditions. Figure 1 shows the effects of RVE domain size on Young's modulus and Poisson's ratio for 80% degree of hydration; in addition a comparison with the "Asymptotic Expansion Homogenization (AEH)" method. Our current work also considered the effects of volume fraction of fly ash on elastic properties.
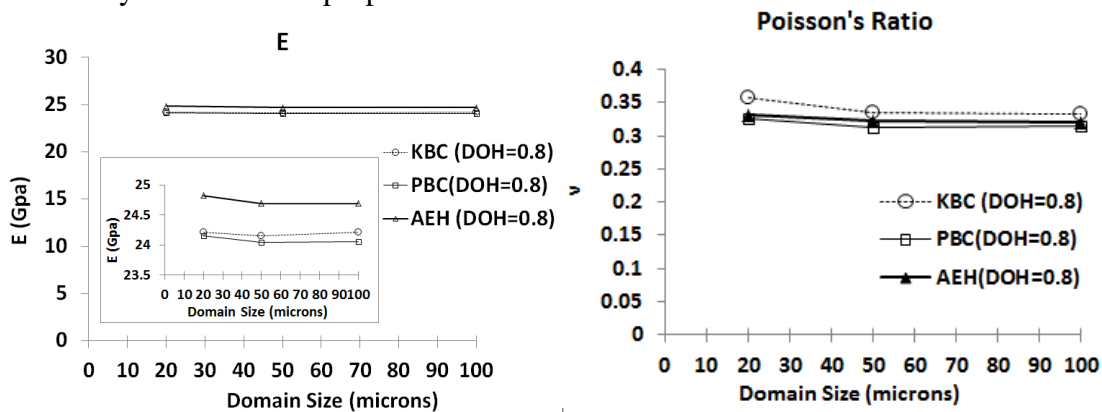

Figure 1. Effect of domain size on material properties for DOH=0.8 for KBC, PBC, and AEH on Youngs Modulus (E) and Poisson's ratio.

REFERENCES

[1] The software package, CEMHYD3D V.3, developed by NIST researchers, MD, USA.

[2] D.P. Bentz, "Three-Dimensional Computer Simulation of Portland Cement Hydration and Microstructure Development," *J. Am. Ceram. Soc.*, 80(1), pp. 3-21, 1997.

[3] ABAQUS, a commercial code, The Abaqus Software is a product of Dassault Systèmes Simulia Corp., Providence, RI, USA.