

Multibody approach for reactive transport and poromechanical modeling in discontinuous porous media

A. Socié¹, F. Dubois^{2,3}, M. Neji⁴, Y. Monerie^{2,3} and F. Perales^{2,4}

¹ : Department of Earth, Ocean and Atmospheric Sciences, University of British Columbia, Canada

² : Laboratoire de micromécanique et intégrité des structures, IRNS-CNRS-UM

³ : Laboratoire Mécanique et Génie Civil - Université de Montpellier, France

⁴ : Institut de Radioprotection et de Sécurité Nucléaire, St Paul lez Durance, France

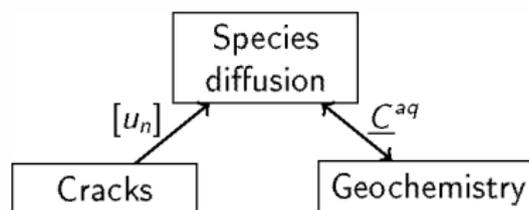
December 9th 2021



Challenges of the modelling

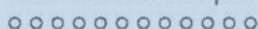
\underline{C}^{aq} : Species concentrations

$[u_n]$: Crack opening



Aims of the study

- Mesoscale modeling of chemical attack in saturated mature concrete
- Reactive transport in discontinuous heterogeneous porous medium



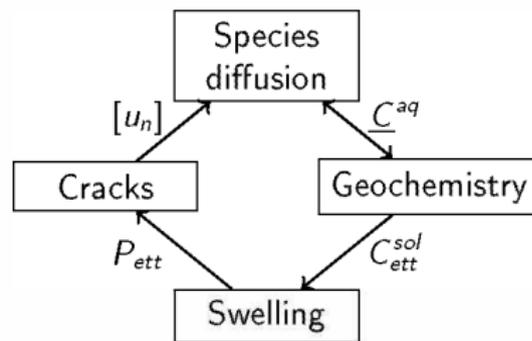
Challenges of the modelling

\underline{C}^{aq} : Species concentrations

$[u_n]$: Crack opening

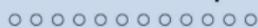
P_{ett} : Pressure induced by ettringite

C_{ett}^{sol} : Ettringite concentration



Aims of the study

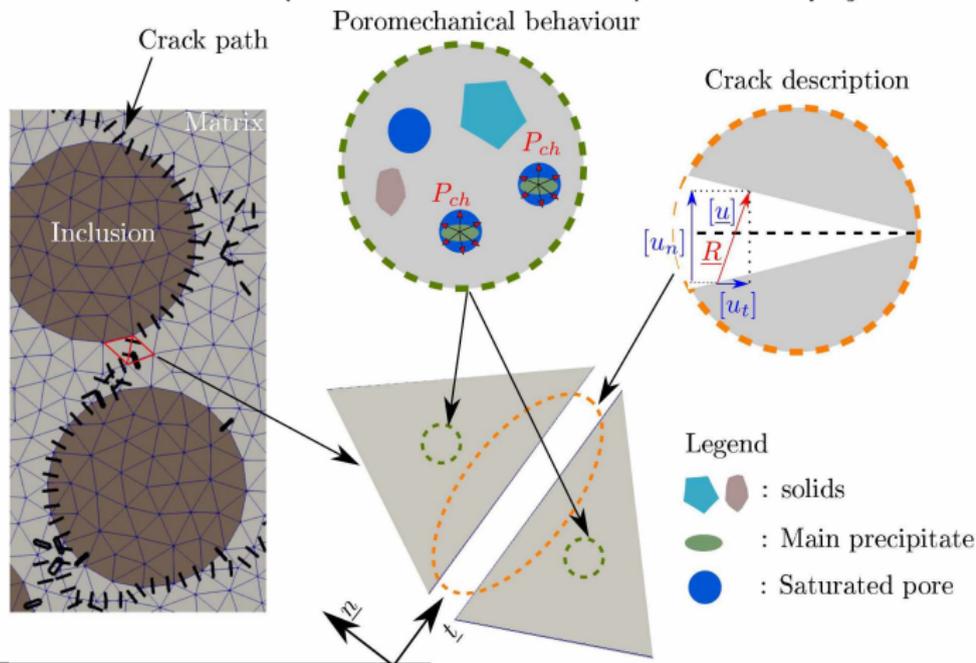
- Mesoscale modeling of chemical attack in saturated mature concrete
- Reactive transport in discontinuous heterogeneous porous medium
- Coupling between reactive transport and mechanics
- Generic implementation in XPER IRSN platform



Multibody approach

■ Bulk behavior (Finite Element): undamaged porous medium

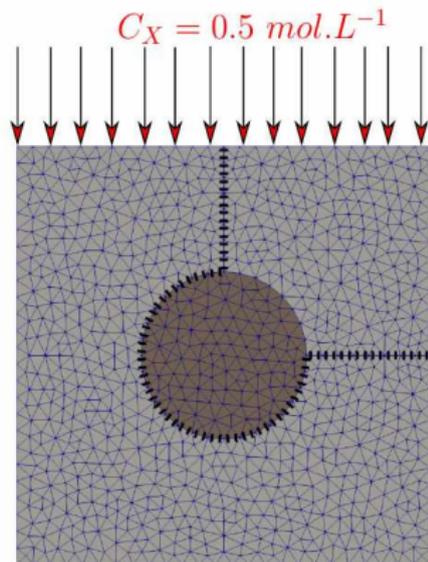
■ Interfacial behavior (Cohesive Zone Model): fracture physics



Species transport in a cracked porous medium

Porous medium: $\frac{\partial \phi C^{aq}}{\partial t} = \text{div}(D \nabla C^{aq}) + \underbrace{r^{\xi}}_{\text{chemistry impact}}$

In cracks: $\frac{\partial (C^{aq})^c}{\partial t} = -\Phi_{ts}^c + \underbrace{r^{\xi c}}_{\text{chemistry impact}}$



Species transport in a cracked porous medium

| Porous medium: $\frac{\partial \phi C^{aq}}{\partial t} = \text{div}(D \nabla C^{aq}) + \underbrace{r^{\xi}}_{\text{chemistry impact}}$

| In cracks: $\frac{\partial (C^{aq})^c}{\partial t} = -\Phi_{ts}^c + \underbrace{r^{\xi c}}_{\text{chemistry impact}}$

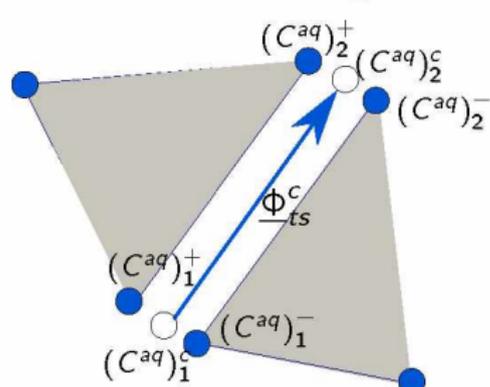
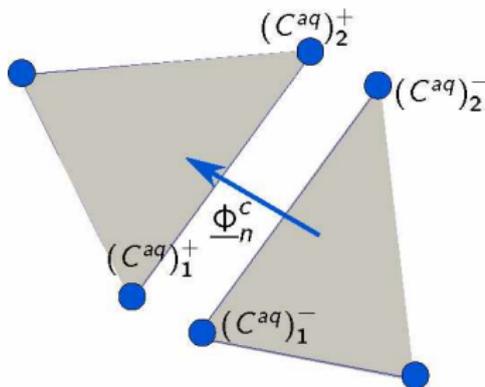
Species transport in a cracked porous medium

- Transport through the crack, e cohesive characteristic length

$$\underline{\phi}_n^c = -D_i^c \frac{[C_i^{aq}]}{e} = D^c \frac{(C^{aq})^+ - (C^{aq})^-}{e} \underline{n}$$

- Transport in cracks

$$\underline{\phi}_{ts}^c = -D^c \cdot \nabla(C^{aq})^c \cdot (\mathbf{I} - \underline{n} \otimes \underline{n}) \quad \text{with} \quad (C^{aq})^c = \frac{(C^{aq})^+ + (C^{aq})^-}{2}$$



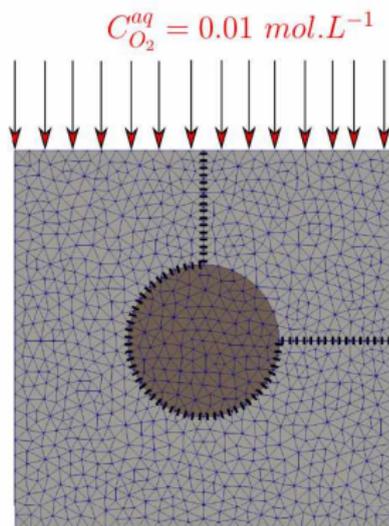
Species transport in a cracked porous medium

█ Crack diffusion model $\begin{cases} D_i^c = D_i^0 \frac{[u_n]}{[u_{ref}]}, & \text{if } [u_n] < [u_{ref}] \\ D_i^c = D_i^0 \end{cases}$

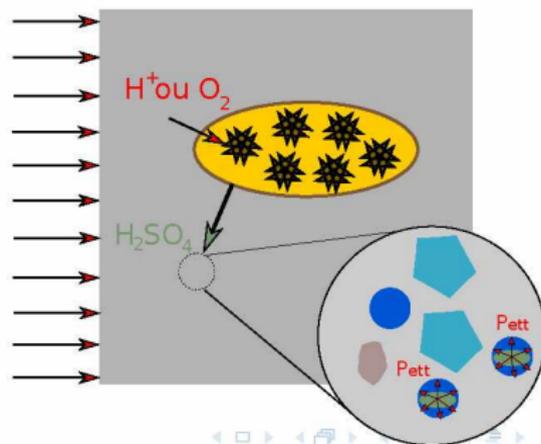
Reactive transport

Porous medium: $\frac{\partial \phi C^{aq}}{\partial t} = \text{div}(D \nabla C^{aq}) + \underbrace{r^\xi}_{\text{chemistry impact}}$

In cracks: $\frac{\partial (C^{aq})^c}{\partial t} = -\Phi_{ts}^c + \underbrace{r^{\xi c}}_{\text{chemistry impact}}$



H^+ ou O_2



Reactive transport

| Porous medium: $\frac{\partial \phi C^{aq}}{\partial t} = \text{div}(D \nabla C^{aq}) + \underbrace{r^{\xi}}_{\text{chemistry impact}}$

| In cracks: $\frac{\partial (C^{aq})^c}{\partial t} = -\phi_{ts}^c + \underbrace{r^{\xi c}}_{\text{chemistry impact}}$

Reactive transport

$$\left\{ \begin{array}{l} \underline{C}_{tot}^{aq} - \left[\underline{C}^{aq} + (\mathbf{s}^{sol})^T \underline{C}^{sol} \right] = 0 \quad \text{Mass balance} \\ \underline{\xi}^{sol} = 1 - \frac{\prod_{j=1}^{N^s} (C_i^{aq} \gamma_i)^{S_{i,j}^s}}{K_i^s} = 0 \quad \text{Law of mass action, } \forall C^{sol} \\ \underline{C}^{aq} \geq \underline{0}, \quad \underline{C}^{sol} \geq \underline{0} \end{array} \right.$$



Reactive transport

Reactive transport

$$\left\{ \begin{array}{l} \underline{C}_{tot}^{aq} - \left[\underline{C}^{aq} + (\mathbf{s}^{aq})^T \cdot \underline{\xi}^{aq}(\underline{C}^{aq}) + (\mathbf{s}^{ad/aq})^T \cdot \underline{\xi}^{ad}(\underline{C}^{aq}, \underline{C}^{ad}) + (\mathbf{s}^{sol})^T \cdot \underline{C}^{sol} \right] = \underline{0} \\ \underline{C}_{tot}^{ad} - \left[\underline{C}^{ad} + (\mathbf{s}^{ad/ad})^T \cdot \underline{\xi}^{ad}(\underline{C}^{aq}, \underline{C}^{ad}) \right] = \underline{0} \\ (\underline{\xi}^{sol}(\underline{C}^{aq}))^T \underline{C}^{sol} = 0, \quad \xi^{el}(\underline{C}^{aq}) = \sum_{i=1}^{N^{aq}} z_i C_i^{aq} = 0 \\ \underline{C}^{aq} \geq \underline{0}, \quad \underline{C}^{ad} \geq \underline{0}, \quad \underline{C}^{sol} \geq \underline{0}, \quad \underline{\xi}^{sol}(\underline{C}^{aq}) \geq \underline{0} \end{array} \right.$$

Chemical reaction

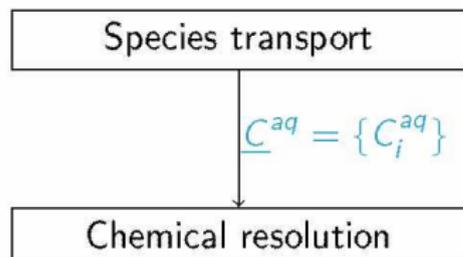
- | | |
|-------------|----------------------|
| 1. Solid | 3. Aqueous |
| 2. Sorption | 4. Electroneutrality |

Logarithmic resolution to ensure positive concentration

[?, ?, ?]

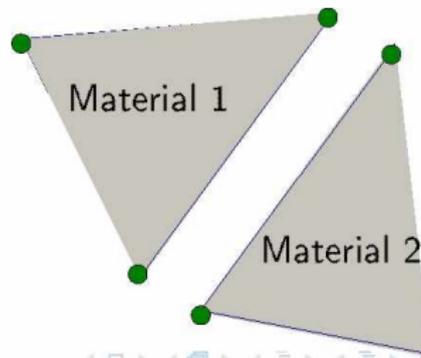
Reactive transport: numerical resolution

- Geochemical model based on thermodynamic equilibrium assumption
- Reactive transport solved by Sequential Non Iterative Approach (SNIA)
- Chemical resolution at nodes
- Multibody approach to solve heterogeneous material



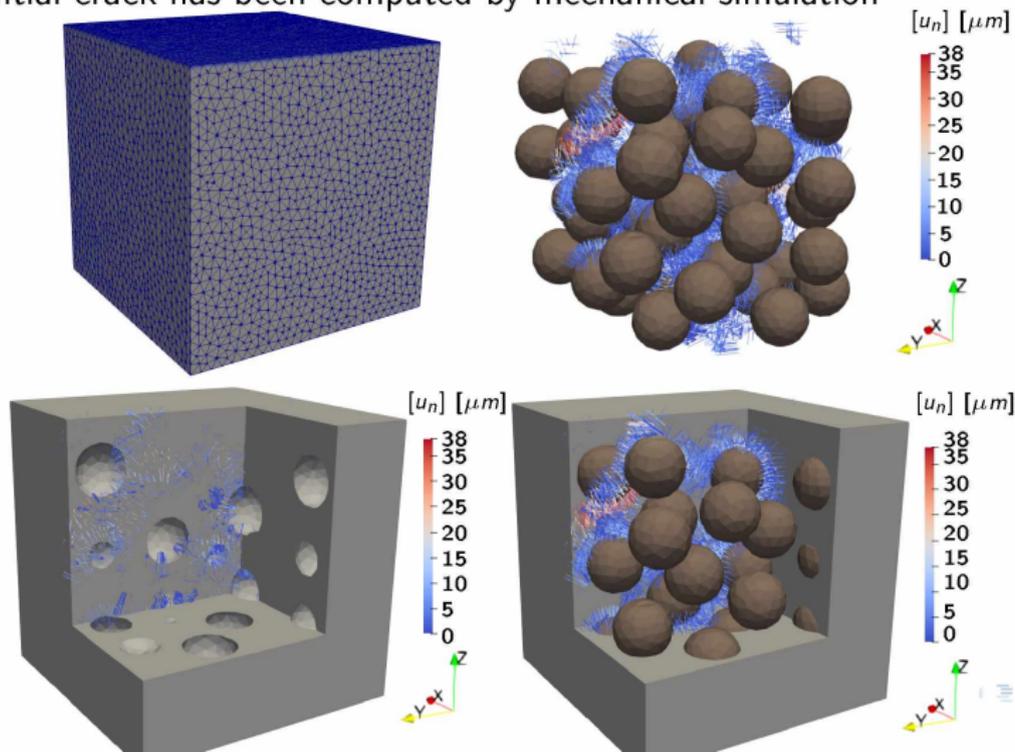
[?, ?, ?]

Chemical resolution at nodes



Reactive transport simulation of cracked concrete

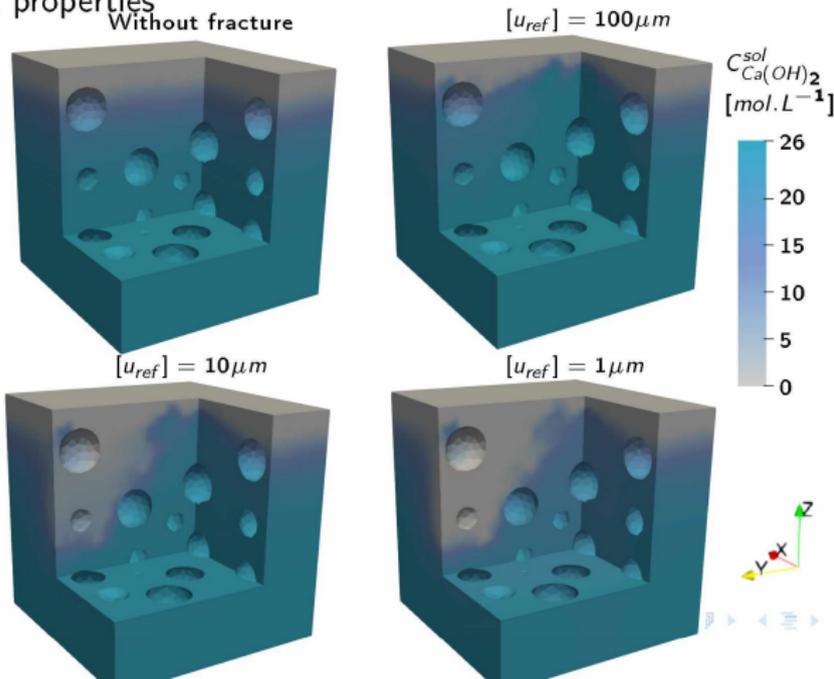
- Concrete cube ($5 \times 5 \times 5 \text{ cm}^3$) with 35% volume fraction of aggregates. Initial crack has been computed by mechanical simulation



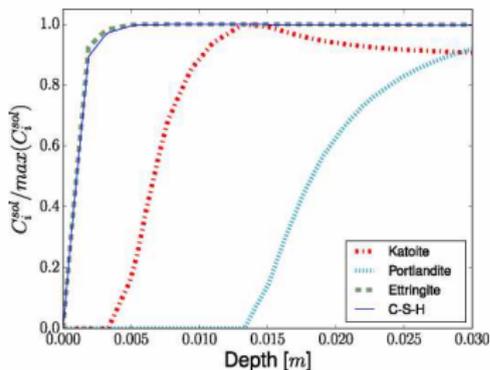
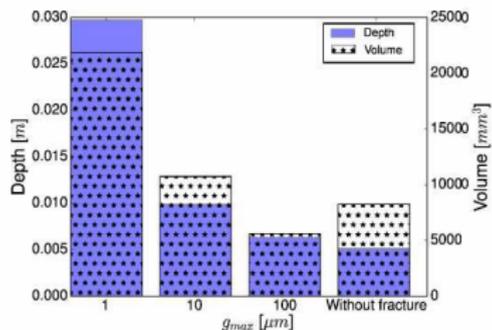
Calcium leaching

Impact of crack on diffusivity: $D_i^c = D_i^0 \max\left(\frac{[u_n]}{[u_{ref}]}, 1\right)$

Calcium leaching induces the dissolution of hydrated mineral that affect the mechanical properties

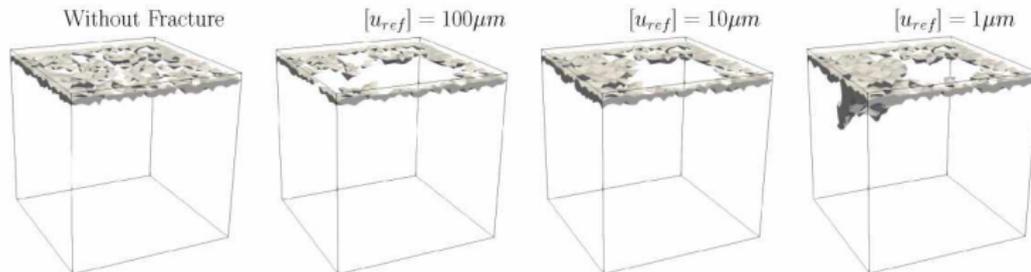


Calcium leaching



Evolution of the depth and the volume of portlandite dissolution

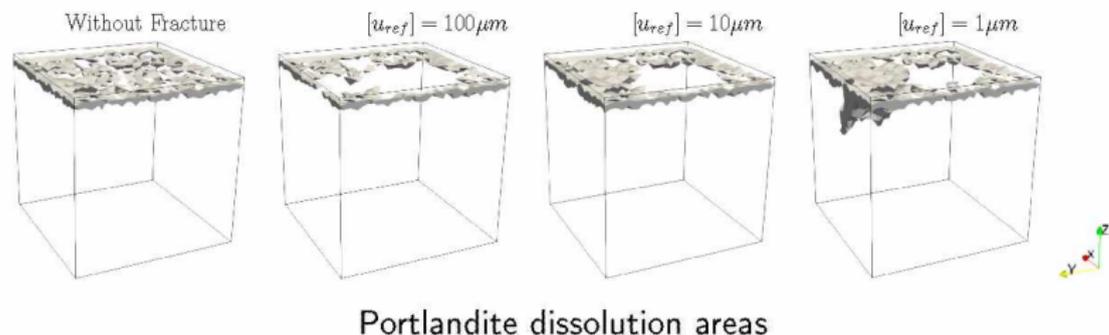
Solid concentrations fraction, 0 is the attack surface area



Portlandite dissolution areas

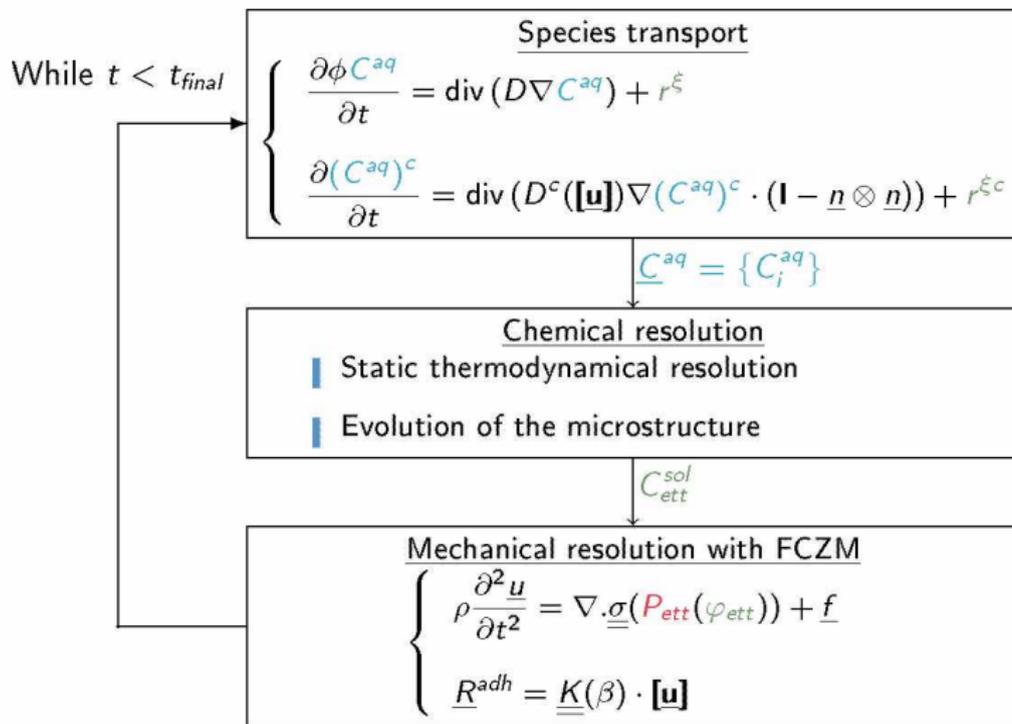
Calcium leaching

- The diffusivity of the gap and the critical gap values impact the chemical degradation area
- Discontinuities localize the chemical degradation
- The depth is not sufficient to describe the degradation, more general 3D effects have to be taken into account



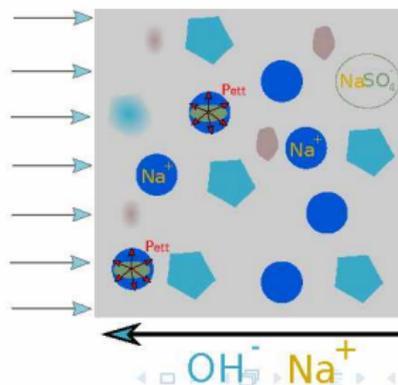
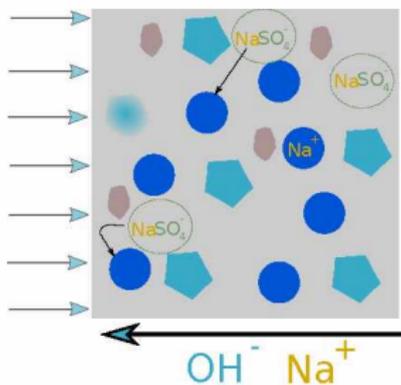
Portlandite dissolution areas

Staggered resolution: coupling strategy



Delayed Ettringite Formation

- Sulfates are initially sorbed, sodium Na^+ leaching induces ettringite precipitation
- Geochemical model
 - 2 sorbed reactions
 - 3 solid reactions
 - Electroneutrality
 - 4 aqueous species



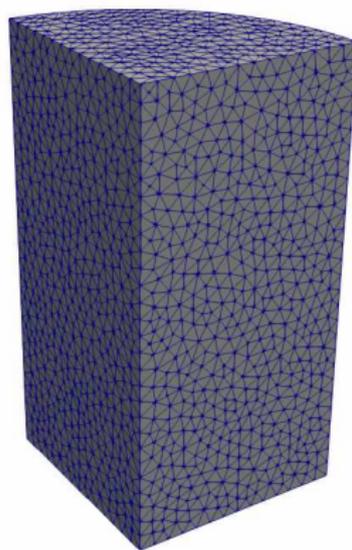
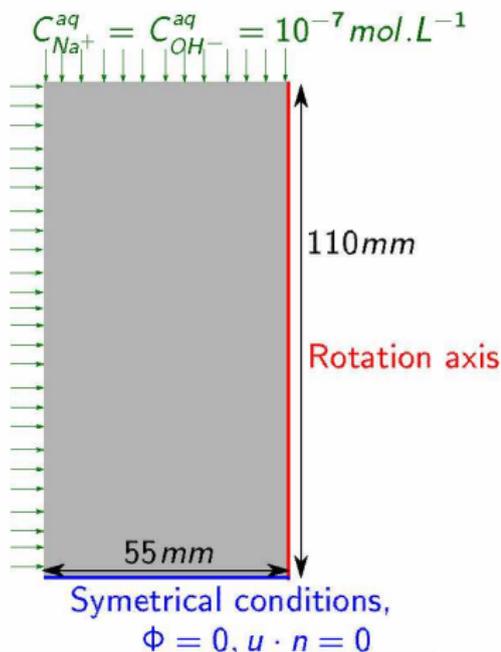
Delayed Ettringite Formation

- | Sulfates are initially sorbed, sodium Na^+ leaching induces ettringite precipitation
- | Geochemical model
 - 2 sorbed reactions
 - 3 solid reactions
 - Electroneutrality
 - 4 aqueous species
- | To accelerate the degradation of the DEF, the samples are immersed

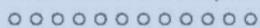


Delayed Ettringite Formation: 3D simulations of mortar

- 1/4 of 110×220 mm mortar sample
- The chemical conditions represent the immersion of the sample in water



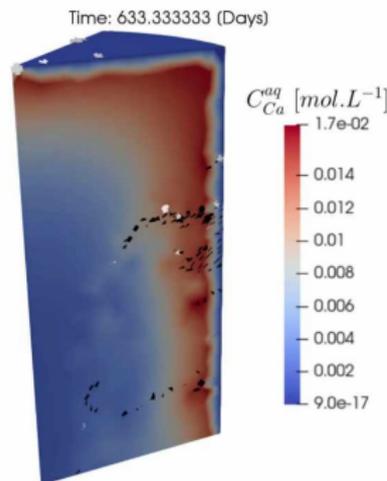
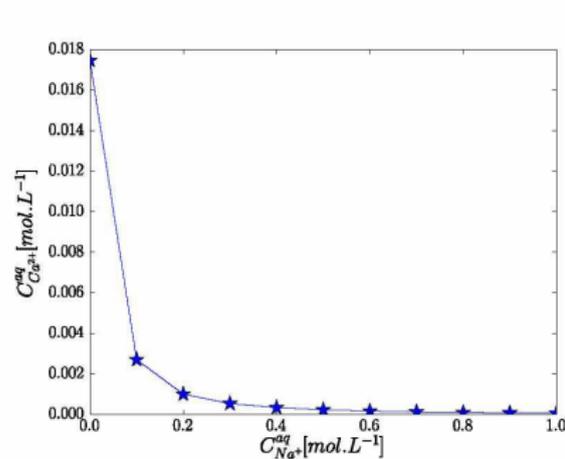
Delayed Ettringite Formation: 3D simulations of mortar



Delayed Ettringite Formation: 3D simulations of mortar

Delayed Ettringite Formation: 3D simulations of mortar

- Sodium and calcium are the main cations
- Sodium leaching impact calcium concentration via electroneutrality and portlandite [?]

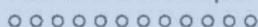


Conclusion

- Chemical-mechanical model in cracked heterogeneous porous medium
 - Multibody approach applied to reactive transport of cracked heterogeneous porous medium
 - Coupling reactive transport and mechanics
 - Generic approach that can take into account different chemical attacks

Conclusion

- Chemical-mechanical model in cracked heterogeneous porous medium
 - Multibody approach applied to reactive transport of cracked heterogeneous porous medium
 - Coupling reactive transport and mechanics
 - Generic approach that can take into account different chemical attacks
- In progress
 - SIA solver for reactive transport
 - Kinetic dissolution reaction
 - Coupling geochemical software CHESS with XPER
 - External Sulfate Attacks (Ph.D. Julie Pouya) and Alkali Silica Reaction (Ph.D. Lucie Gomez)



Bichet, L. (2017).

Mécanisme de transport dans la fissuration des matériaux hétérogènes : application a la durée de vie d'exploitation des centrales nucléaires.

PhD thesis, Université de Montpellier II.



Brunetaud, X. (2005).

Etude de l'influence de différents paramètres et de leurs interactions sur la cinétique et l'amplitude de la réaction sulfatique interne au béton.

PhD thesis, Ecole Centrale des Arts et Manufactures "Ecole Centrale Paris".



De Dieuleveult, C., Erhel, J., and Kern, M. (2009).

A global strategy for solving reactive transport equations.

Journal of Computational Physics, pages 228 : 6395 – 6410.



Djerbi, A., Bonnet, S., Khelidj, A., and Baroghelbouny, V. (2008).

Influence of traversing crack on chloride diffusion into concrete.

Cement and Concrete Research, pages 38 : 877 – 883.



Eddy, L., Awasthi, A., Matsumoto, K., Nagai, K., and Asamoto, S. (2017).

Mesoscopic analysis of different expansion causes in concrete by 3d rigid body spring model.

[Seisan Kenkyu](#), pages Volume 69, Issue 4 : 181–185.



Erhel, J. and Migot, T. (2018).

Characterizations of solutions in geochemistry: existence, uniqueness, and precipitation diagram.

[Computational Geosciences](#), pages 1 – 13.



Idiart, A., López, C., and Carol, I. (2011).

Chemo-mechanical analysis of concrete cracking and degradation due to external sulfate attack: A meso-scale model.

[Cement and Concrete Composite](#), pages 33 : 411 – 423.



Leblond, J.-B., Bergheau, J.-M., Lacroix, R., and Huin, D. (2017).

Implementation and application of some nonlinear models of diffusion/reaction in solids.

Finite Elements in Analysis and Design, pages 132 : 8 – 26.



Michel, J., Suquet, P., and Thébaud, F. (1994).

Une modélisation du rôle des interfaces dans le comportement des composites à matrice métallique.

Revue Européenne des Éléments, pages 3 (4), 573 – 595.



Monerie, Y. and Acary, V. (2001).

Formulation dynamique d'un modèle de zone cohésive tridimensionnel couplant endommagement et frottement.

Revue européenne des éléments finis, pages 10 : 489 – 503.



Perales, F., Bourgeois, S., Chrysochoos, A., and Monerie, Y. (2008).

Two field multibody method for periodic homogenization in fracture mechanics of non linear heterogeneous materials.

[Engineering Fracture Mechanics](#), pages 75 : 3378 – 3398.



Poyet, S., Sellier, A., Capra, B., Foray, G., Torrenti, J.-M., Cognon, E., and Bourdarot, E. (2007).

Chemical modelling of Alkali Silica reaction: Influence of the reactive aggregate size distribution.

[Materials and Structures](#), pages 40 : 229 – 239.



Sabit, S. (2014).

[Les méthodes numériques de transport réactif](#).

PhD thesis, Université de Rennes.



Segura, J. and Carol, I. (2004).

On zero-thickness interface elements for diffusion problems.

[International journal for numerical and analytical methods in geomechanics](#), pages 28 : 947 – 962.



Socié, A., Dubois, F., Monerie, Y., Neji, M., and Perales, F. (2021a).

Simulation of internal and external sulfate attacks of concrete with a generic reactive transport-poromechanical model.

[European Journal of Environmental and Civil Engineering.](#), page Under review.



Socié, A., Dubois, F., Monerie, Y., and Perales, F. (2021b).

Multibody approach for reactive transport modeling in discontinuous-heterogeneous porous media.

[Computational Geosciences.](#), pages 1473 – 1491.