Towards a multiscale approach for long-term chemical concrete degradation

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Contributors

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  - Cooperation with
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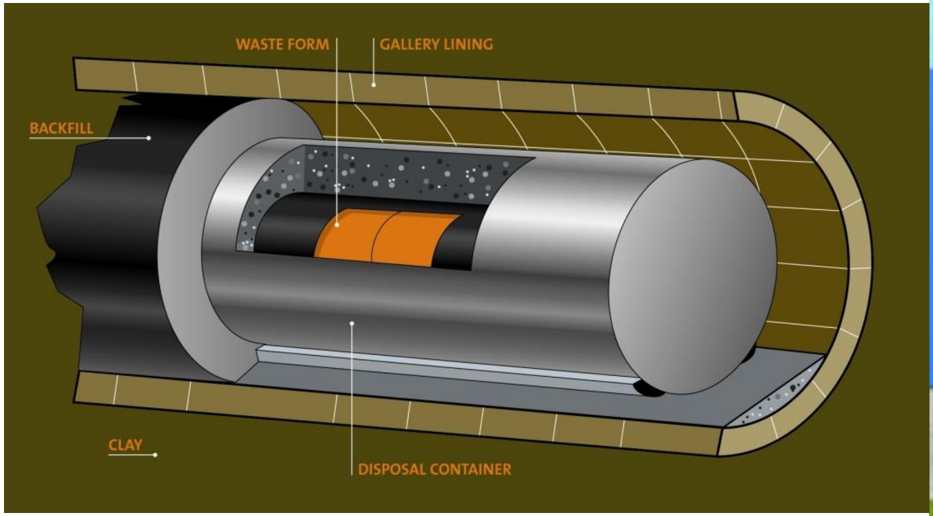
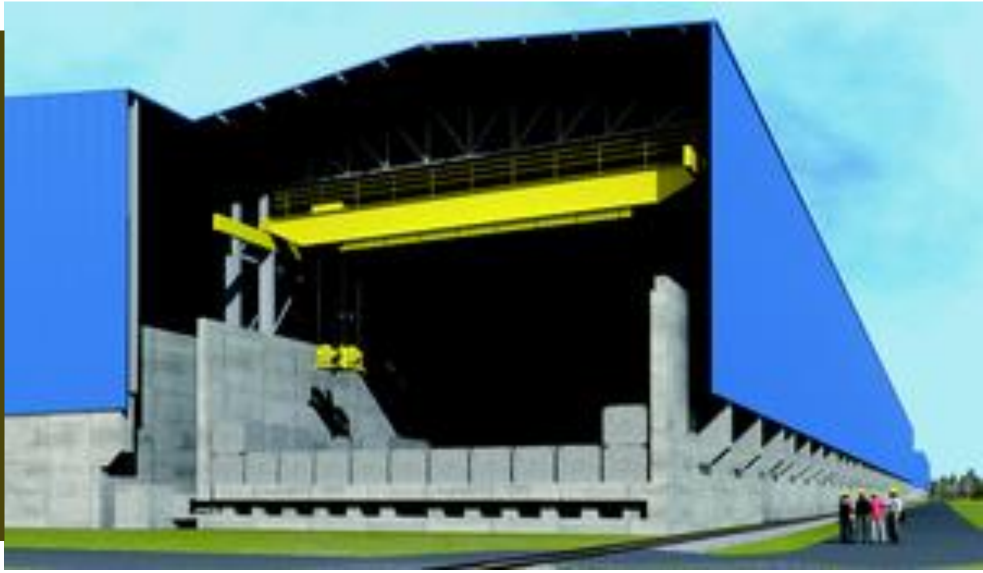
    - TUDelft: Guang Ye, Klaas Van Breugel
- Scientific collaborators at SCK•CEN
  - Norbert Maes
  - Janez Perko
  - Suresh C. Seetharam

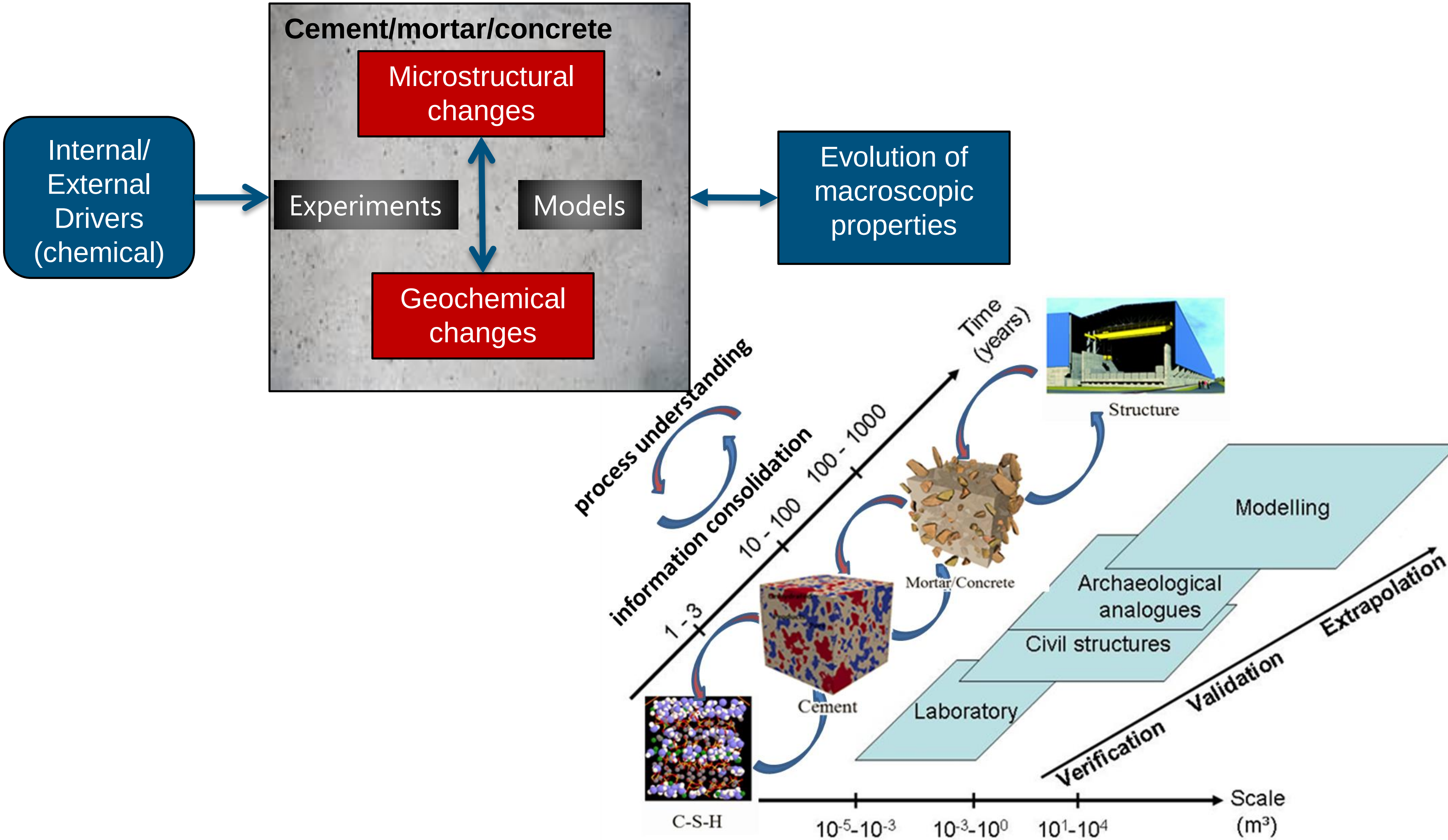
Cement-based materials in disposal systems





- Geomechanical stability
- Operational safety
- **Contribution to long term safety**
  - **Geochemical stable conditions**
  - **Limiting water flow**
  - **Limiting radionuclide migration**

Long-term behaviour during chemical degradation



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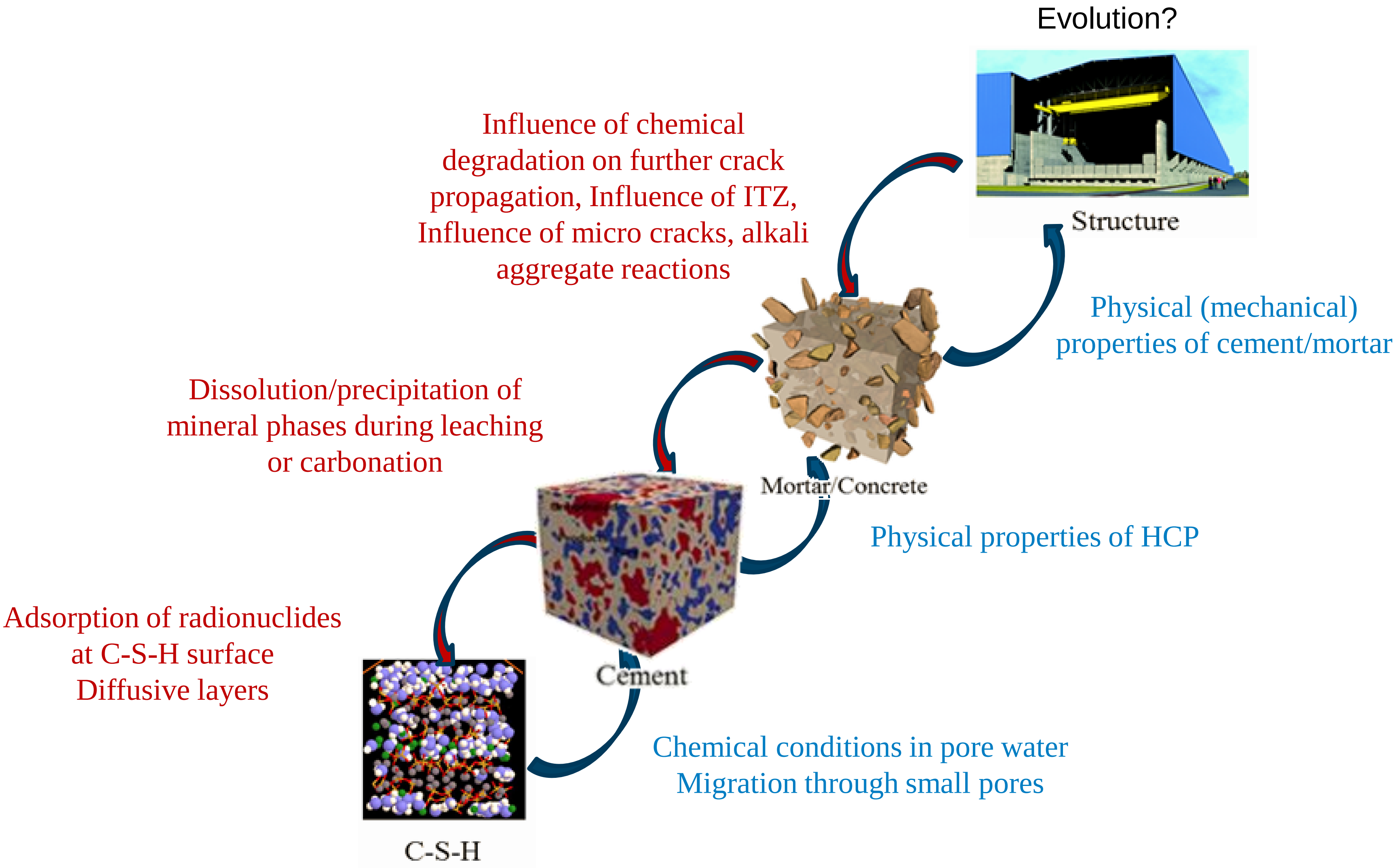
Concrete at different scales of heterogeneity



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Aim

- Give an overview of research at SCK to assess long-term chemical degradation of concrete
  - Consequences for macroscopic properties
  - Consequences for long-term safety

- To highlight some points in a multiscale framework

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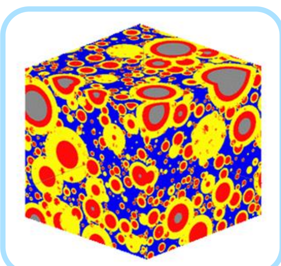
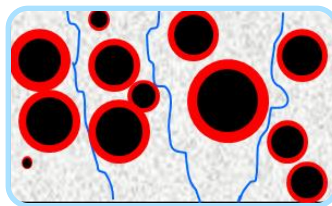
Experimental Studies

Leaching and carbonation HCP

"micro-scale"
phases in
hardened cement paste



"meso-scale"
components in
mortar/concrete



"macro-scale"
mortar/concrete
(cracks)

Pore-scale reactive model Lattice Boltzmann

Finite element modelling

Continuum scale modelling at small scale

Flow & transport in cracked media

Upscaling by model abstraction

Modelling Studies

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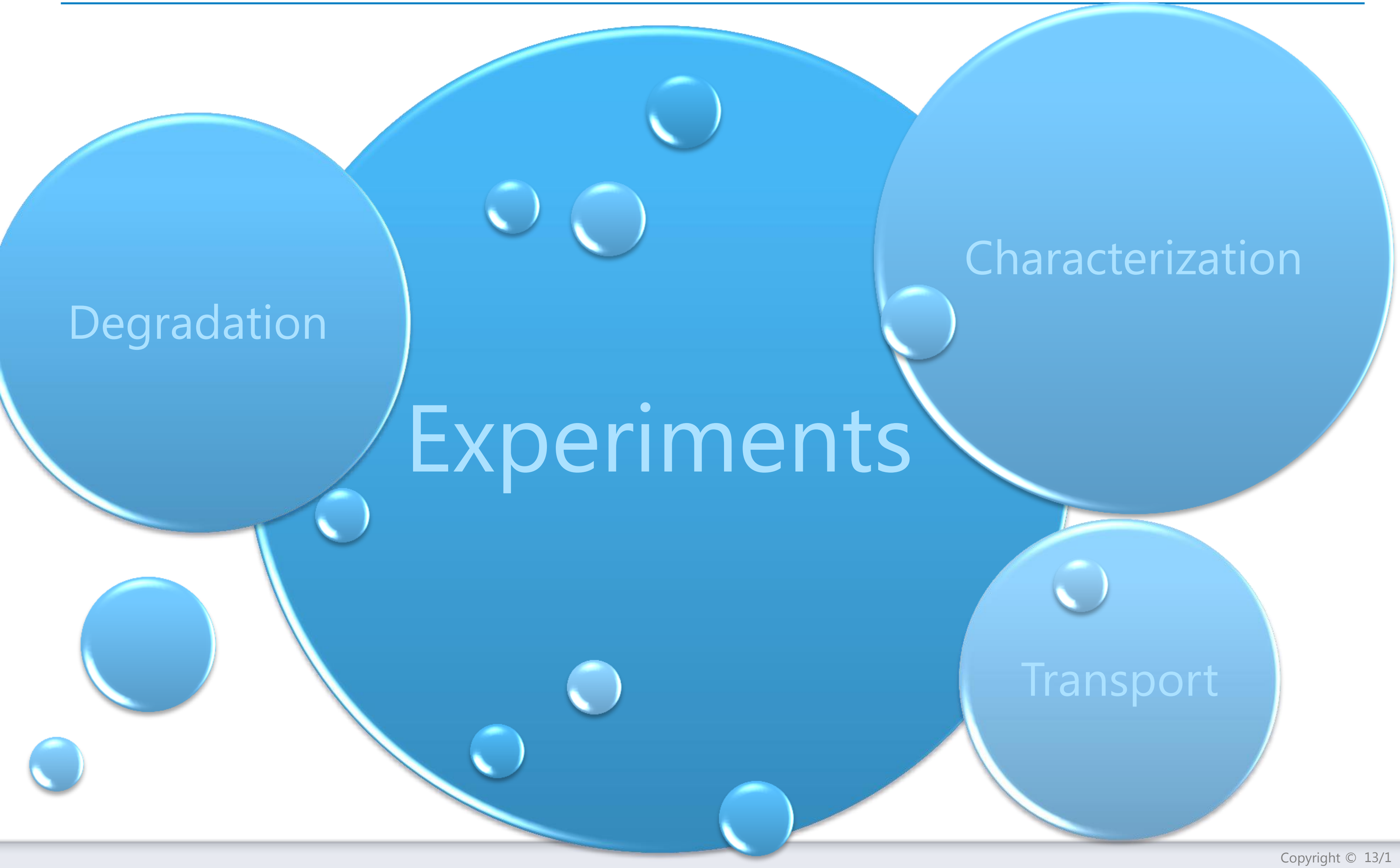

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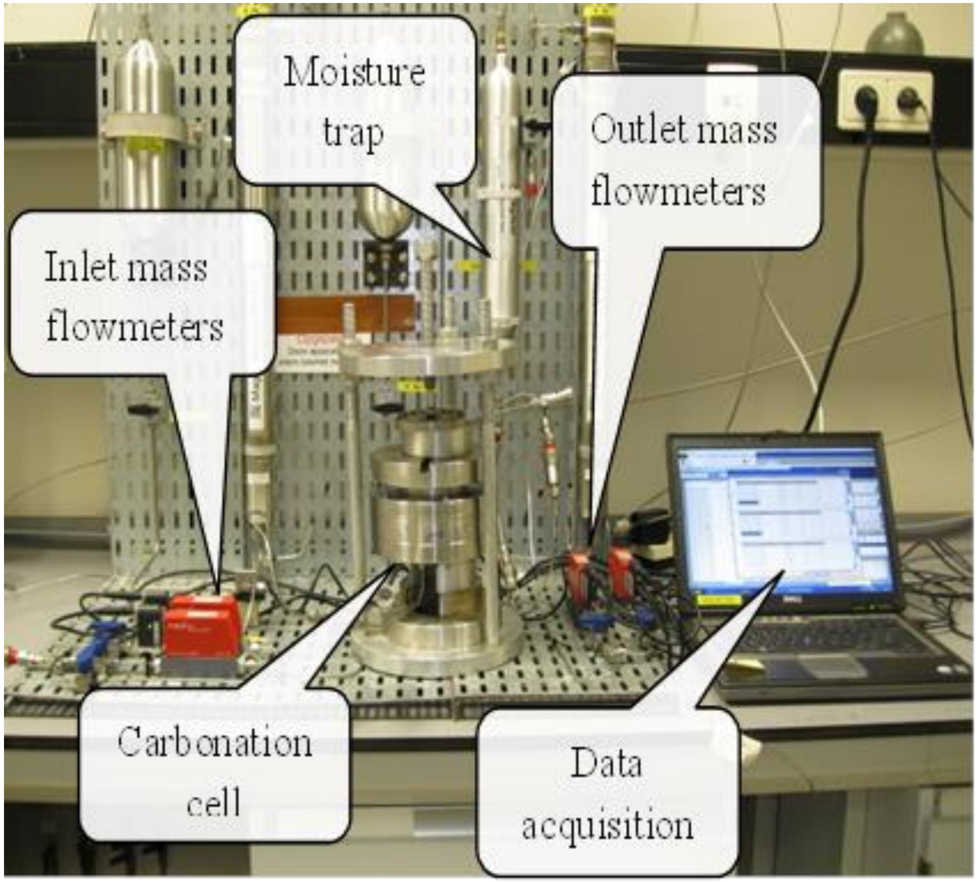
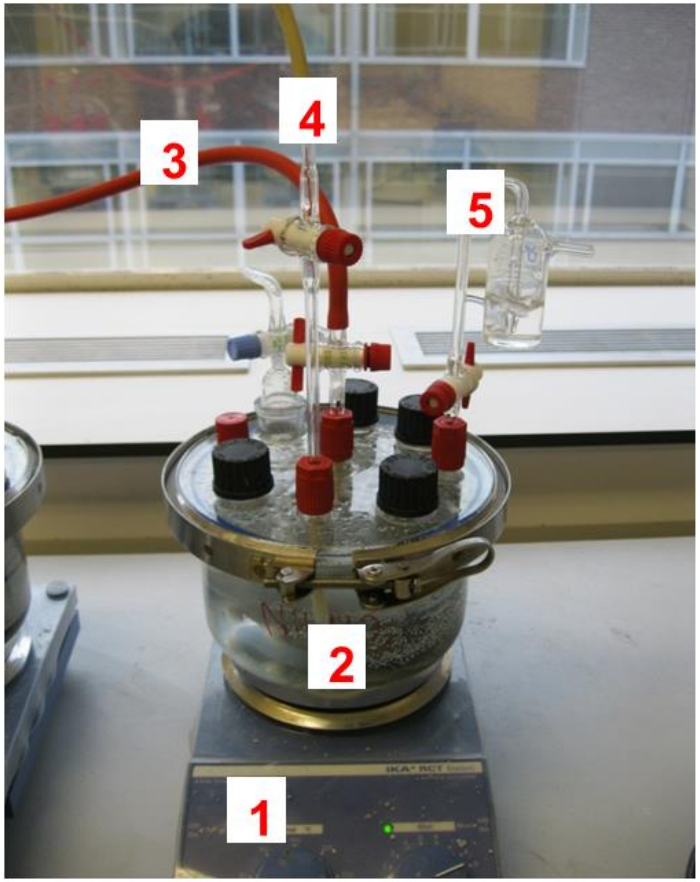
Accelerated chemical degradation
Carbonation - Leaching





1 - Magnetic stirrer 2 - NH_4NO_3 vessel

3 - Nitrogen line 4 - Extraction line

5 - Bubbler

Phung (2015)

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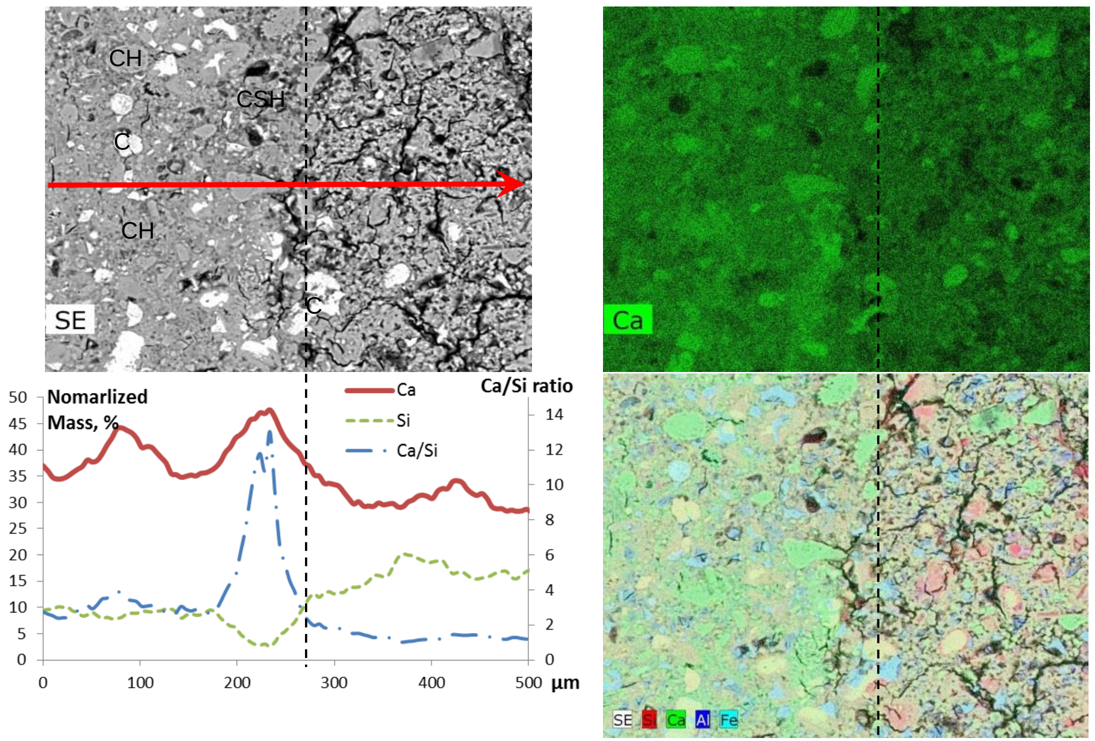
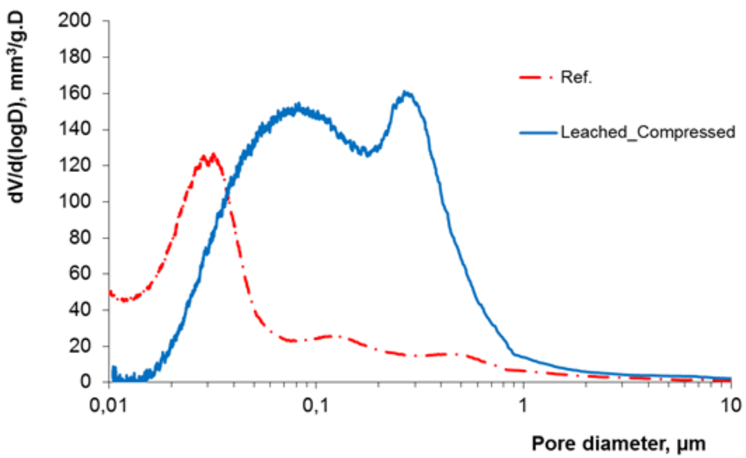
Characterization of degraded material



Characterisation of the Ca-leached degradation front (SEM-EDX)



Opening of pores due to Ca-leaching (N_2 adsorption and Hg-porosimetry)

Phung (2015)

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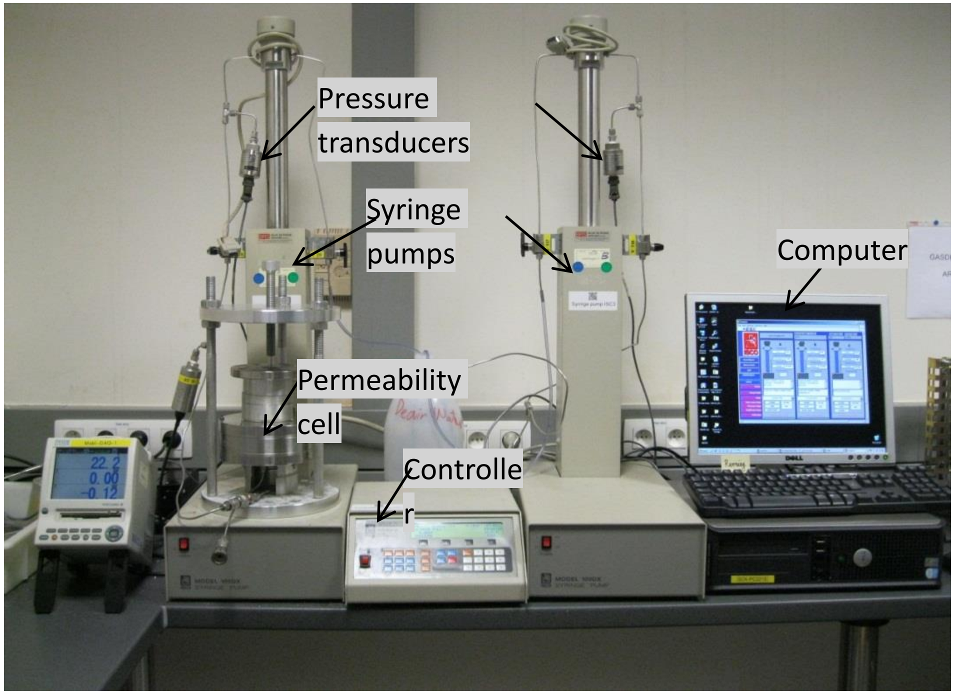
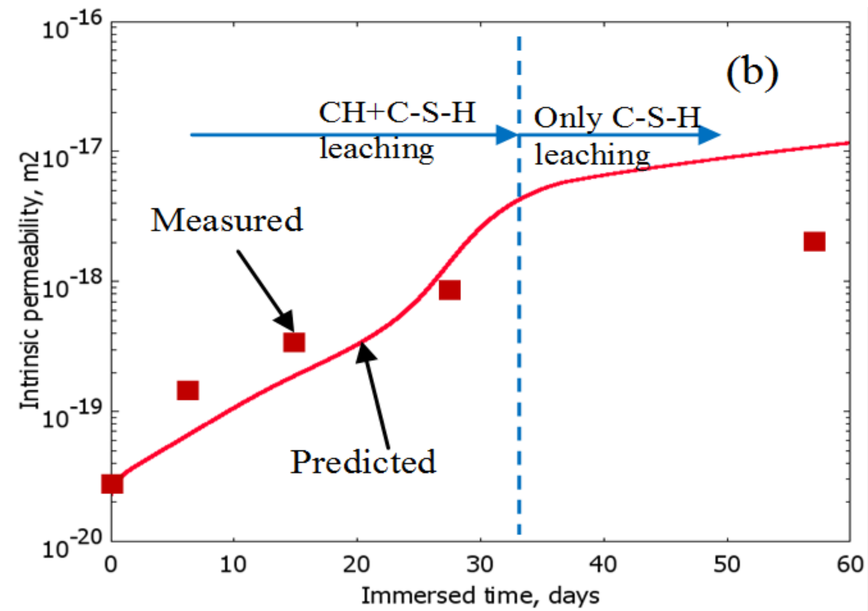
Quantification of effect of degradation on effective properties (Permeability)



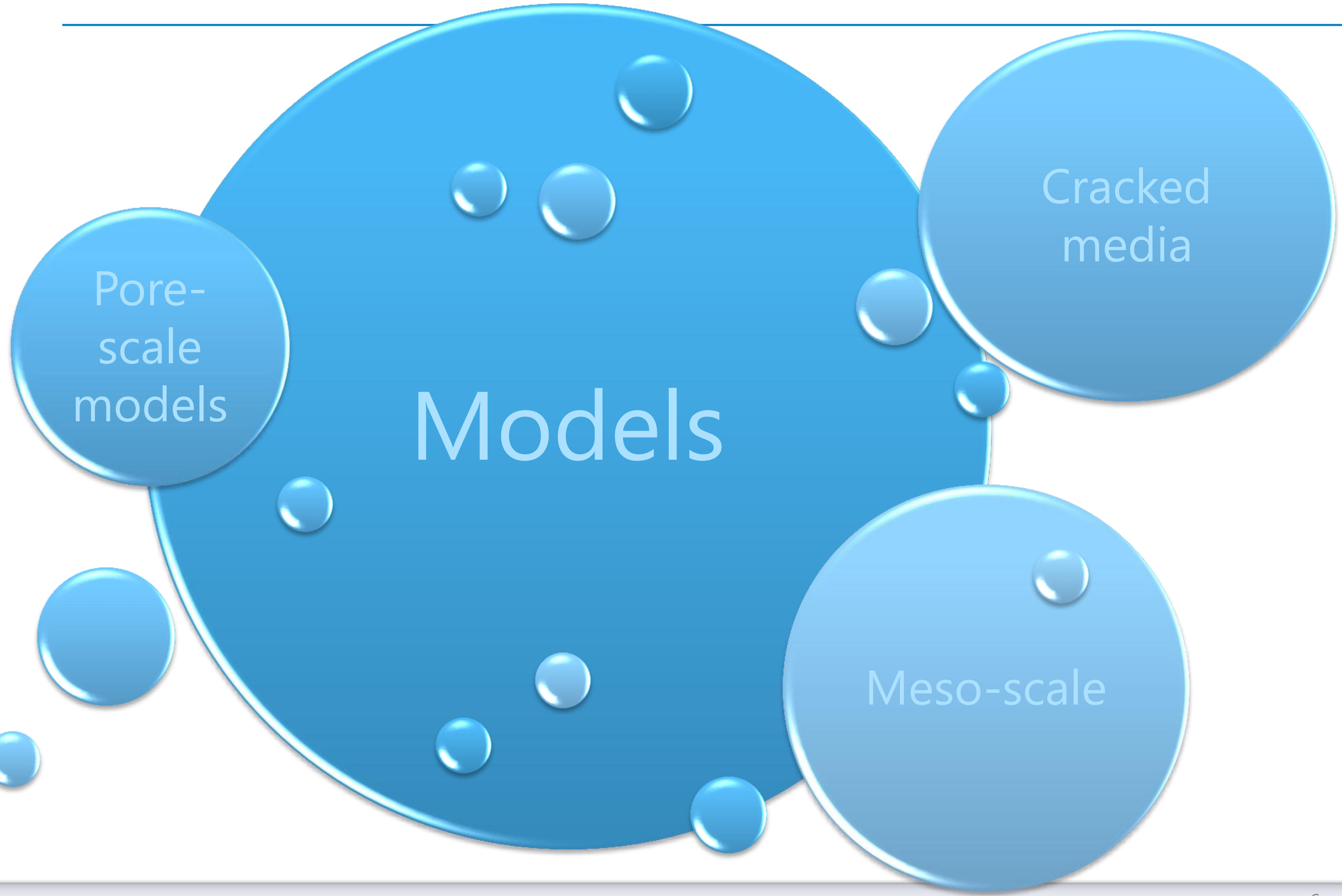


Determination of the permeability of cementitious samples.

Evolution of the permeability as function of leaching time (exp. vs. predicted)

Via phenomenological model for leached material

Phung (2015)



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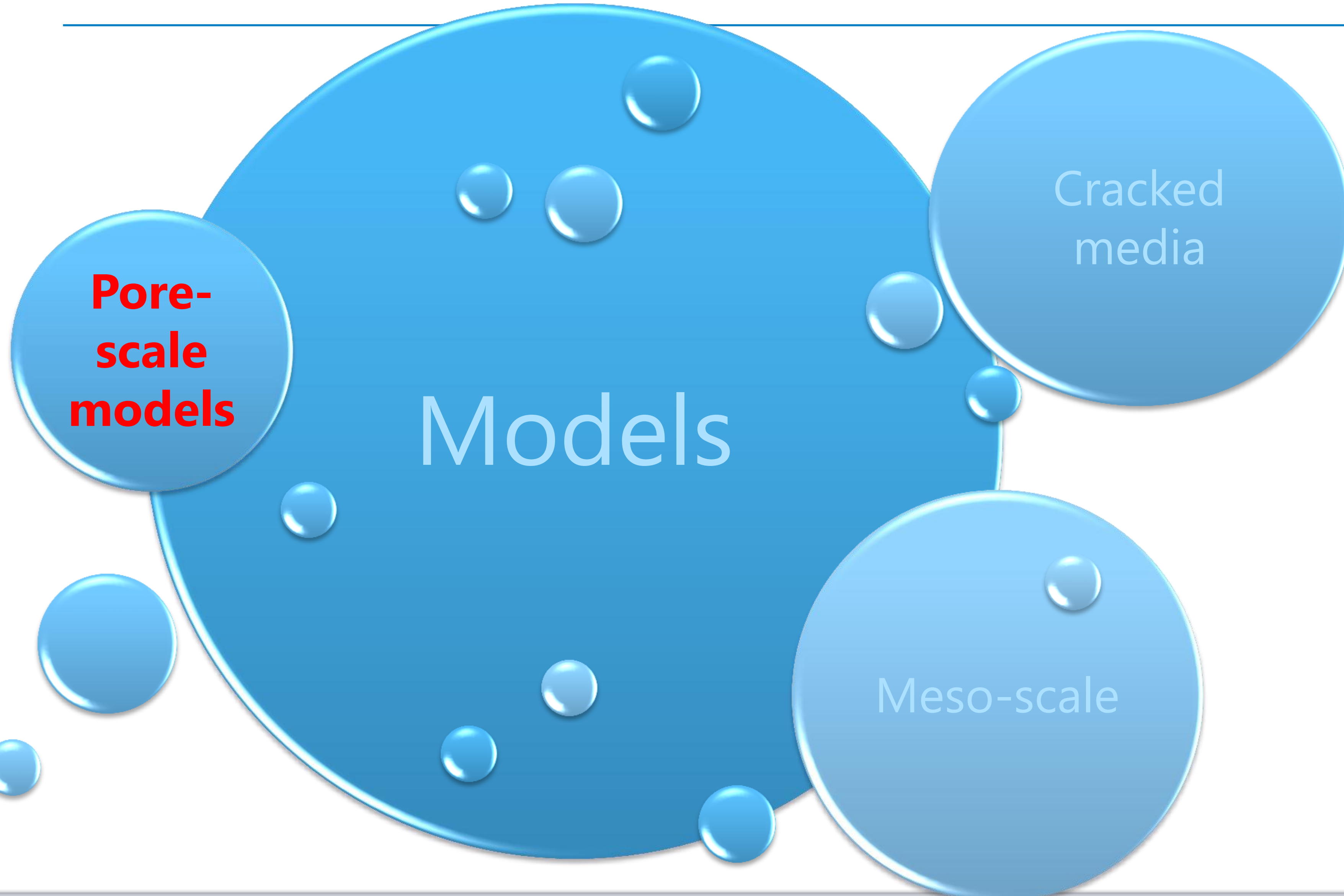

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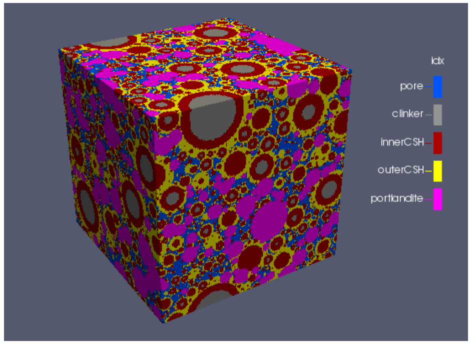
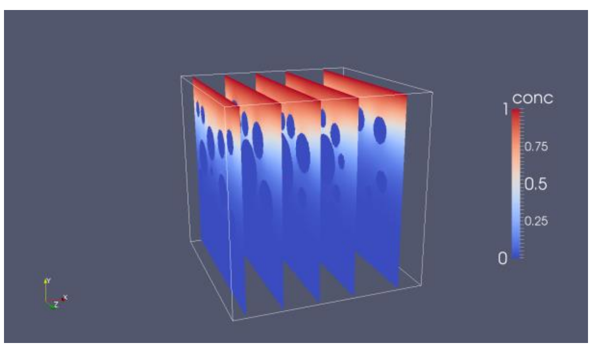
A versatile reactive transport framework at the pore-scale



Virtual microstructure from a cement hydration model

Initial microstructure of Hardened cement Paste

Lattice Boltzmann method

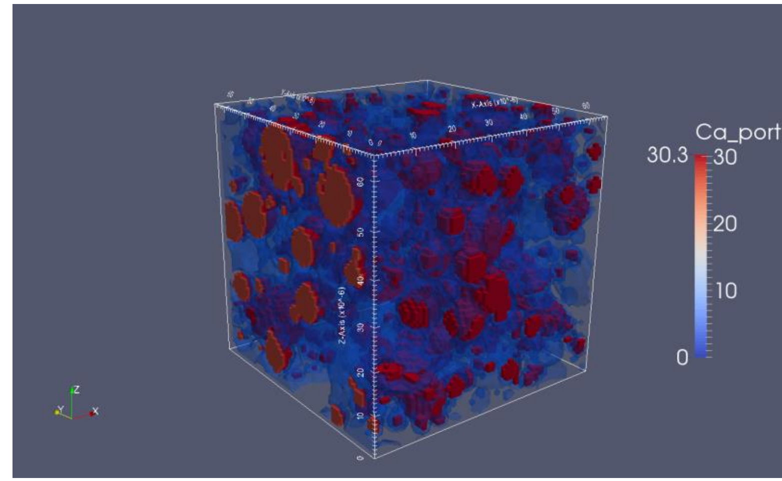


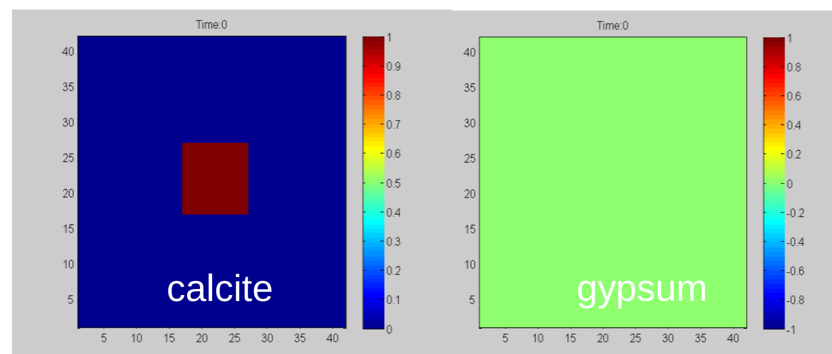
Flow and transport through HCP microstructure

Patel et al (2014), Perko and Patel (2014)

Reactive transport + pore structure evolution

Leaching of cement paste





Precipitation of secondary minerals

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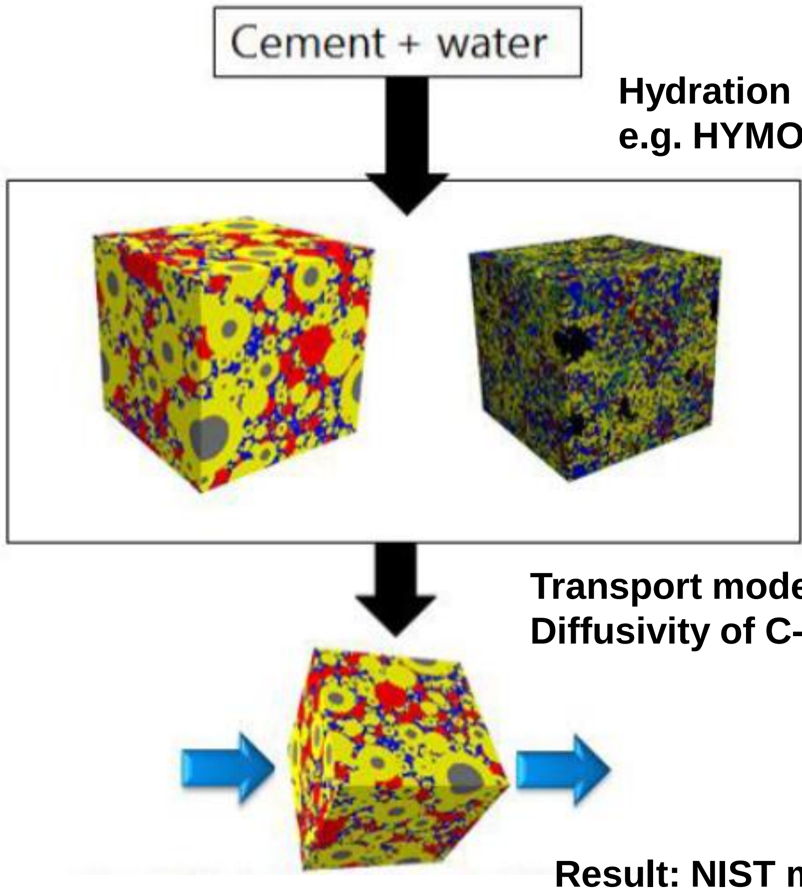
Yantra tool - Features

- Reactions included as sink/source term instead as flux in lattice Boltzmann method which allows
  - First time coupling with geochemical solver (i)PHREEQC
  - Flexibility to introduce other solvers or abstracted geochemical models
- Numerical scheme to deal with heterogeneities in diffusion properties
  - Multi-scale implementation to compute diffusion in C-S-H phases
- Flexibility in defining microstructures
  - Virtual based on hydration model
  - From 2D/3D images
- Extension for other processes and physics possible
  - Multi-physics problems can be solved (e.g. thermal, flow, etc.)

Patel et al (2014), Perko and Patel (2014)

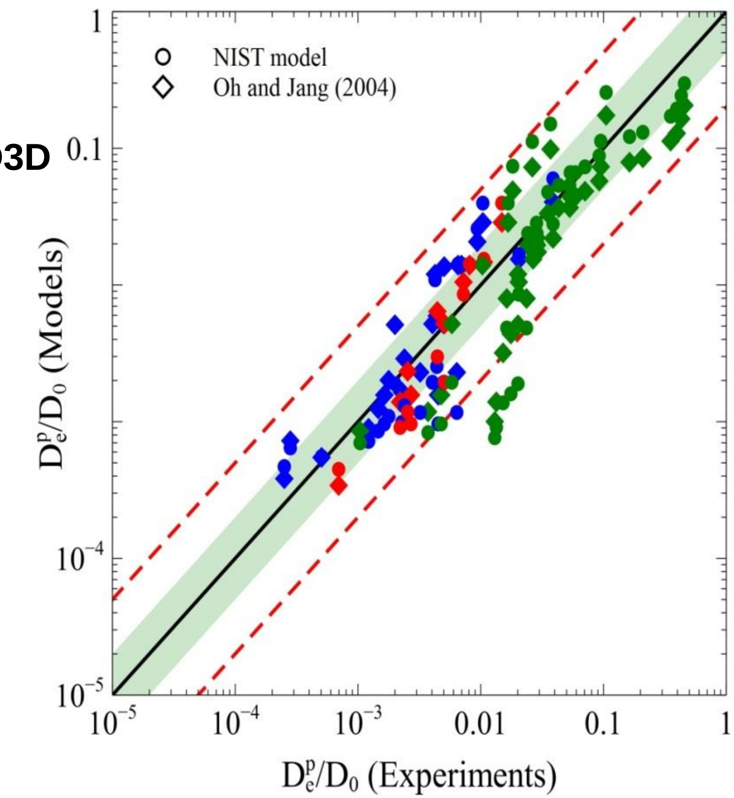
Example 1 – Estimation of effective diffusion coefficient

Virtual experiment



Hydration model
e.g. HYMOSTRUC, CEMHYD3D

Transport model
Diffusivity of C-S-H: constant



Result: NIST model linking
Effective Diffusion Coefficient to capillary porosity

Patel (2015)

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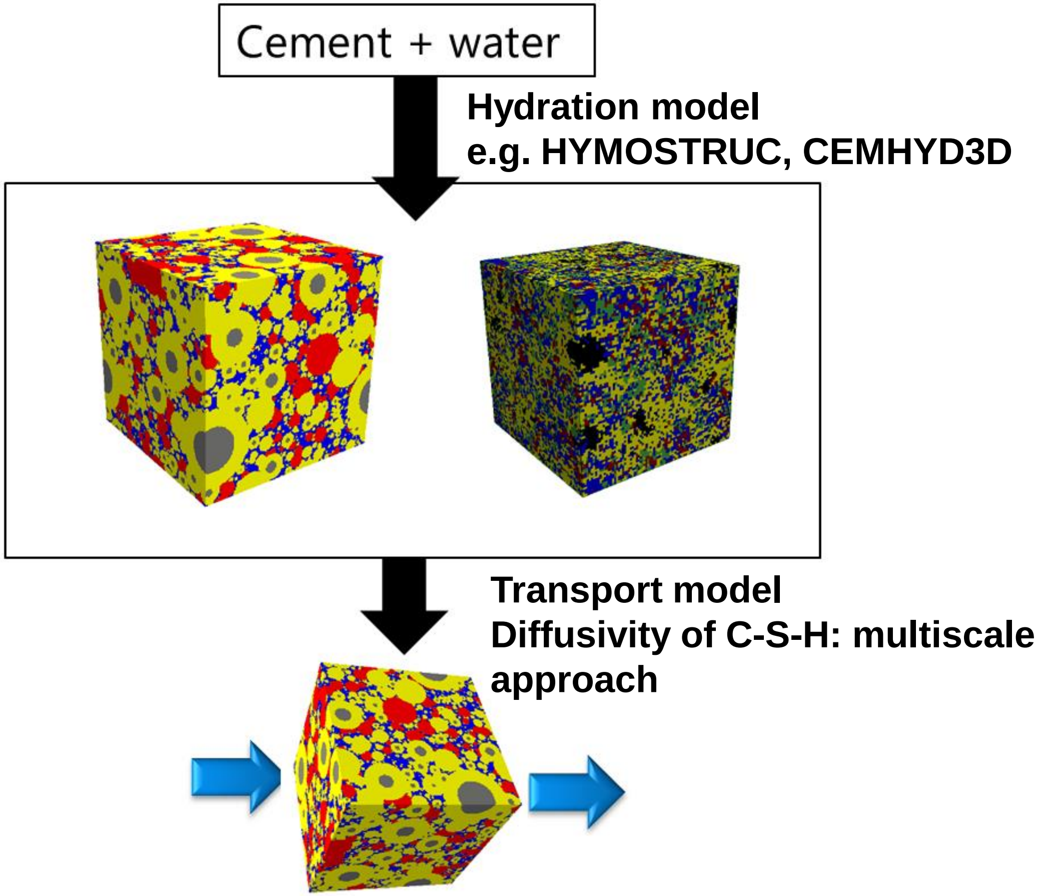
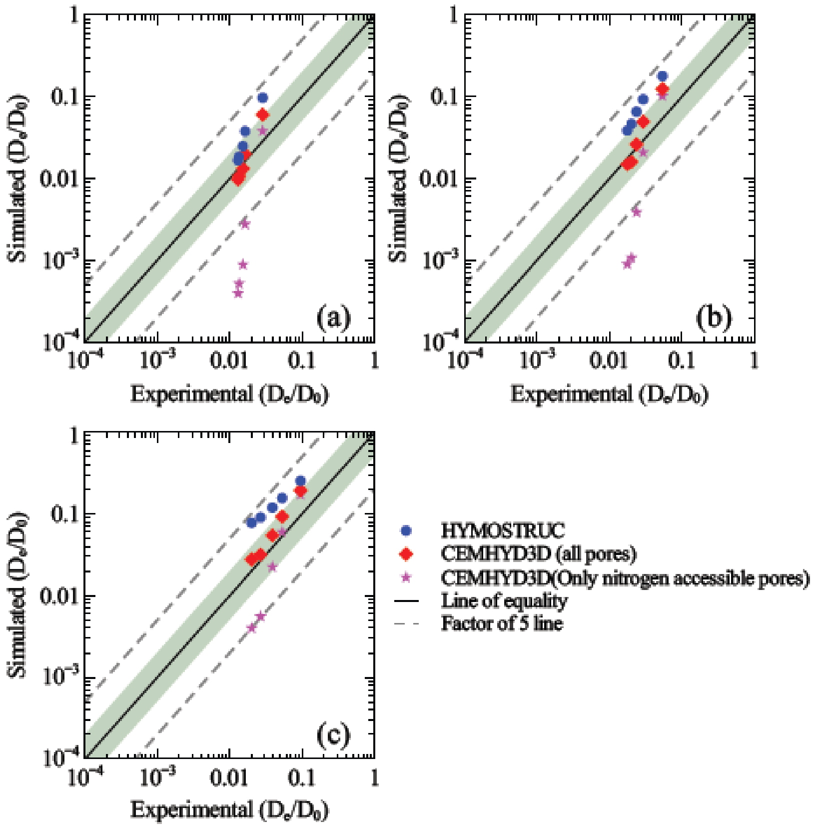
Virtual experiment



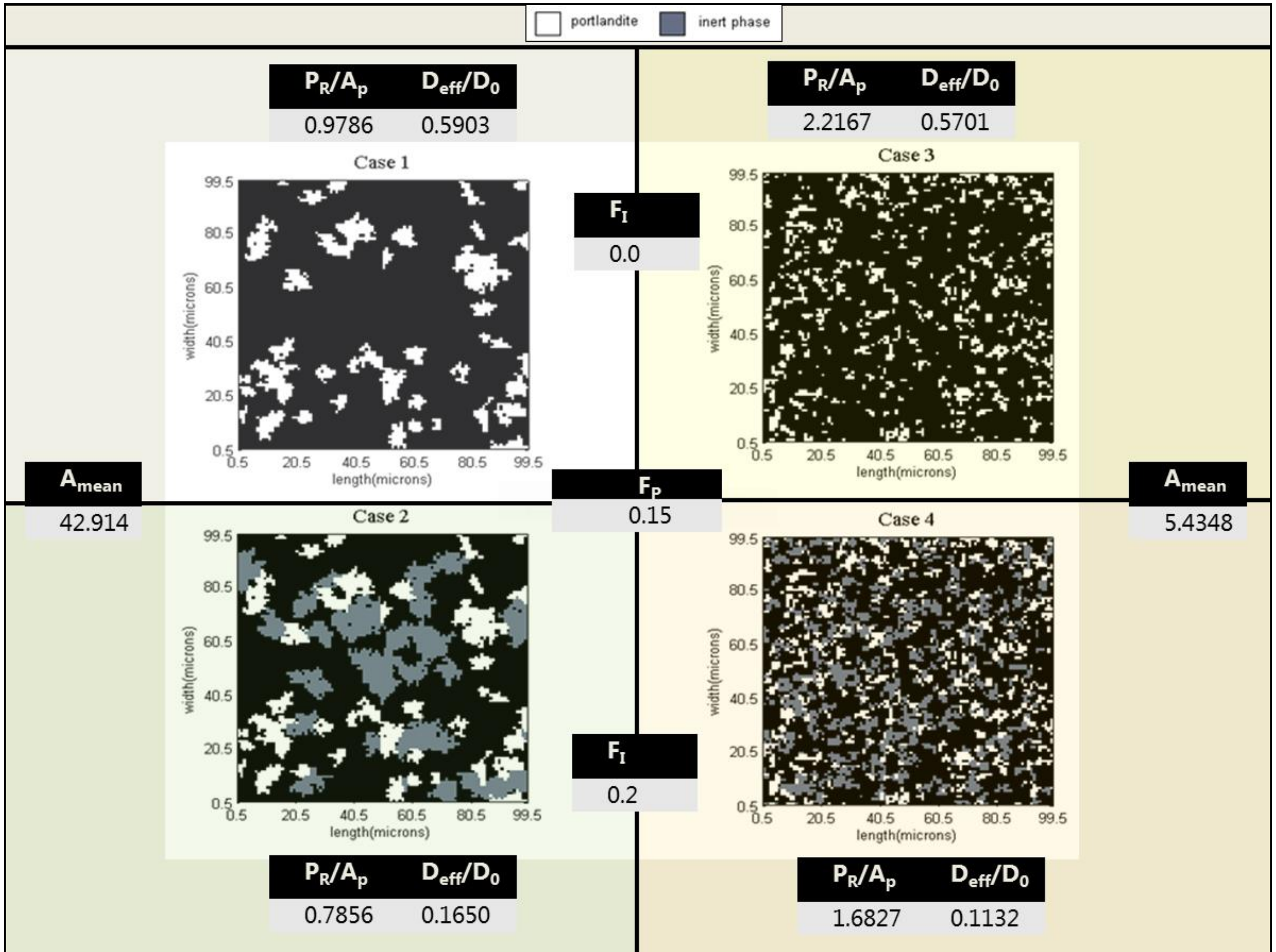
Electric resistivity measurements



Data from Ma etl al. (2012)

Patel (2015)

Example 2 – Influence of pore structure on dissolution



F_I : fraction of inert material

P_R/A_p: perimeter of reactive surface over area of portlandite particles

D_{eff}/ D_0 : ratio of effective diffusivity of medium to diffusivity of ion in free water

A_{mean} : mean area of particle

Patel (2015)

C_{eq}=19.48 mM

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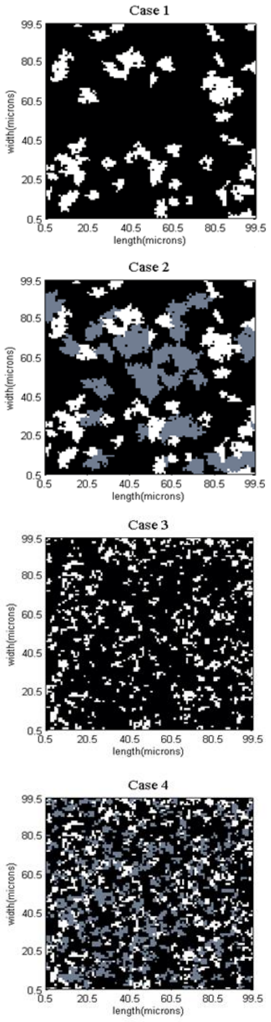
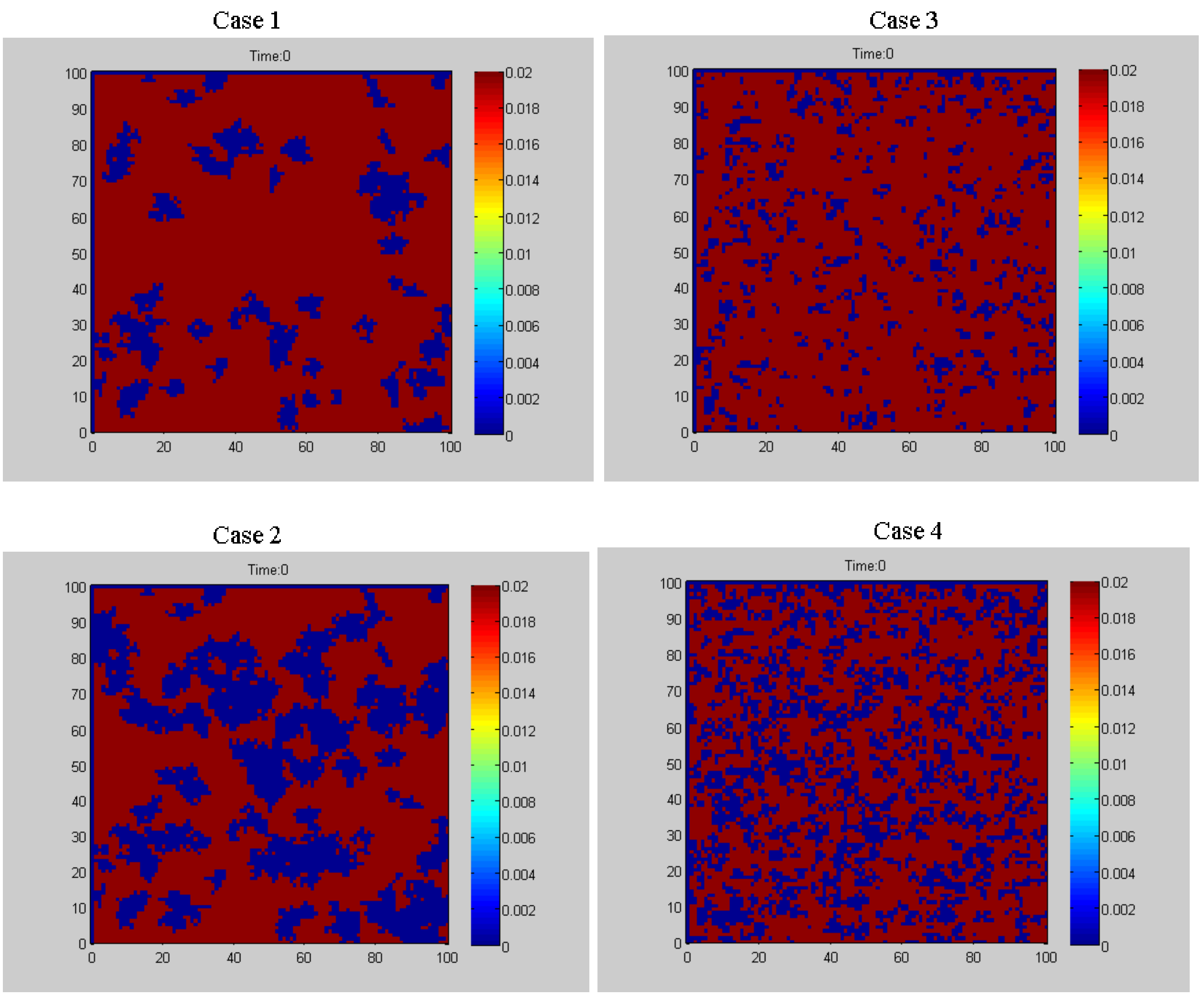
Example 2 – Influence of pore structure on dissolution



$D_{eff}/D0$
0.5903
0.1650
0.5701
0.1132

Patel (2015)



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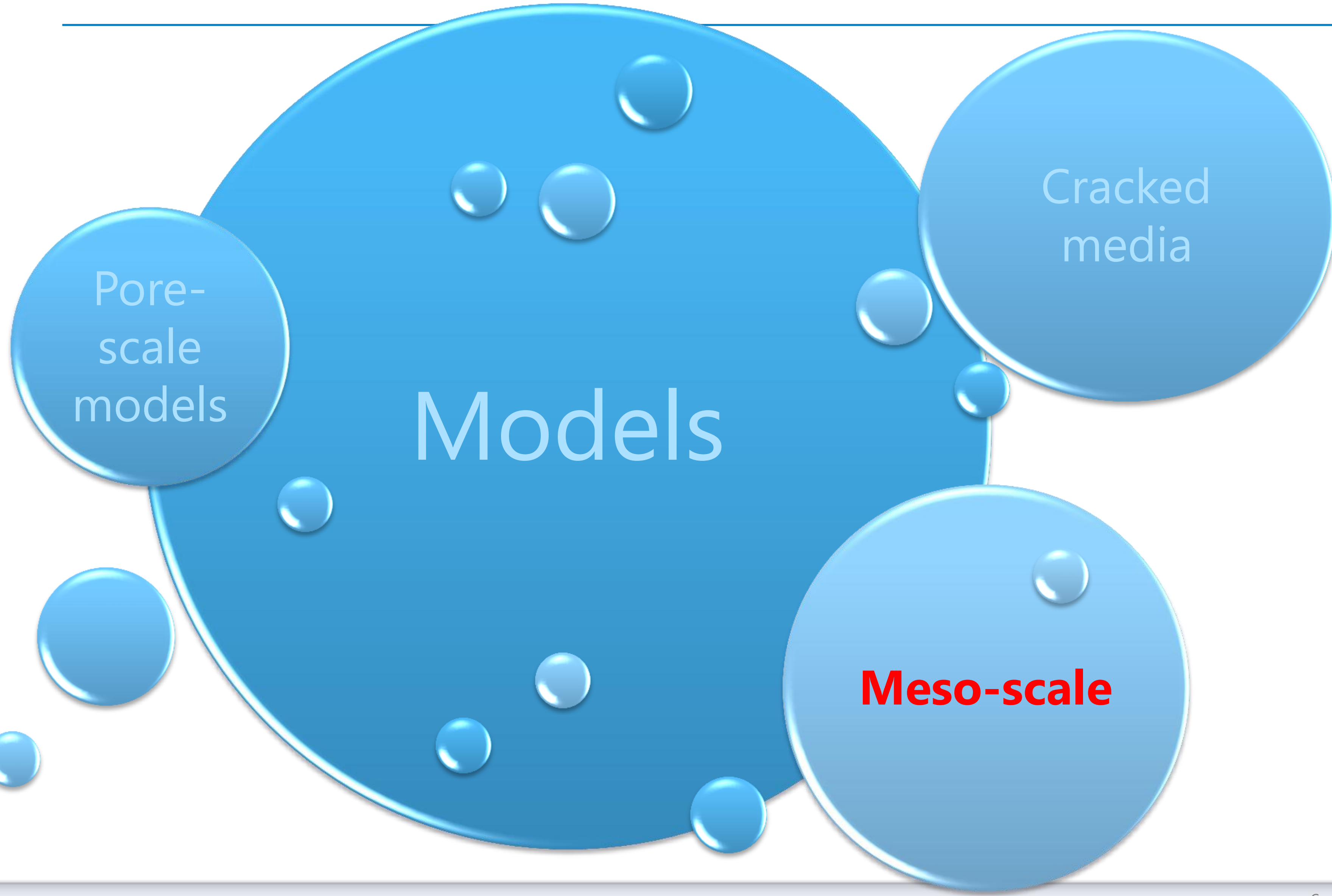

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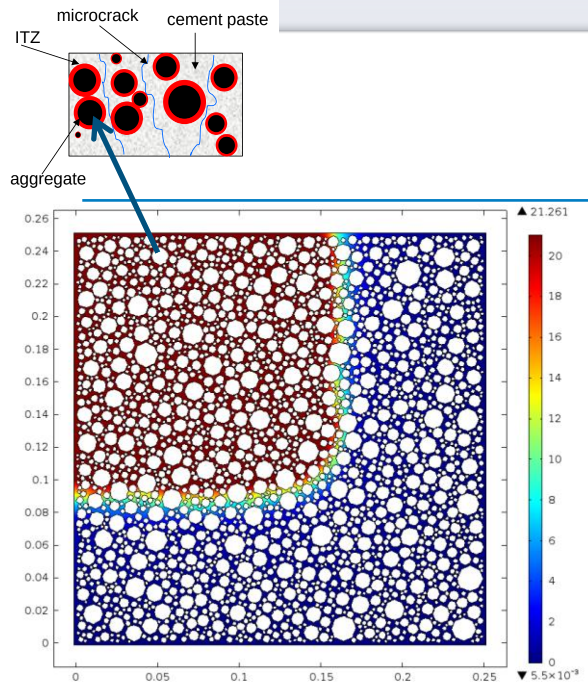
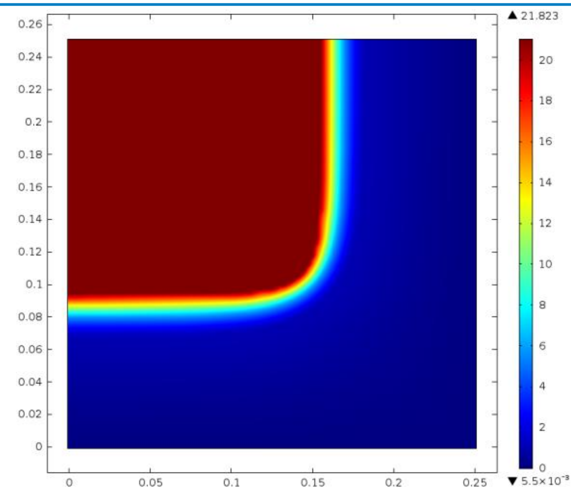
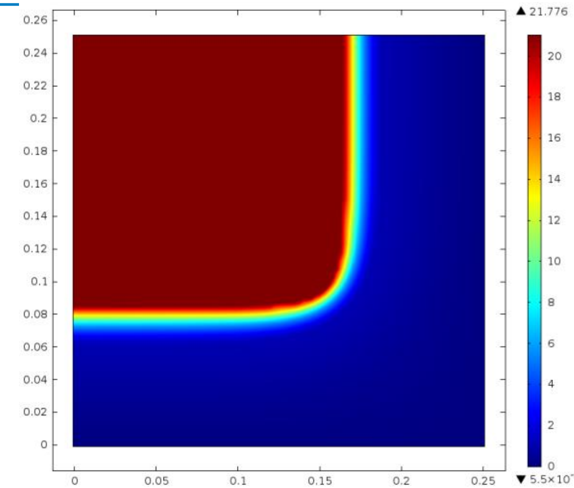
Meso-Macro Model (Ongoing work) – Ca leaching of concrete after 3000 years



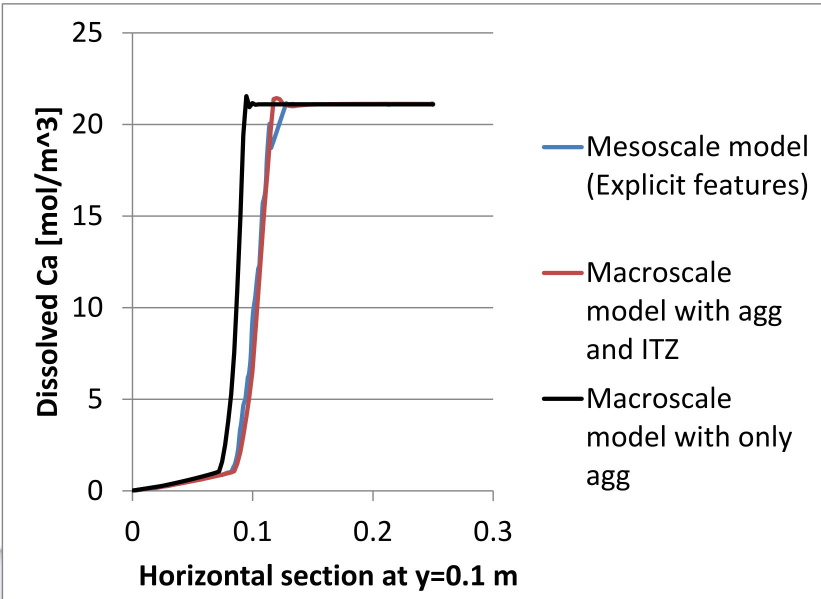
Mesoscale with aggregates and ITZ explicitly considered



Macroscale with aggregates and ITZ effect incorporated in the effective diffusivity



Macroscale with only aggregates effect incorporated in the effective diffusivity but no ITZ



- In upscaling techniques, often only aggregates are considered.
- Preliminary results suggest that the effect of ITZ should also be considered to capture leaching fronts.
- At this stage, based on hypothetical parameters.

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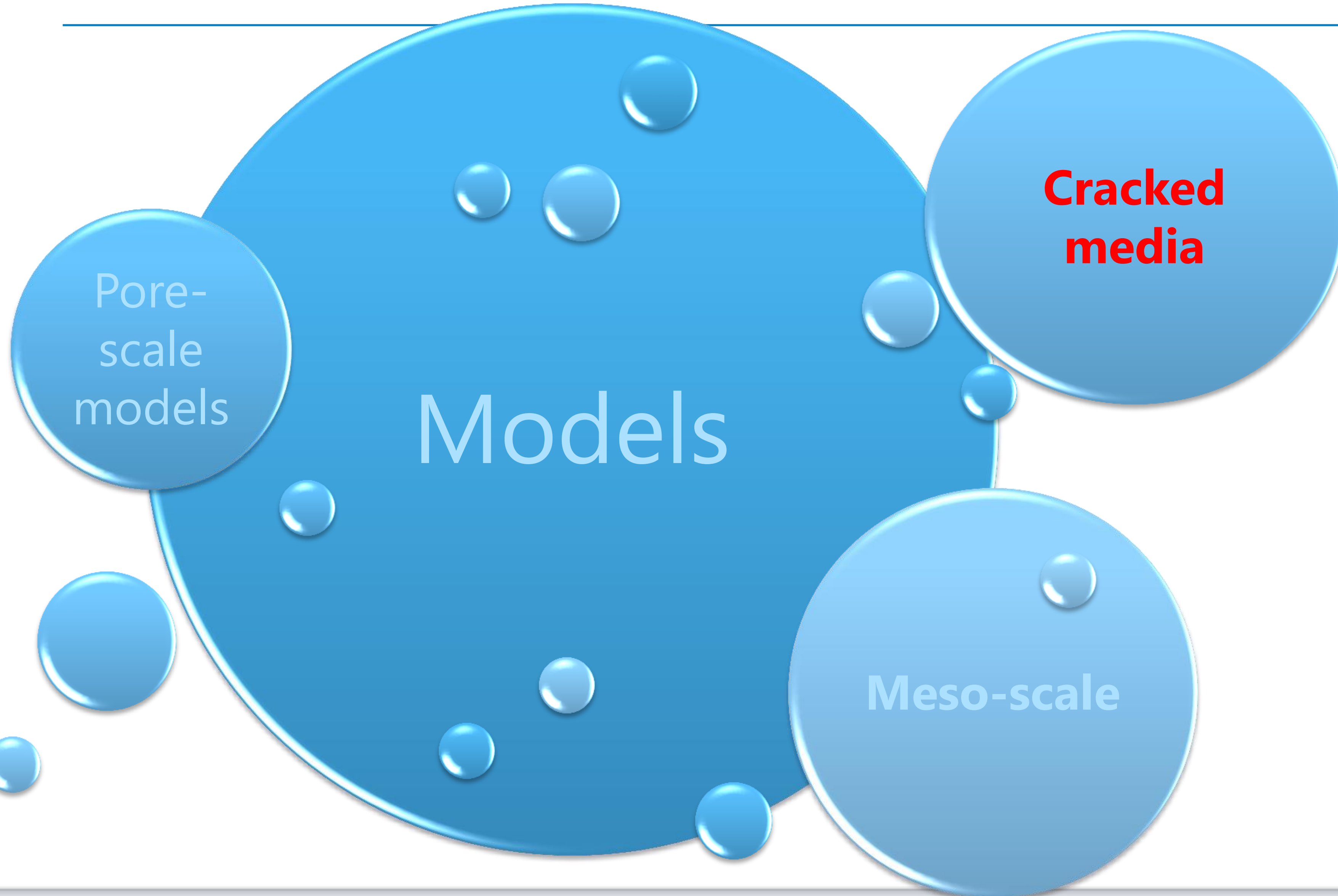

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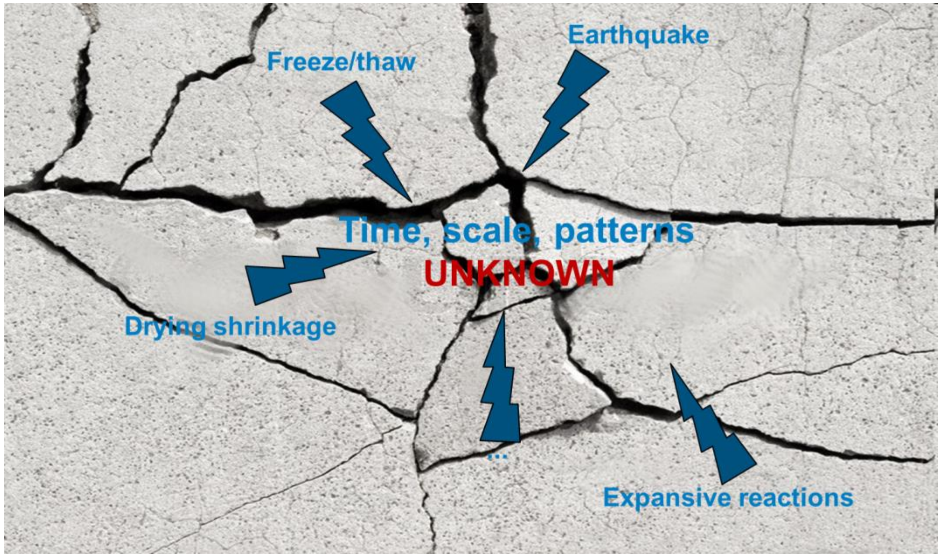
Flow and transport in heterogeneous media with discrete features (fractures)



Fractures

- Geometrical properties
- Connectivity
- Flow and transport properties

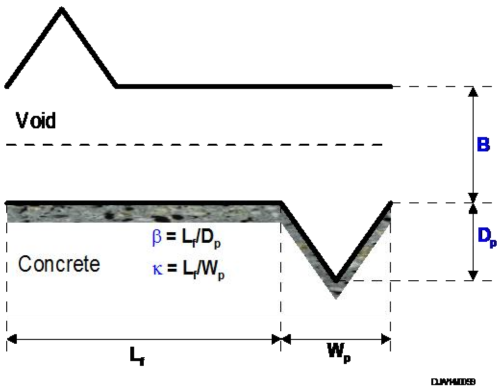
Matrix

- Evolution of physical and chemical properties

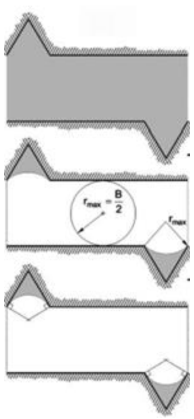
- Models are used to
  - Give support for expected phenomenological long-term evolution
  - Justify Safety and Performance Assessment (SA/PA) models
    - Simplification / Abstraction
    - Conservatism

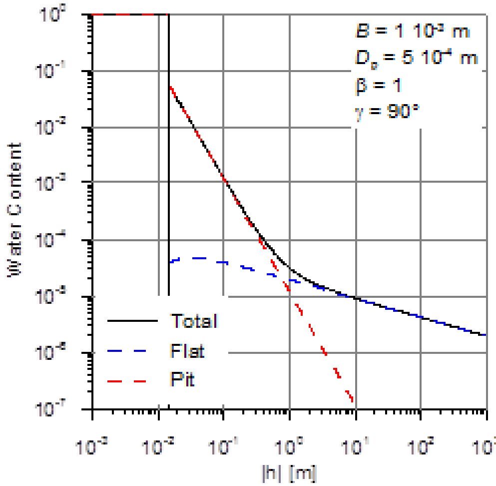
Example 1 - Water flow and saturation

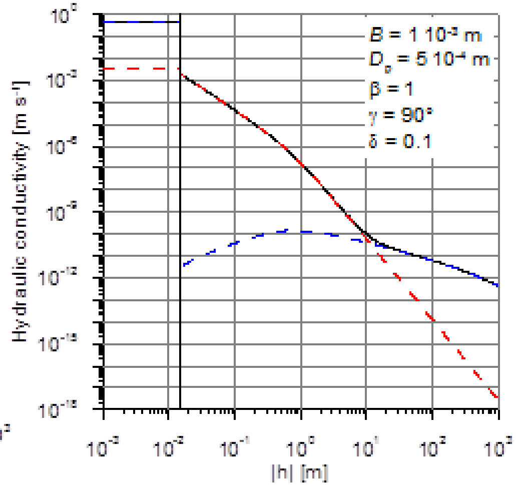
GEOMETRICAL MODEL (Tuller and Or approach)



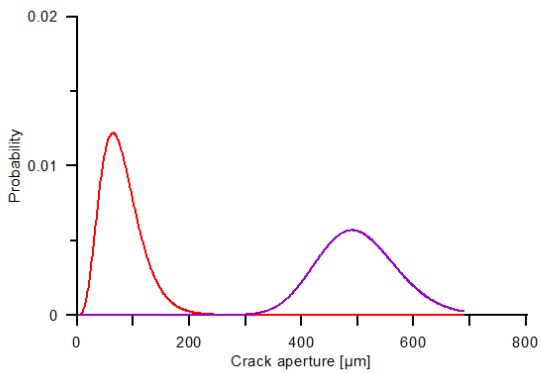
FLOW PROPERTIES FRACTURE



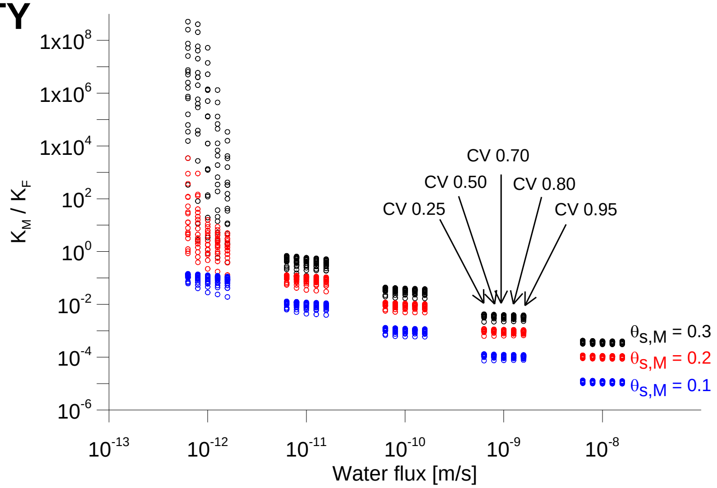




FLOW PROPERTIES NETWORK



UNCERTAINTY



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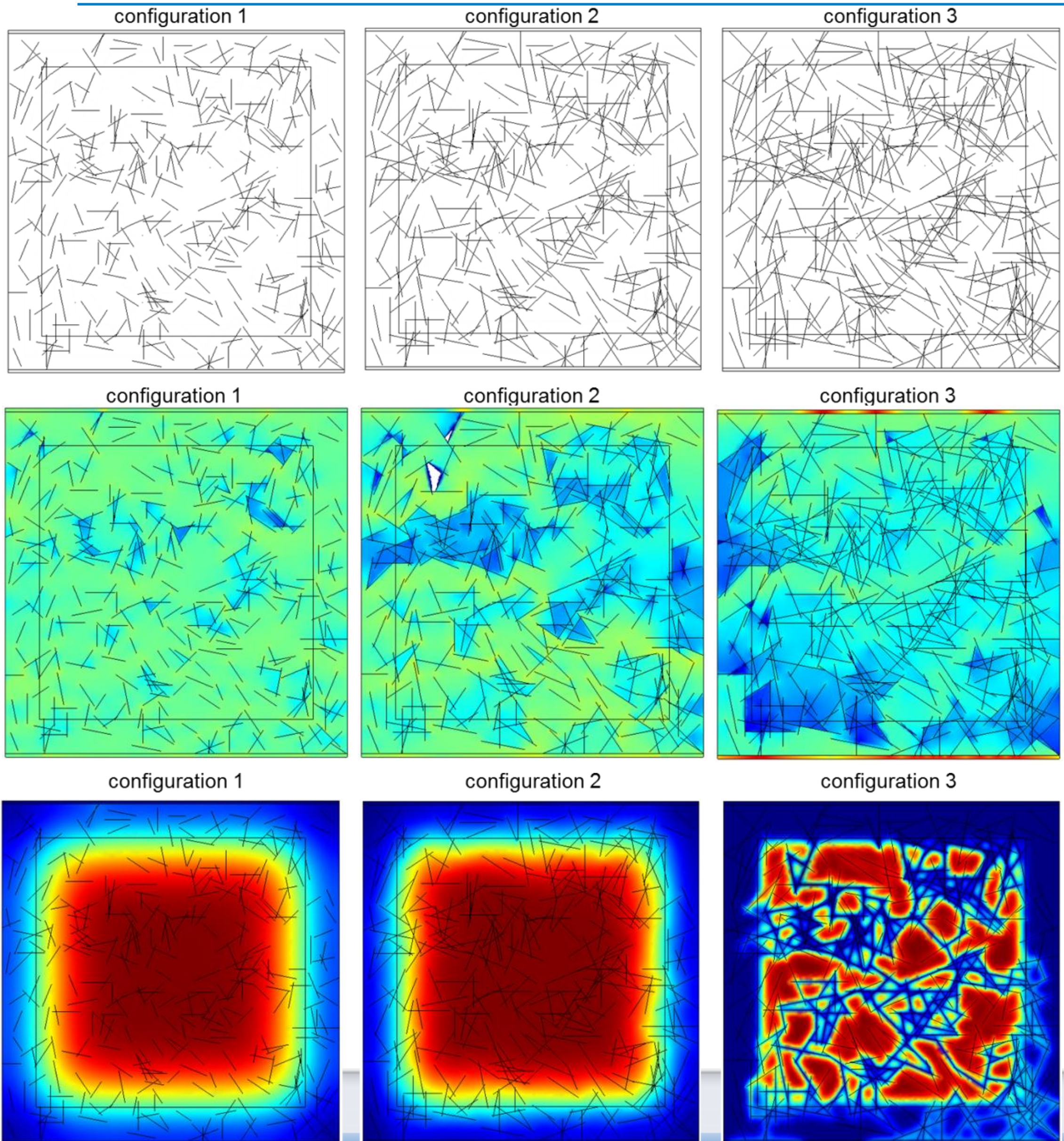
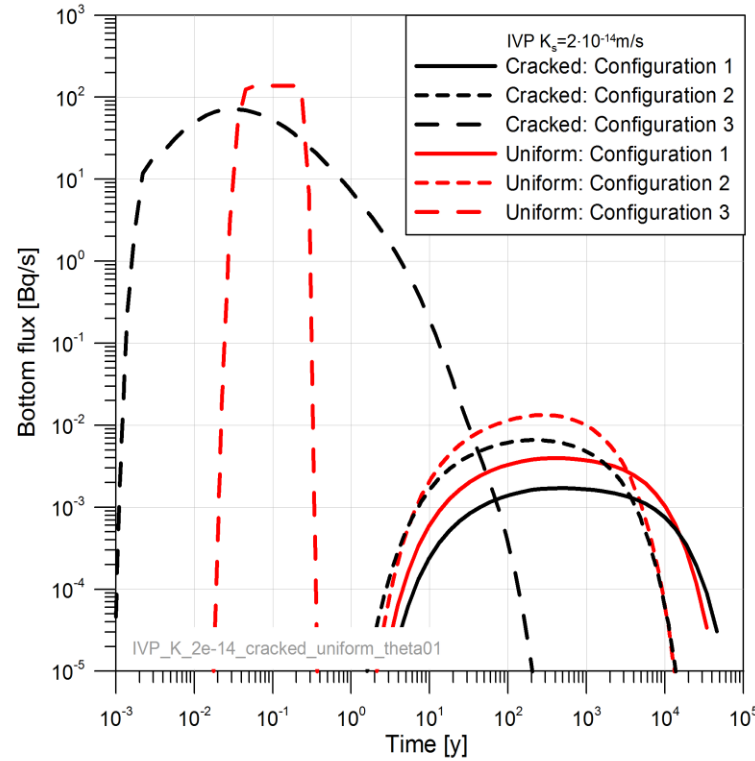
Example 2 – Leaching from a cracked concrete





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Summary

- Research question

  How chemical detrimental processes will affect concrete properties and processes in concrete at relevant time and spatial scales?
- Treated within a multi-scale framework

- Where are we now?
  - Develop methods for accelerated degradation and measurement of transport properties
  - Pore-scale framework to treat degradation at the micro-scale
  - Include fractures at the macro-scale including geometrical features to determine their properties

- Next steps

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Experimental Studies

Leaching and carbonation HCP

Using images from real HCP

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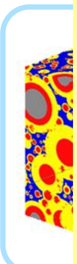

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mortar/concrete
(cracks)

Pore-
model
Lattice Boltzmann

Continuum scale modelling at small scale

Flow & transport in cracked media

Upscaling by model abstraction

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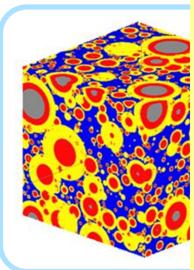

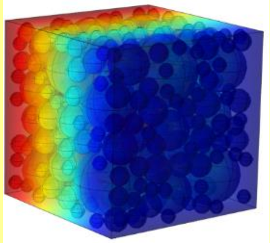

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Degradation under 'natural' conditions

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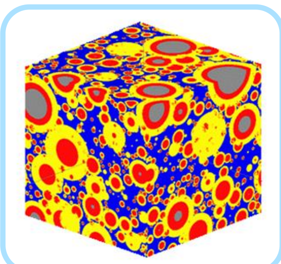

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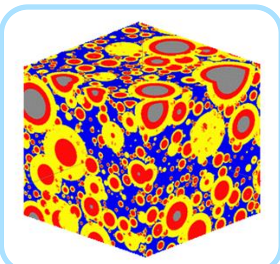

Fracture characterization Processes in fractures and at fracture/matrix interface

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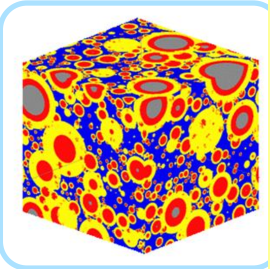

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