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Strategy for predicting transport-based durability properties of concrete based on DEM approach

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Outline

- Transport-based durability issues of concrete
- Discrete element method (DEM)
- Pore network characteristics of hydrated paste
- Simulation of hydrated structure on nano-scale
- Conclusions

Transport-based durability issues of concrete

Durability problems of concrete

Fluid, ion transport in concrete

Pore structure affects its strength and durability

Transport-based durability issues of concrete

Three types of pores in cement-based materials:

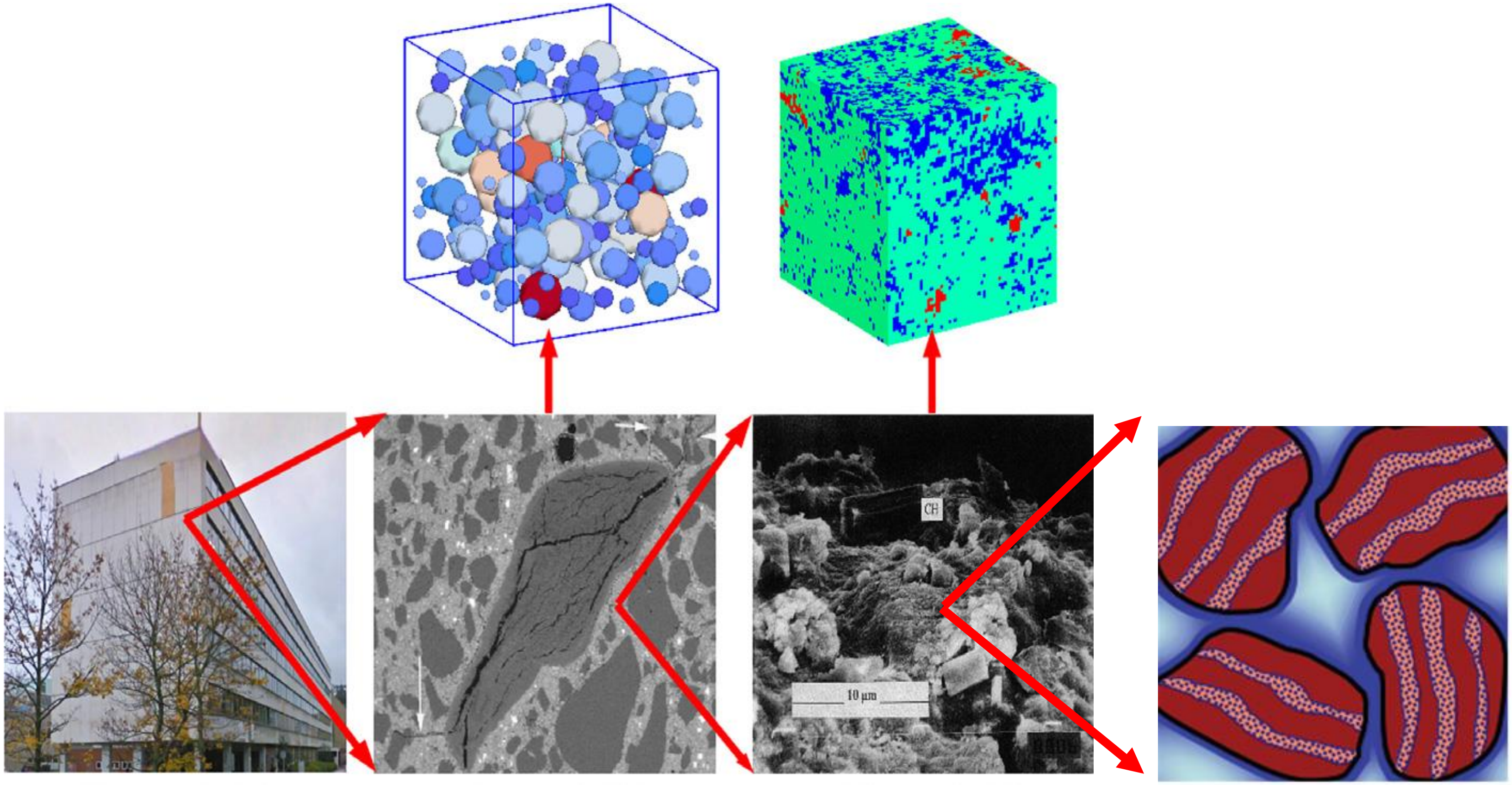
•Gel pores	few nanometers
•Capillary pores	1 nm – 10 μm
•Macro-pores (air voids)	lager than 10 μm

Jing Hu, PhD thesis, Delft, 2004

Available techniques for pore exploration:

- MIP (Mercury Intrusion Porosimetry)
- IA (Images Analysis)
- Computer Simulation

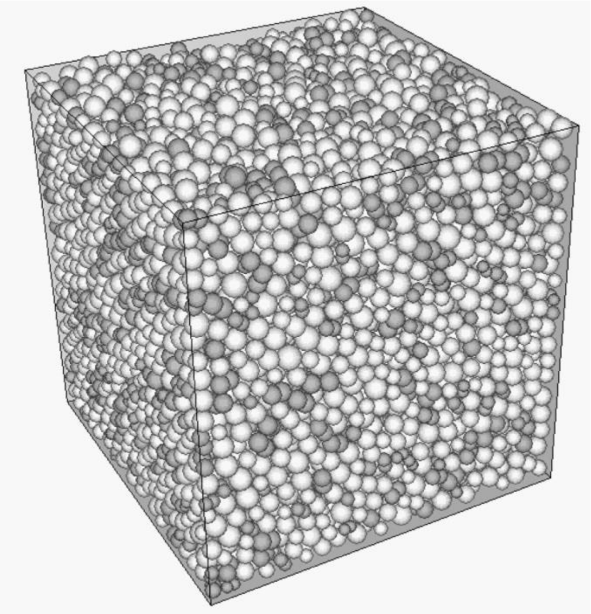
Transport-based durability issues of concrete

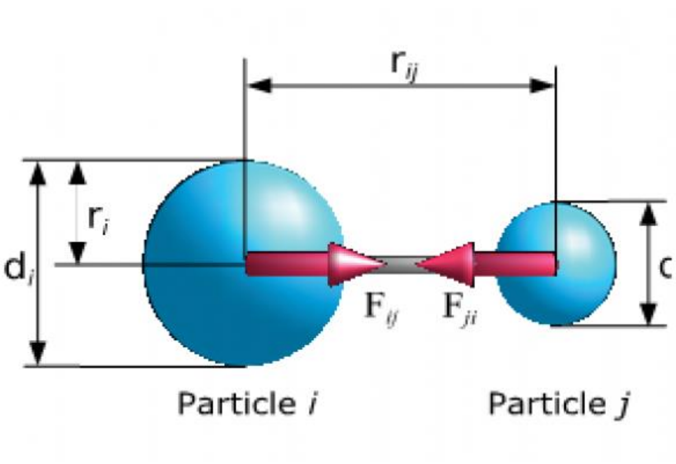


Macroscale Mesoscale Microscale Nanoscale

Multi-scale investigation for concrete nowadays!

Discrete element method (DEM)





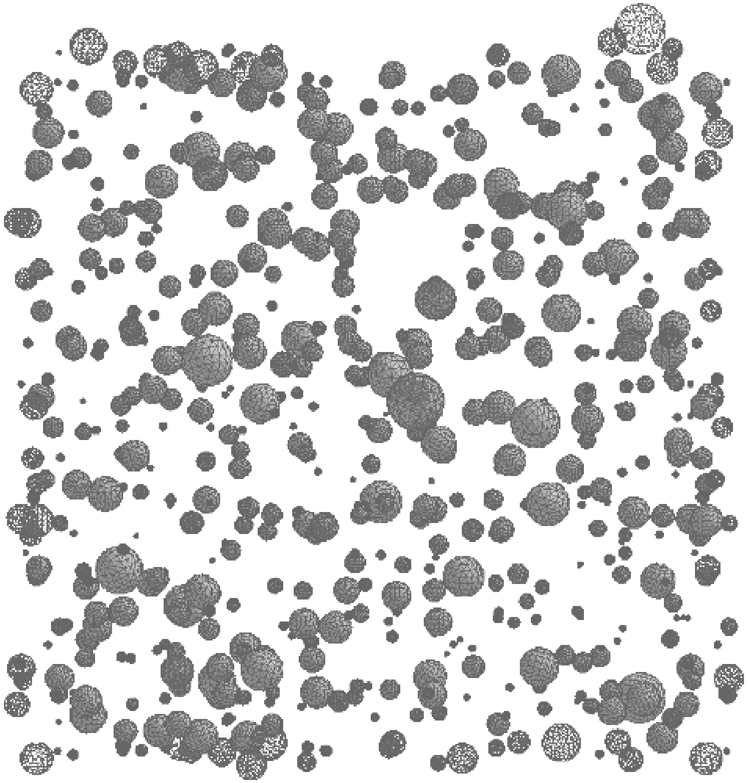
Newtonian system with particles (HADES package)

Linear direction: $$F_i = \sum_j f_{ij} = m_i \frac{\partial v_i}{\partial t}$$

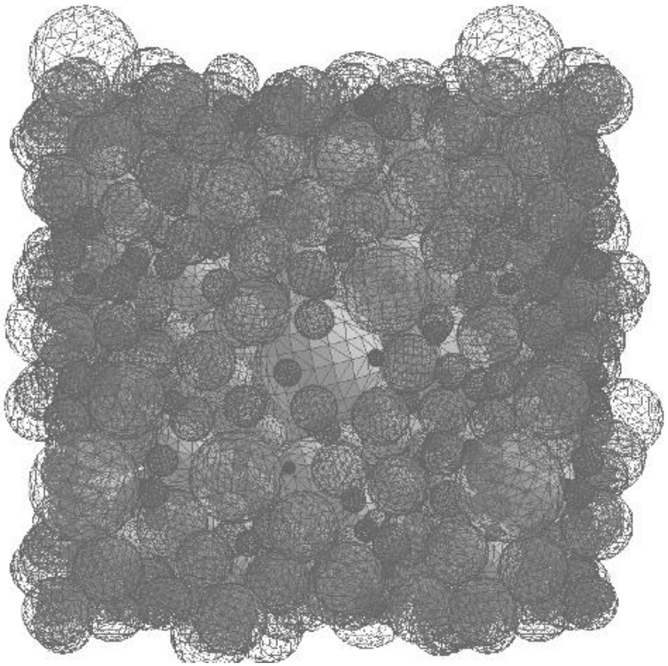
Angular direction: $$M_i = \sum_j m_{ij} = I_i \frac{\partial \omega_i}{\partial t}$$

Pore network characteristics of hydrated paste

HADES: dynamic DEM for packing simulation of fresh cement grains (Rosin-Rammler distribution).



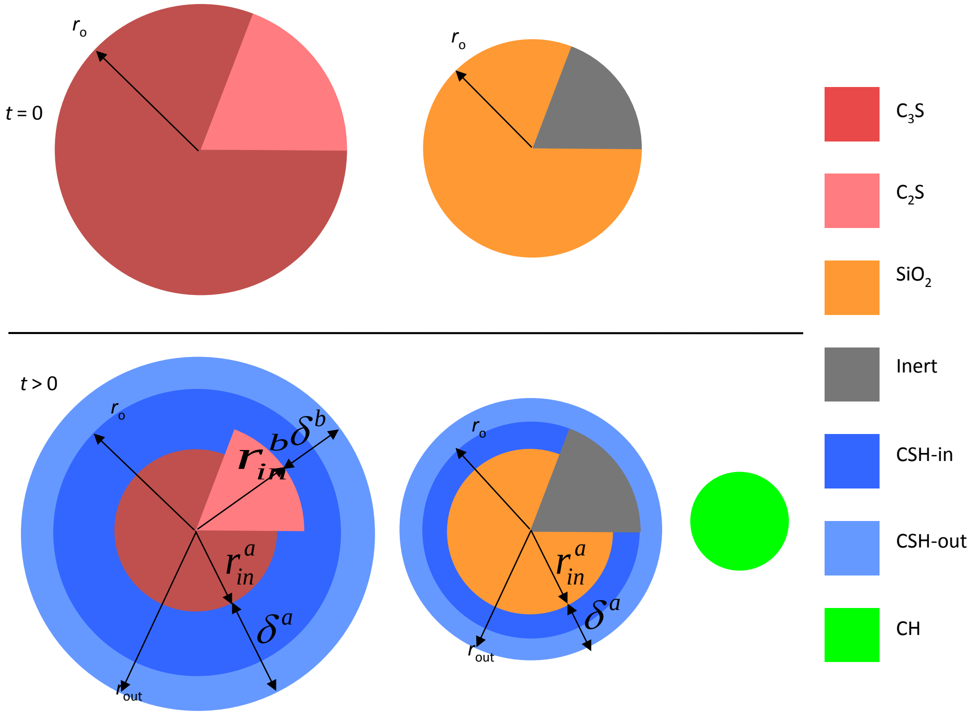
(a) Initial state (loose)

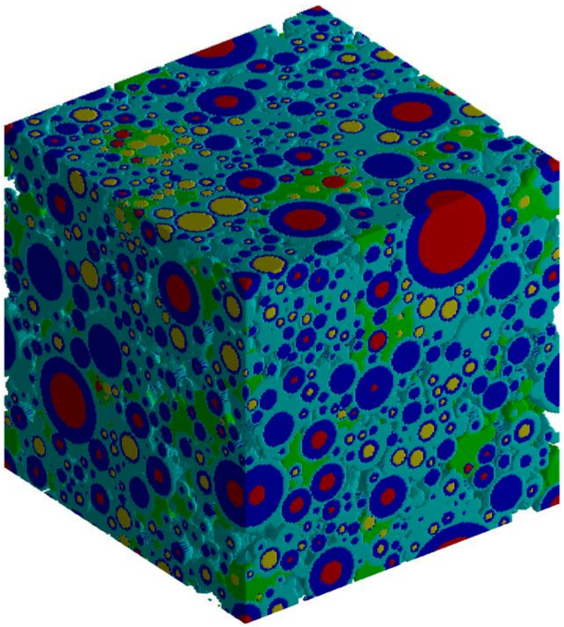


(b) Final state (dense)

Pore network characteristics of hydrated paste

XIPKM: extended integrated particle kinetics method for simulation of fresh multi-component cement system.





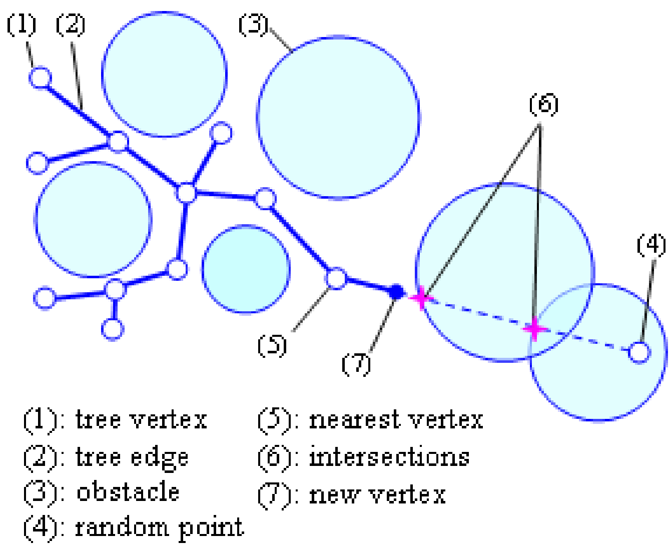
(left) particle model for multi-component cement grain

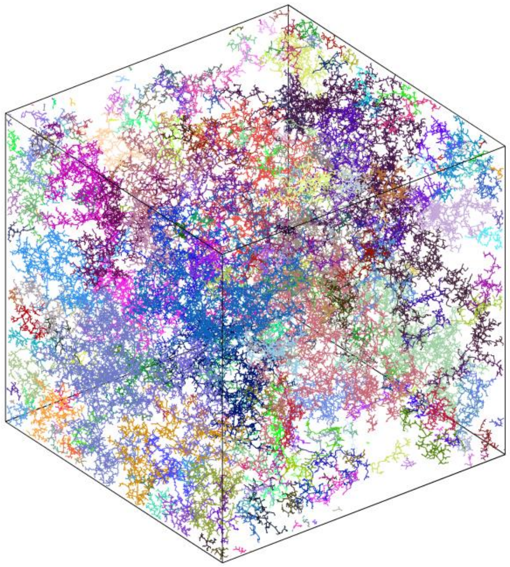
(right) differently color-coded microstructure of hydrated paste

Pore network characteristics of hydrated paste

DRaMuTS: double random multiple tree structuring system for delineating the complete pore network system and for topology assessment.

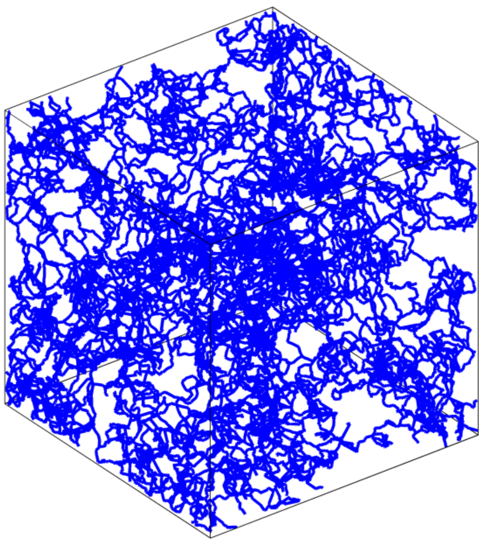
Illustration of DRaMuTS





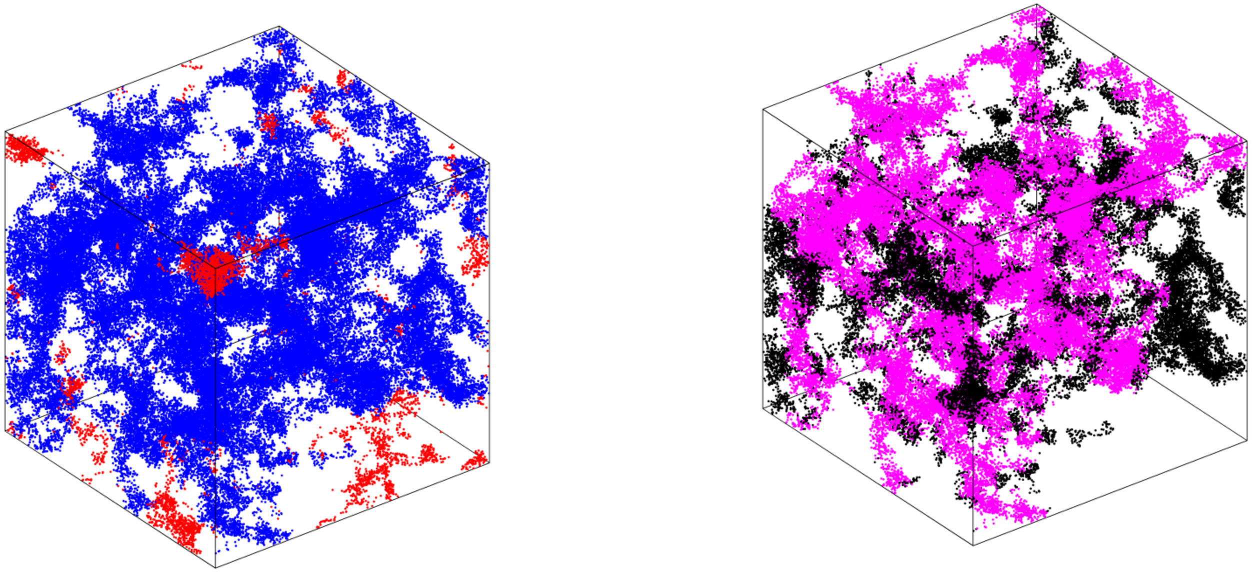
Different colors is for trees from different seeds

The main trunks in continuous pore channels



Pore network characteristics of hydrated paste

Main trunks and connectivity of pore network



points in percolated pores

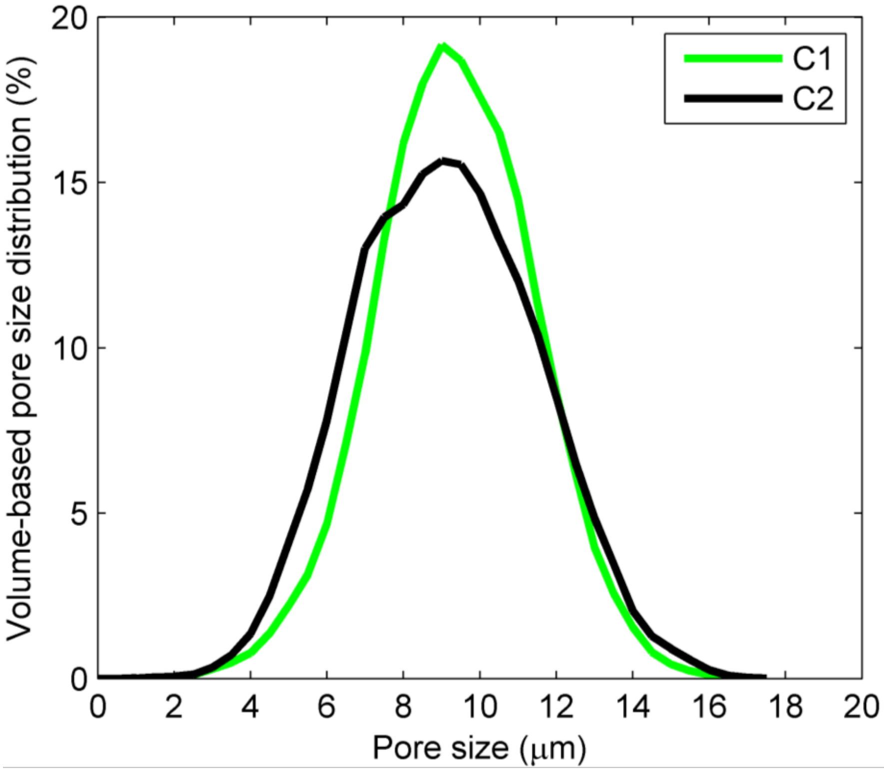
points in isolated pores

points in main channels

points in dead-end pores

Pore network characteristics of hydrated paste

SVM: star volume measurements in uniformly random point system inside the pore network



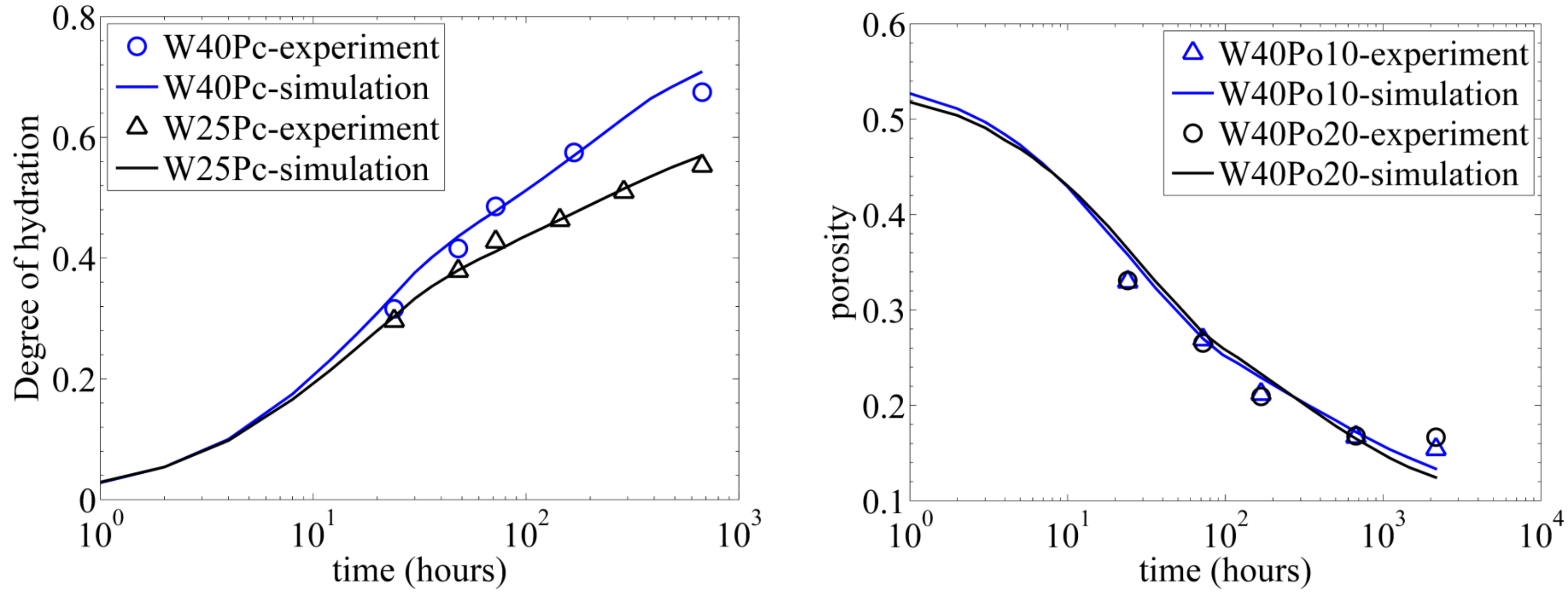
C1: 6P
C2: 4P+2R

P: periodic boundaries
R: rigid boundaries

Pore size distribution in 1-30 μm fully hydrated PC with w/c=0.3

Pore network characteristics of hydrated paste

Validation



Hydration curves of PC (left) and porosity curves of RHA-blended PC samples for prolonged hydration (right). Note that 40/25 means wc=0.4/0.25; 10/20 % PC blending.

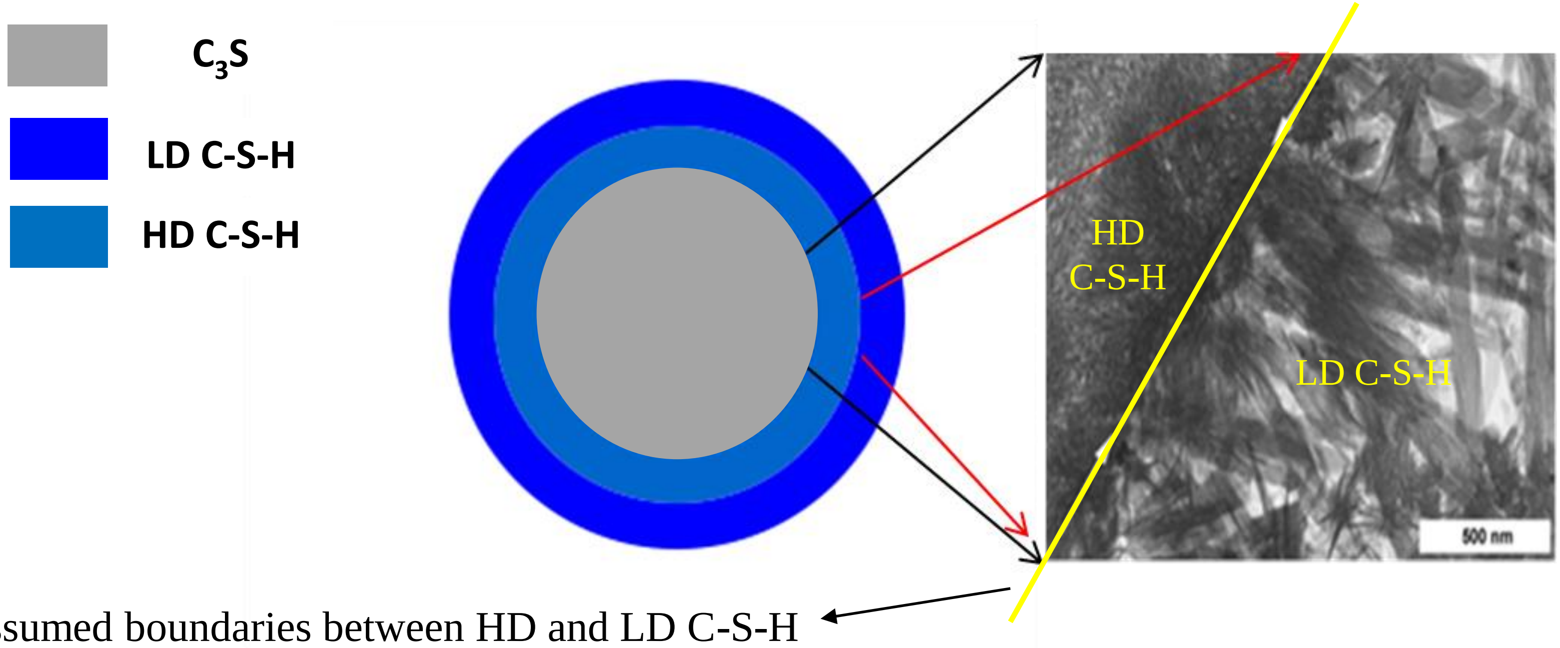
Simulation of hydrated structure on nano-scale

However, "overestimation" of pore size distribution does exist……

Besides, for investigating transport-based durability properties of cementitious materials, surface roughness of hydration product needs to be taken into account……

If we move from micro-level to nano-scale, probably solutions to our problems can be found……

Simulation of hydrated structure on nano-scale



Hydration products represented by HD and LD C-S-H

I.G. Richardson, Cement and Concrete Research, 34 (2004) 1733-1777

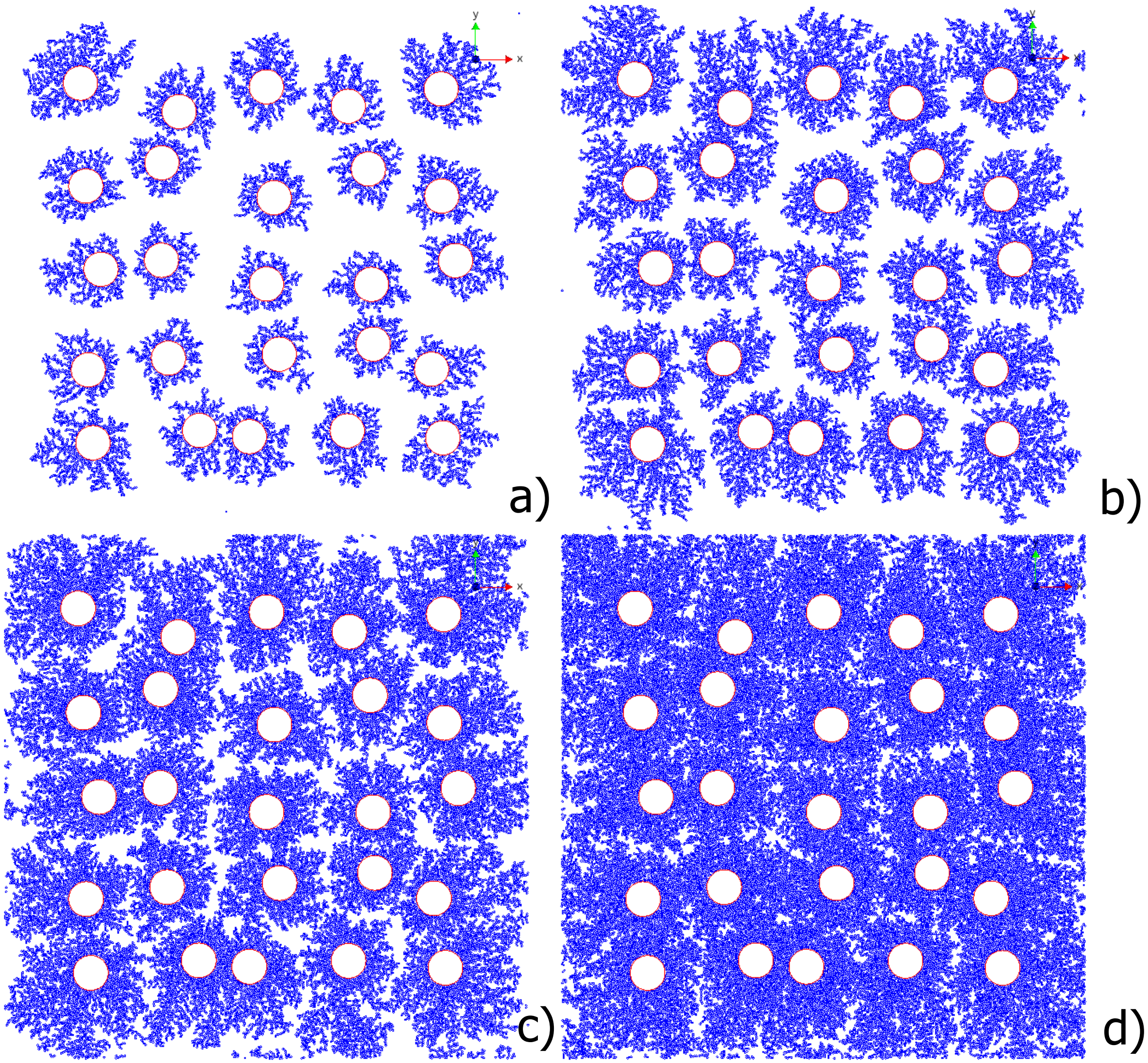
Simulation of hydrated structure on nano-scale

- C-S-H (calcium silicate hydrate), the main hydration product, important but complex gel.

- Granular nature and fractal dimension of C-S-H is suggested by Jennings' colloidal model, meanwhile, fibrous morphology is revealed by experimental techniques.

- New mechanism should be employed based on existing Information to produce more realistic product.

2D illustration of hydrated structure on nano-scale



a: stage 1

b: stage 2

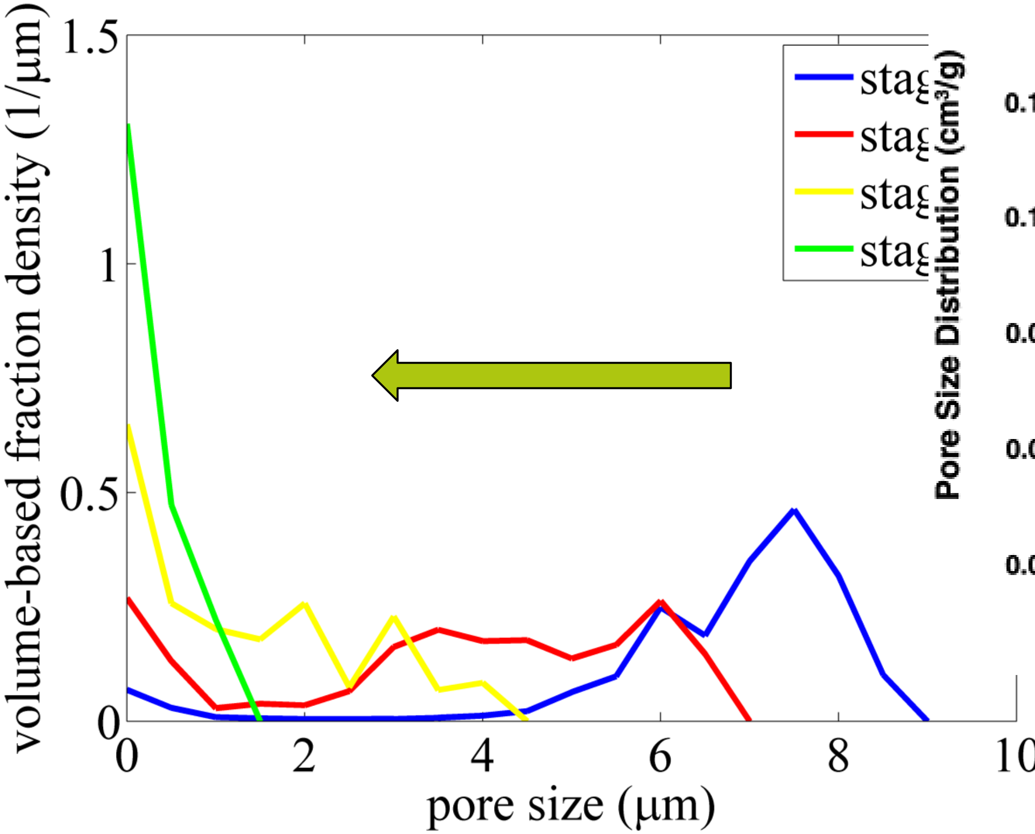
c: stage 3

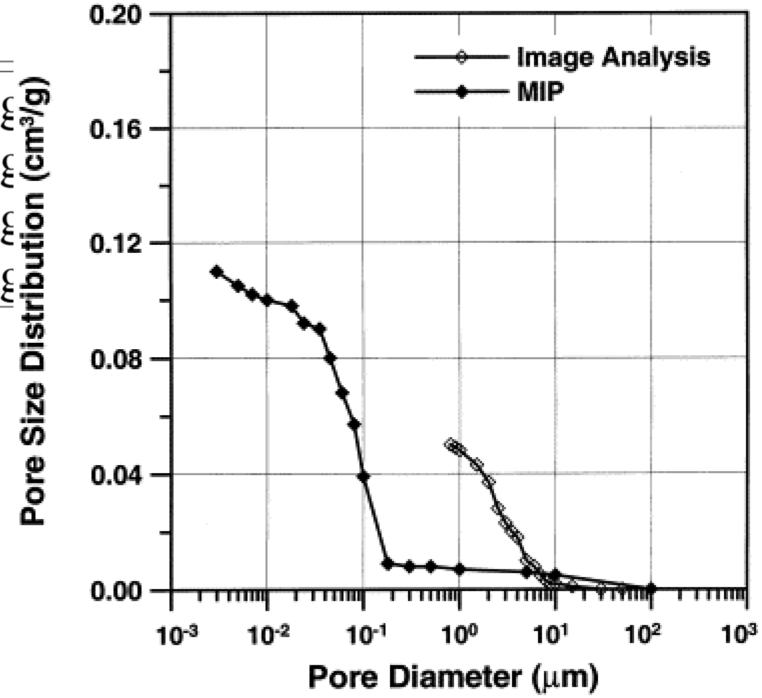
d: stage 4

red: cement grain
blue: outer C-S-H
white: pore space

Simulation of hydrated structure on nano-scale

Structural analysis – pore size distribution





S. Diamond, Cement and Concrete Research, 30 (2000) 1517-1525

Conclusions

- Micro-level porosimetry approaches are useful for durability estimation purposes.
- The full range of cement particles should be involved for estimating transport properties.
- The nano-level approach could provide more realistic structure and morphology product, compared to the classical vector approach.

Conclusions

- A realistic shape factor should be added to the resulting expressions.
- A multi-scale techniques should be developed to bridge the gap between micro- and nano-level.

Thanks for your attention!