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14. ABSTRACT
The current work focuses on evaluation of the effective elastic properties of cementitious materials through a voxel based FEA approach. Voxels are generated for a heterogeneous cementitious material (Type-I cement) consisting of typical volume fractions of various constituent phases from digital microstructures. The microstructure is modeled as a micro-scale representative volume element (RVE) in ABAQUS to generate cubes several tens of microns in dimension and subjected to various prescribed deformation modes to generate the effective elastic tensor of the material. The RVE calculated elastic properties such as moduli and Poisson's ratio are validated through an

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Report Title

Micromechanics Based Representative Volume Element Modeling of Heterogeneous Cement Paste

ABSTRACT

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Multi-Scale Modeling of Cementitious Materials

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Abstract

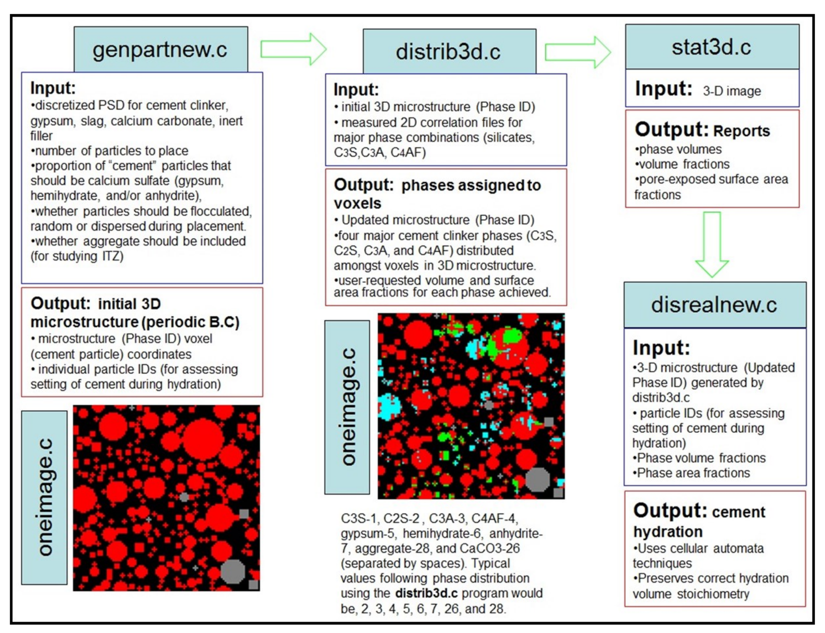
- ❑ Effective elastic properties of cementitious materials are evaluated through a voxel based FEA approach.

Introduction

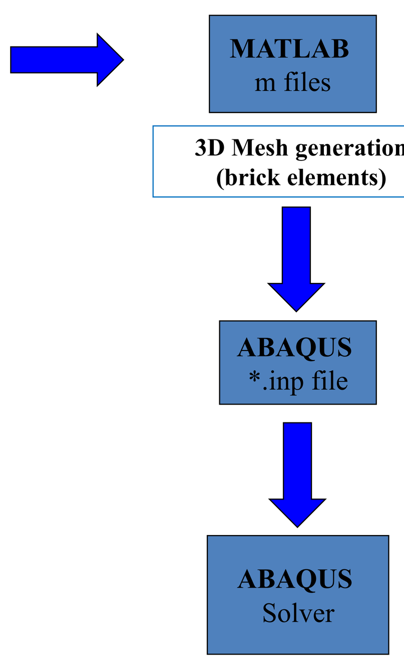
- ❑ A methodology has been developed for computing the elastic properties of heterogeneous C-S-H (calcium oxide- silicate oxide- hydroxide) based multi-phase cementitious materials.
- ❑ The primary focus is to predict homogenized properties at macro-levels using micro mechanics based models.
- ❑ Focus is on the determination of elastic properties for hydrated cement paste from un-hydrated constituents when small strain quasi-static loading conditions are applied to micro-scale.

Methodology

- ❑ The representative volume element (RVE) is the smallest volume of material that captures global characteristics of the material and shows the same overall material properties irrespective of the boundary conditions applied.
- ❑ Software package CEMHYD3D V.3 (NIST), simulates the hydration process and formation of the digitally generated micro-structure for a typical Type-I general purpose cement.
- ❑ Initial 3D microstructure is created based on measured geometrical particle size distribution (PSD) as well as volume fractions and surface–area fractions of the constituent phases for cement powder, extracted from 2D composite images of cement at various degrees of hydration (DOH).
- ❑ The RVE-calculated elastic properties such as moduli and Poisson's ratio are validated through an asymptotic expansion homogenization (AEH) and compared with rule of mixtures.
- ❑ Windowing is employed to investigate how anisotropy due to local microstructure leads to overall isotropic behavior of the agglomerate. Windows are analogous to physical core samples prepared by extraction from a hydrated bulk specimen.



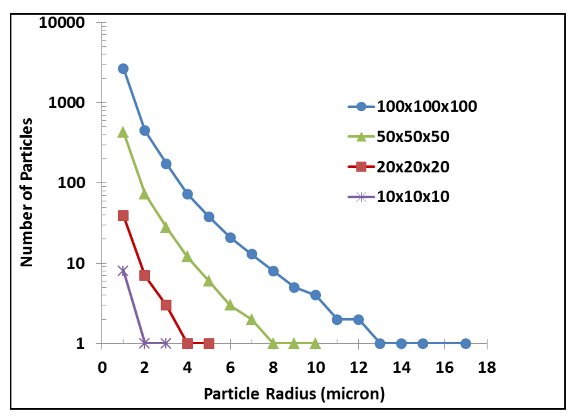
Generation of particle size distributions, voxel coordinates and material type



Linear elastic
Nonlinear Quasi-static
Nonlinear Dynamic Explicit
(wave propagation)

	Phase	Phase ID	Volume Fraction%	E (GPa)	Poisson's ratio ν
1	Water Porosity	0	19.8251	0.001	0.499924
2	Tricalcium Silicate (C_3S)	1	7.1625	117.6	0.314
3	Dicalcium Silicate (C_2S)	2	2.628	117.6	0.314
4	Tricalcium Aluminate (C_3A)	3	1.7376	117.6	0.314
5	Tetracalcium Aluminoferrite (C_4AF)	4	1.1012	117.6	0.314
6	Dihydrate (Gypsum) ($C\bar{S}.H_2$)	5	0.0022	45.7	0.33
7	Hemihydrate ($C\bar{S}.H_{1/2}$)	6	0.0001	62.9	0.3
8	Anhydrite ($C\bar{S}$)	7	0.0005	80	0.275
9	Calcium Hydroxide (CH)	13	14.425	42.3	0.324
10	Calcium Silicate Hydrate Gel (CSH)	14	37.4425	22.4	0.25
11	Hydrogarnet (C_3AH_6)	15	4.2538	22.4	0.25
12	Ettringite ($C_6A\bar{S}_3H_{32}$)	16	6.034	22.4	0.25
13	Iron-rich Stable Ettringite ($ETTRC_4AF$)	17	1.807	22.4	0.25
14	Monosulfate AFM ($C_4A\bar{S}H_{12}$)	18	2.4623	22.4	0.25
15	Iron Hydroxide (FH_3)	19	0.3193	22.4	0.25
16	Gypsum Formed from Hemihydrate and Anhydrite (GYPSUMS)	25	0.003	45.7	0.33
17	ABSGYPS	29	0.2996	45.7	0.33
18	Empty Porosity	45	0.4963	0	0

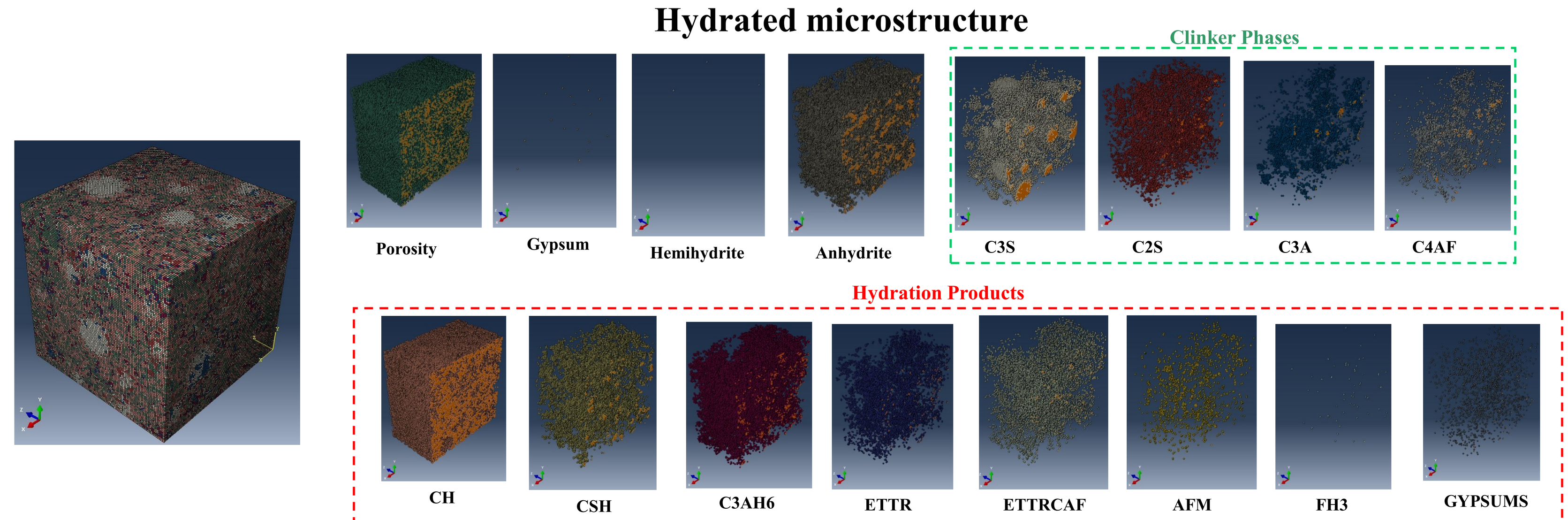
Material properties and volume fractions of constituent phases for a representative Type-I cement

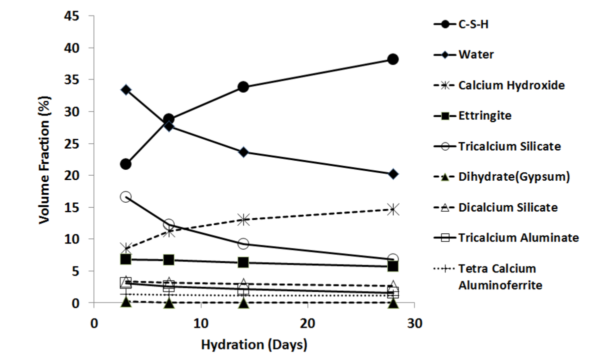


Scaling is required to maintain consistent area and volume fractions of various constituent phases

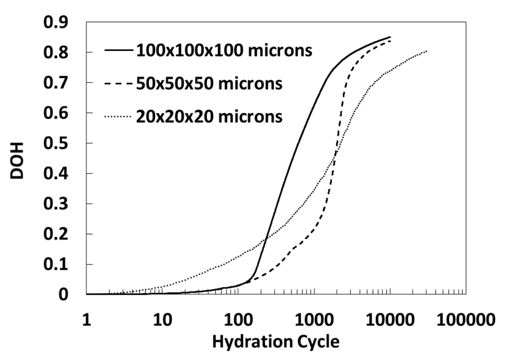
Cement Hydration

Hydrated microstructure

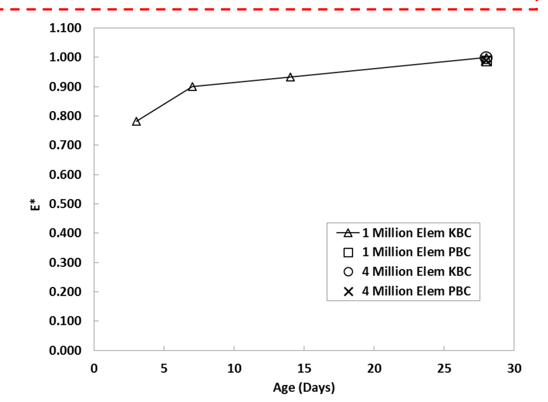




Typical volume fractions of major constituents vs Curing

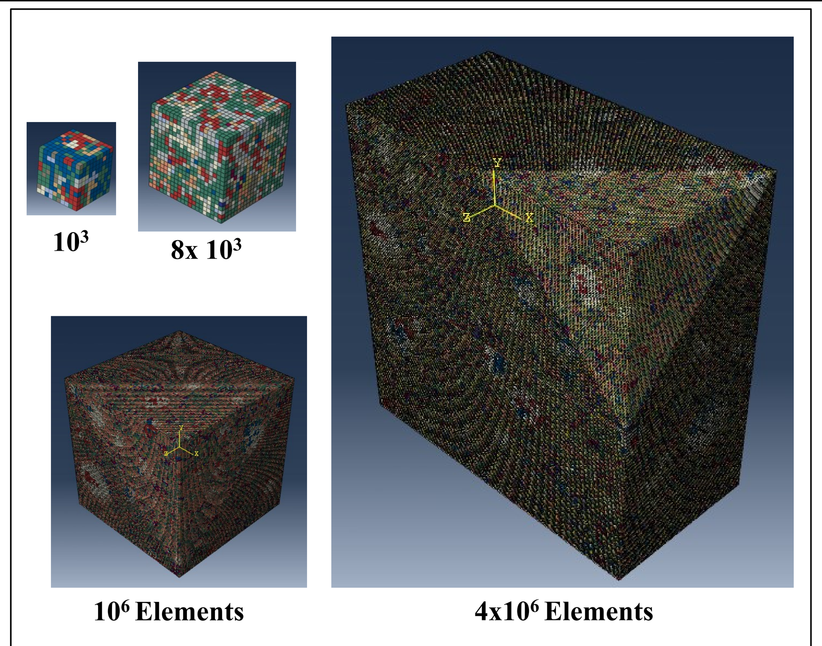


Effect of domain size on DOH



Development of the Young's Modulus

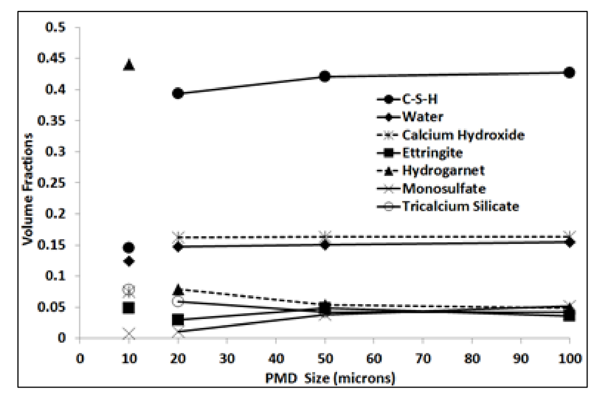
RVE



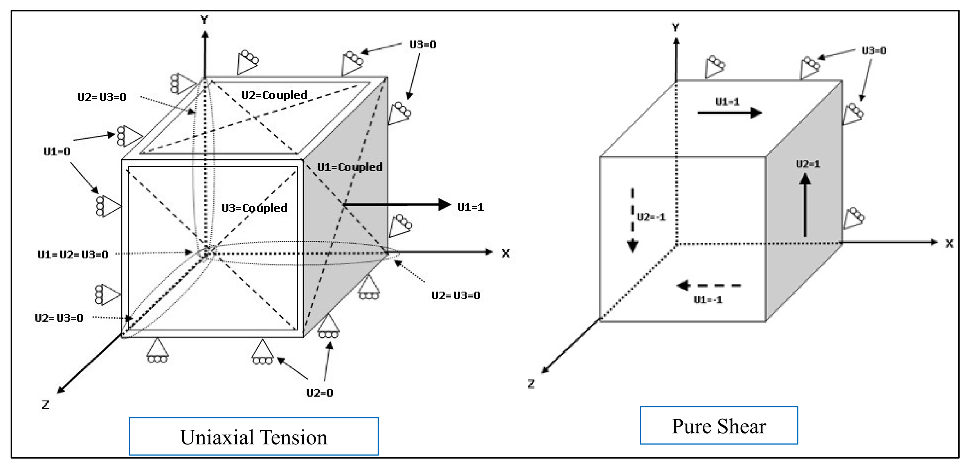
$$\begin{Bmatrix}\sigma_1\\\sigma_2\\\sigma_3\\\sigma_4\\\sigma_5\\\sigma_6\end{Bmatrix}=\begin{bmatrix}C_{11}&C_{12}&C_{13}&0&0&0\\C_{12}&C_{22}&C_{23}&0&0&0\\C_{13}&C_{23}&C_{33}&0&0&0\\0&0&0&C_{44}&0&0\\0&0&0&0&C_{55}&0\\0&0&0&0&0&C_{66}\end{bmatrix}\begin{Bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\\\varepsilon_6\end{Bmatrix}$$

$$U=\frac{1}{2}\cdot\sigma_p^{avg}\cdot\varepsilon_q^{avg}\cdot V_{RVE}$$

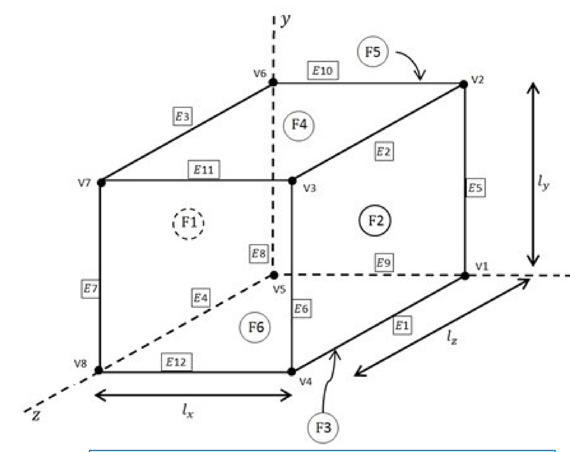
$$E_i=\frac{\sigma_i^{avg}}{\epsilon_i^{avg}}\quad G_{ij}=\frac{\sigma_i^{avg}}{\epsilon_j^{avg}}$$



Volume fractions of major phases for 1K, 8K, 125K and 1M PMDs



Kinematic Boundary Conditions



Periodic Boundary Conditions

Nodes on Faces:

$$u_i^{F2}-u_i^{F1}-L_x\varepsilon_{i1}=0$$
$$u_i^{F4}-u_i^{F3}-L_y\varepsilon_{i2}=0$$
$$u_i^{F6}-u_i^{F5}-L_z\varepsilon_{i3}=0$$

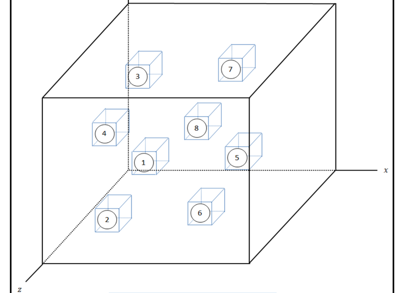
Nodes on Edges:

$$u_i^{E2}-u_i^{E4}-L_x\varepsilon_{i1}-L_y\varepsilon_{i2}=0$$
$$u_i^{E1}-u_i^{E3}-L_x\varepsilon_{i1}+L_y\varepsilon_{i2}=0$$
$$u_i^{E6}-u_i^{E8}-L_x\varepsilon_{i1}-L_z\varepsilon_{i3}=0$$
$$u_i^{E5}-u_i^{E7}-L_x\varepsilon_{i1}+L_z\varepsilon_{i3}=0$$
$$u_i^{E11}-u_i^{E9}-L_y\varepsilon_{i2}-L_z\varepsilon_{i3}=0$$
$$u_i^{E10}-u_i^{E12}-L_y\varepsilon_{i2}+L_z\varepsilon_{i3}=0$$

Nodes on Vertices:

$$u_i^{V3}-u_i^{V5}-L_x\varepsilon_{i1}-L_y\varepsilon_{i2}-L_z\varepsilon_{i3}=0$$
$$u_i^{V2}-u_i^{V8}-L_x\varepsilon_{i1}-L_y\varepsilon_{i2}+L_z\varepsilon_{i3}=0$$
$$u_i^{V7}-u_i^{V1}+L_x\varepsilon_{i1}-L_y\varepsilon_{i2}-L_z\varepsilon_{i3}=0$$
$$u_i^{V4}-u_i^{V6}-L_x\varepsilon_{i1}+L_y\varepsilon_{i2}-L_z\varepsilon_{i3}=0$$

Constraint Equations for PBC



Windowing

AEH

- ❑ Subject to PBC, exact estimate of the effective homogeneous elastic properties can be obtained for linear elastic inhomogeneous microstructures that exhibit perfectly-periodic homogeneity by solving for $\boldsymbol{\chi_k^{mn}}$ in:

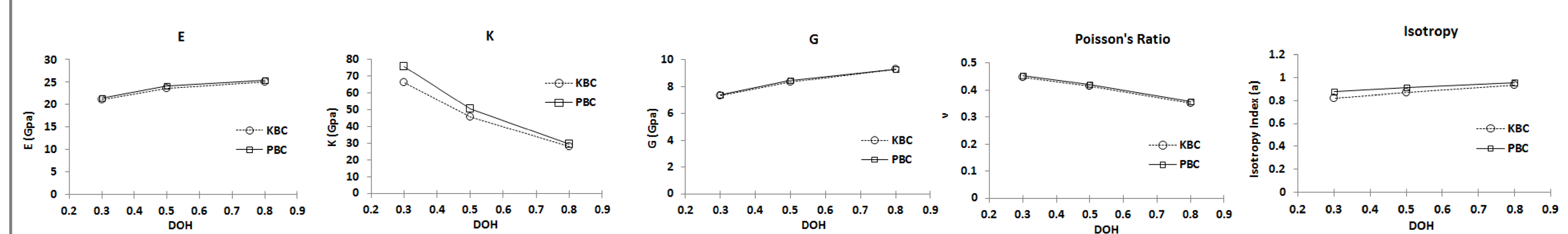
$$\frac{\partial}{\partial y_j}D_{ijkl}(y)\frac{\partial\chi_k^{mn}}{\partial y_l}=\frac{\partial}{\partial y_j}D_{ijmn}(y)$$

- ❑ Vector y_i signifies the coordinates of the microstructure RVE, and $\boldsymbol{D_{ijkl}}$ is the elastic stiffness tensor at a point **y** in the material. The homogenized linear elastic stiffness tensor, $\boldsymbol{D_{ijmn}^{hom}}$ is given:

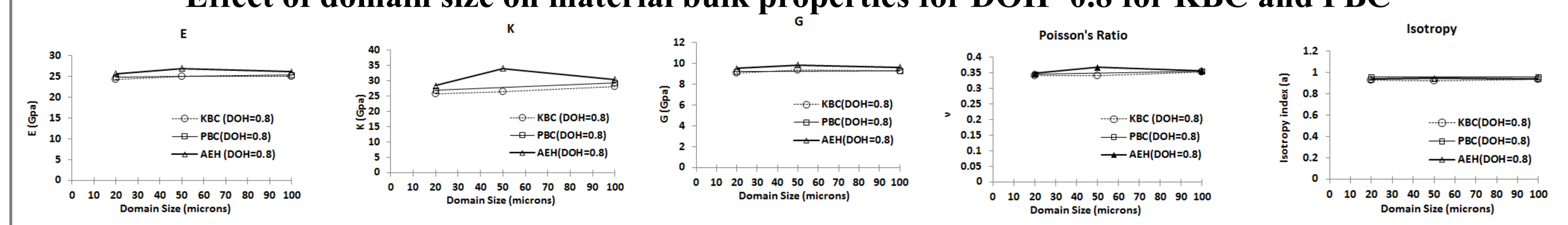
$$D_{ijmn}^{hom}=\frac{1}{|Y|}\int_Y D_{ijmn}(y)\left(\delta_{km}\delta_{ln}-\frac{\partial\chi_k^{mn}}{\partial y_l}\right)d^3y$$

Microstructure Based Homogenization

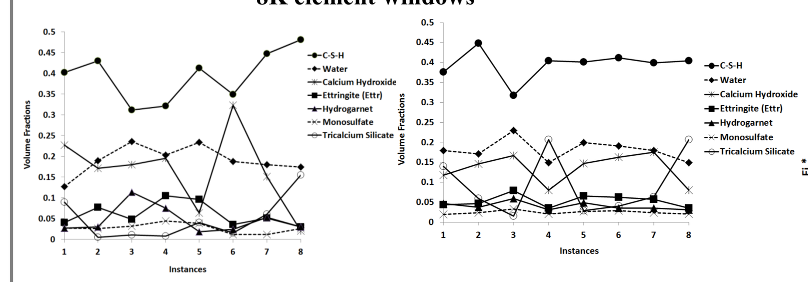
Effect of DOH on material bulk properties for 1M-RVE for KBC and PBC



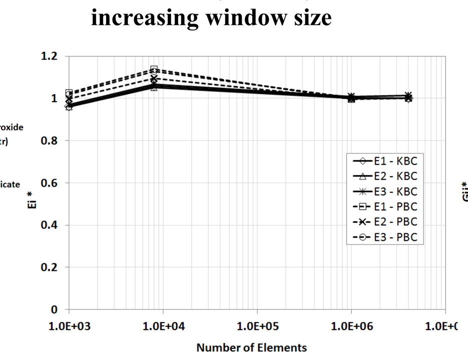
Effect of domain size on material bulk properties for DOH=0.8 for KBC and PBC



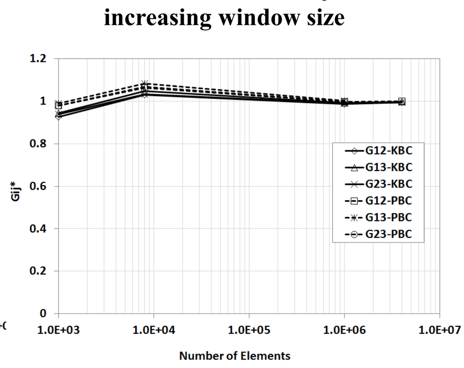
Volume fractions of major phases for (a) 1K element and (b) 8K element windows



Elastic moduli (uniaxial) with increasing window size



Elastic shear modulus G_{ij} with increasing window size



Rule of Mixtures Based Homogenization

- ❑ A rule of mixtures approach independent of the microstructure of the material is used to compute the effective bulk properties of the cementitious material.
- ❑ The theoretical extreme upper and lower bounds on effective material properties of multi-phase materials are the Voigt (1928) and Reuss (1929) bounds.

$$K^*=\sum_{i=1}^{n}f_iK_i\qquad G^*=\sum_{i=1}^{n}f_iG_i$$

$$\frac{1}{K^*}=\sum_{i=1}^{n}\frac{f_i}{K_i}\qquad\frac{1}{G^*}=\sum_{i=1}^{n}\frac{f_i}{G_i}$$

- ❑ Hashin(1962) presented the composite (or coated) spheres model for determining the effective material properties for multi-phase materials, based on the dilute suspension model.

$$\frac{K^*}{K_m}=1+3(1-\nu_m)\sum_{i=1}^{n}\frac{\left(\frac{K_p^i}{K_m}-1\right)c_i}{2(1-2\nu_m)+(1+\nu_m)\left[\frac{K_p^i}{K_m}-\left(\frac{K_p^i}{K_m}-1\right)c\right]}$$

$$\frac{G^*}{G_m}=1+15(1-\nu_m)\sum_{i=1}^{n}\frac{\left(\frac{G_p^i}{G_m}-1\right)c_i}{7-5\nu_m+2(4-5\nu_m)\frac{G_p^i}{G_m}-2(4-5\nu_m)\left(\frac{G_p^i}{G_m}-1\right)c}$$

- ❑ For Hashin and Voigt estimates, the bulk modulus (K) is found to be lower compared to the values computed based on the microstructure (KBC, PBC and AEH). Both the Young's Modulus (E) and shear modulus (G) are determined to be higher than those estimated by microstructure based homogenization.

Conclusion

- ❑ A comparison between the two domain sampling methods shows that windowing produces effective material properties with a larger variation than the PMD due to a higher variation in local phase volume fractions.
- ❑ Macroscopic properties obtained for various DOH and domain sizes, determined by applying Kinematic Boundary Conditions (KBC), Periodic Boundary Conditions (PBC), AEH and rule of mixtures based homogenization are found to be comparable.
- ❑ It is shown that even though cement is a heterogeneous anisotropic material at the micro-level, the bulk properties are effectively isotropic.

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