Multiscale modelling of carbonation in concrete made with RCA

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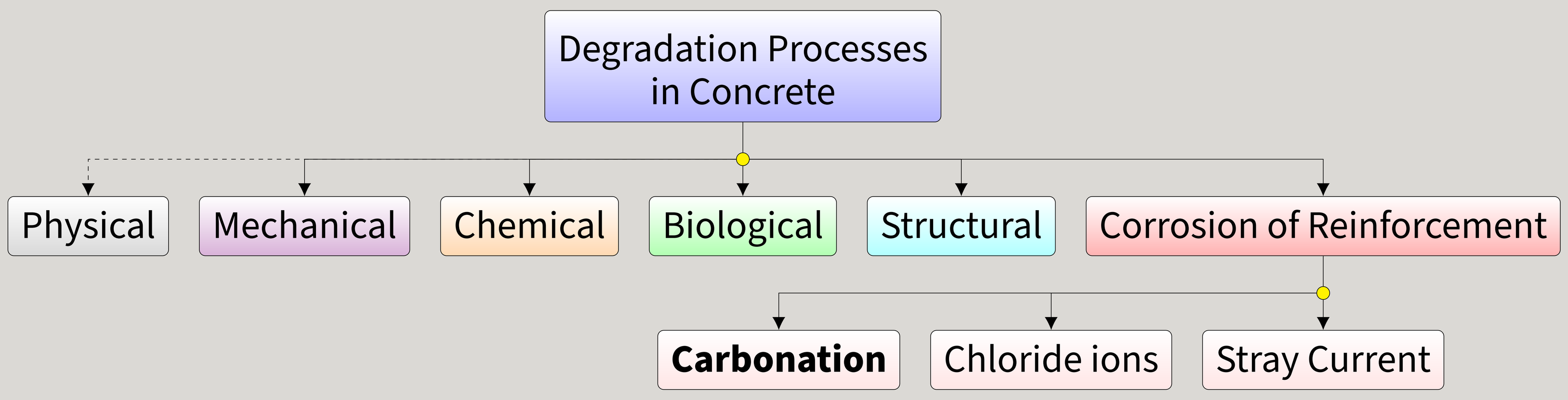
1. Context

Problematic:
- Limited raw material resources (2.5×10^9 t/yr of natural aggregates produced in the EU)
- CO_2 emissions
- Construction and demolition waste (374×10^6 t/yr in the EU)

Solution: Recycling concrete into recycled concrete aggregates (RCA) for concrete production

3. Durability properties



Caution is advised when introducing new materials, as their long-term durability performance is often uncertain and requires thorough evaluation.

Reinforcement corrosion:
- Causes aesthetic degradation
- Reduces structural durability and safety
- Requires frequent repairs
- Necessitates continuous monitoring
- Represents a significant global cost
- Two main causes:
  - Chloride ion penetration
  - **Carbonation**

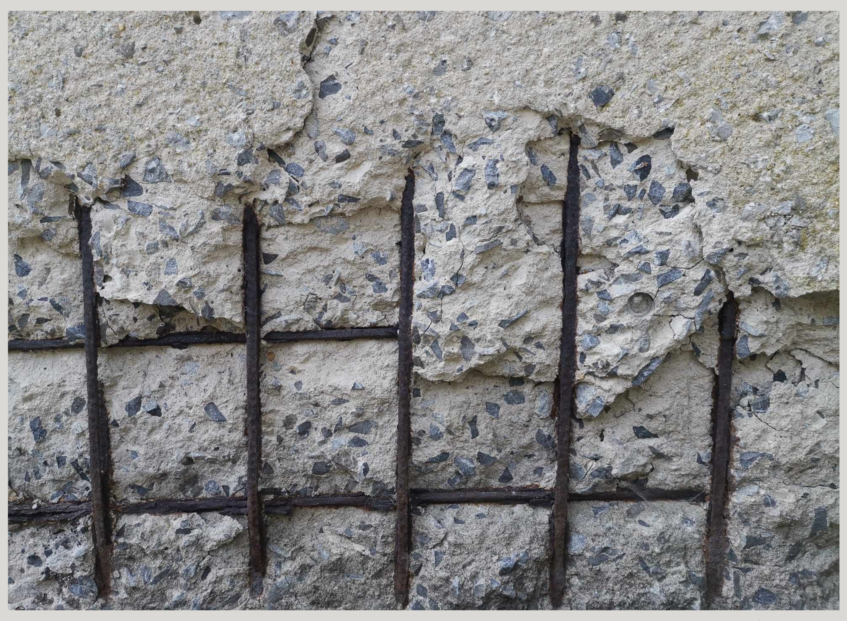


Figure 2: Corroded rebar in B6 Building (ULiège)

5. Central research question

How can the carbonation of concrete incorporating recycled concrete aggregates be modelled to accurately predict and assess its impact on durability and performance ?

6. Experimental study

Goals:
- Calibrate key input parameters of the numerical model
- Compare simulation results with real-world observations

Compositions :

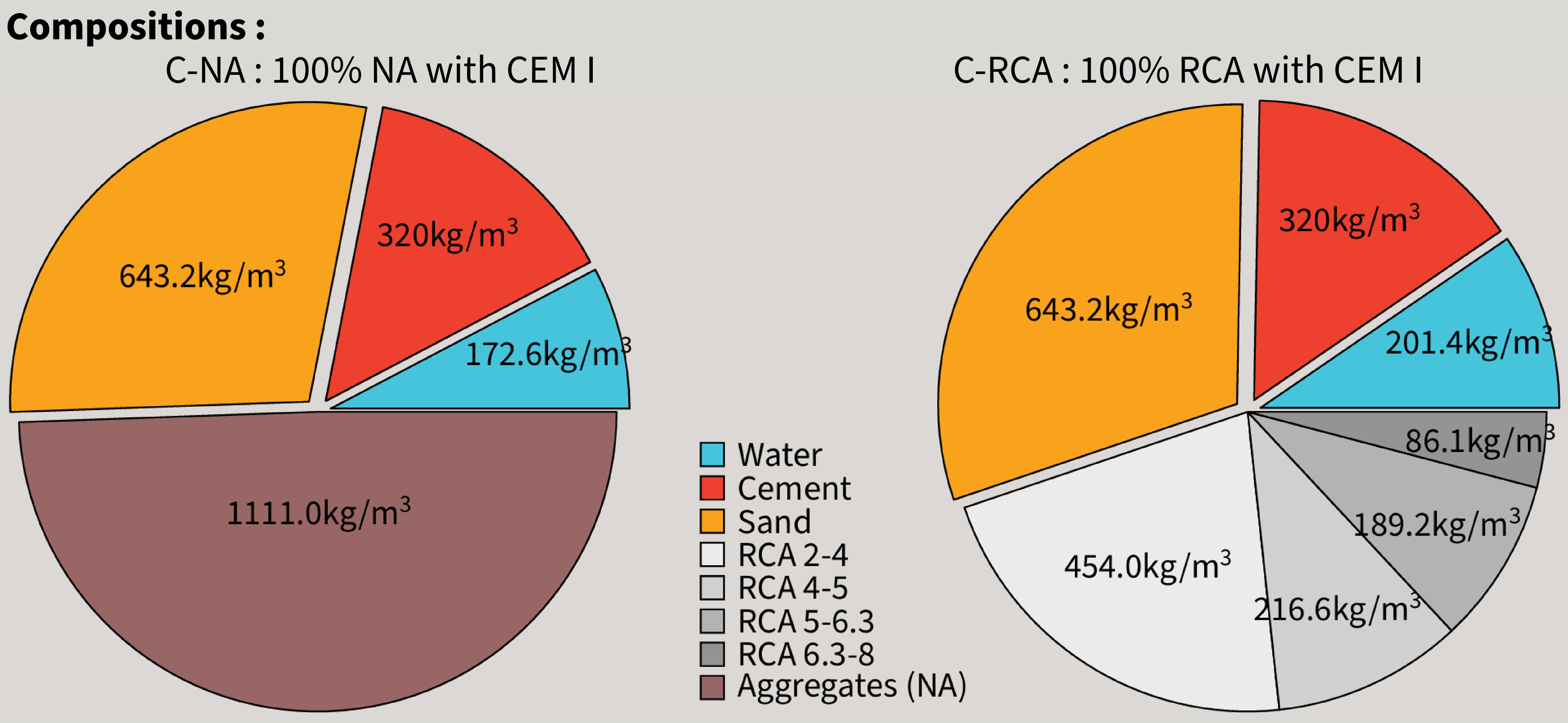


Figure 4: Micro-concrete composition with and without RCA [3]

A matching mortar, with the same paste composition as the concretes, was also included.

Planned tests :
- Fresh state tests
  - Workability, Air content, Bulk density
- Hardened state tests
  - Compressive strength, water permeability, CO_2 diffusion, static sorption-desorption...
- Carbonation tests
  - Phenolphthalein indicator, TGA, gamma densitometry

8. Objectives

- Promote the use of recycled concrete aggregates (RCA) to reduce natural resource consumption and construction waste.
- Investigate the impact of RCA on the carbonation process and its implications for durability.
- Develop and validate experimental and numerical tools to predict carbonation in RCA-based concrete.
- Support the safe and durable integration of RCA in structural applications.

References

[1] Mi, R., Pan, G., Li, Y., Kuang, T., & Lu, X. (2019). *Distinguishing between new and old mortars in recycled aggregate concrete under carbonation using iron oxide red*. Construction and Building Materials, 222, 601–609. https://doi.org/10.1016/j.conbuildmat.2019.06.171

[2] Thiery, M. (2005). *Modelling of atmospheric carbonation of cement based materials considering the kinetic effects and modifications of the microstructure and the hydric state*. PhD thesis, Ecole des Ponts ParisTech.

[3] Fanara, A. (2024). *FE2 multiscale modelling of chloride ions transport in recycled aggregates concrete*. Doctoral thesis, Université de Liège.

[4] Saetta, A. V., Schrefler, B. A., & Vitaliani, R. V. (1993). *The carbonation of concrete and the mechanism of moisture, heat and carbon dioxide flow through porous materials*. Cement and Concrete Research, 23(4), 761–772. https://doi.org/10.1016/0008-8846(93)90030-D

2. Recycled concrete aggregate (RCA)

- is obtained by crushing concrete from construction and demolition waste
- is a natural aggregate (NA) surrounded by mortar
- is a porous aggregate due to the presence of the adhered mortar
- contains unreacted cement and carbonatable materials within the mortar

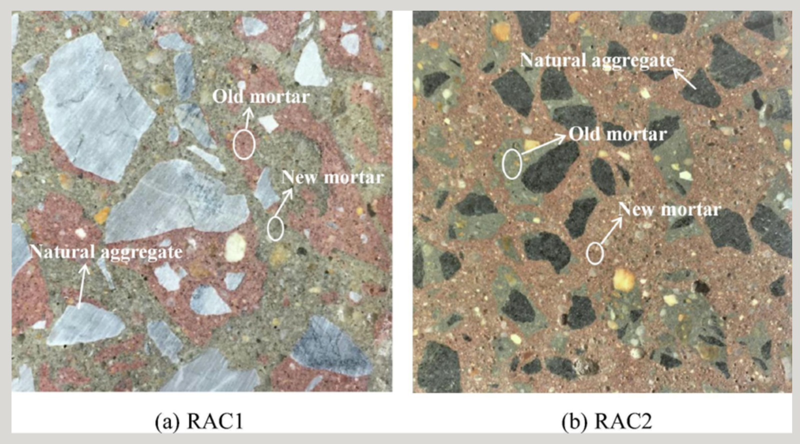


Figure 1: Phases in concrete with RCA [1]

4. Carbonation chemistry

Global reactions :
- $Ca(OH)_2 + CO_2 \xrightarrow{water} CaCO_3 + H_2O$
- $C_xS_yH_z + xCO_2 \xrightarrow{water} xCaCO_3 + (ySiO_2 \cdot tH_2O) + (x - t + z)H_2O$
- ...

This is a significant simplification of the actual chemical processes, as shown in Figure 3 for the $Ca(OH)_2$ reaction.

Consequences :
- Reduction in porosity
- Corrosion by carbonation
  - Decrease in pH
  - Depassivation of reinforcements
  - Potential corrosion of reinforcements

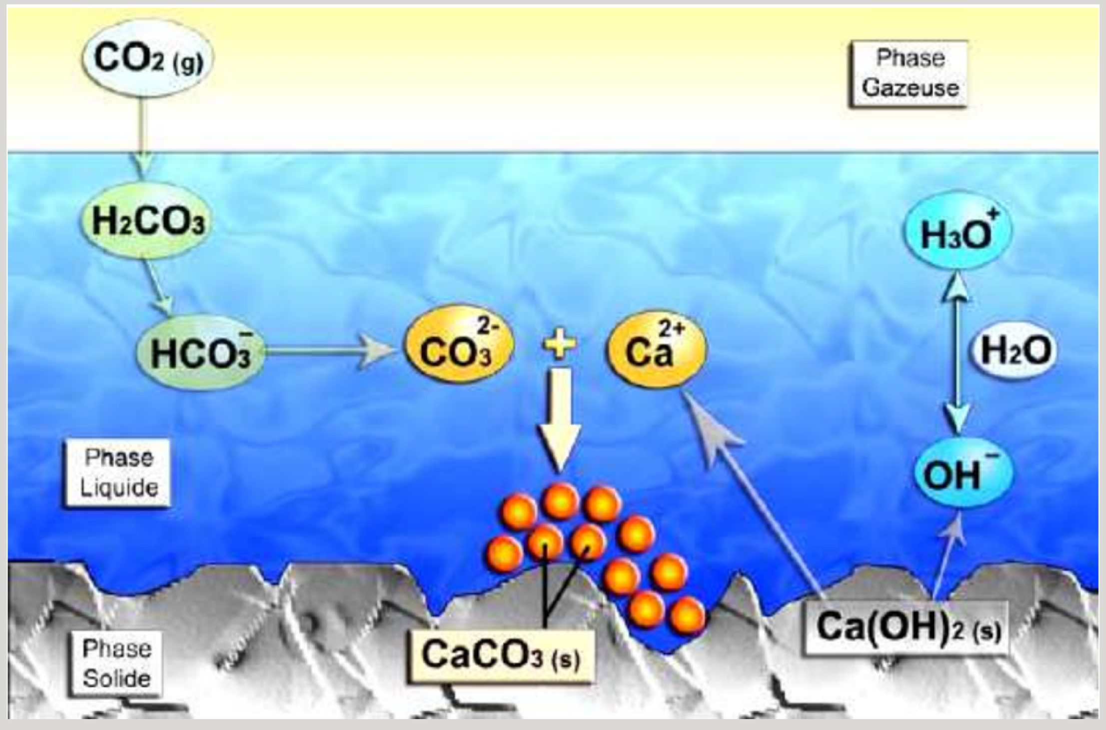


Figure 3: Carbonation mechanism of $Ca(OH)_2$ [2]

7. Numerical study

Goals :
1. Development of a macroscopic model
2. Development of the multi-scale model

1. Macroscopic model
- Model based on the work of Saetta [4]
- Focused solely on the reaction: $Ca(OH)_2 + CO_2 \xrightarrow{water} CaCO_3 + H_2O$
- Various simplifications applied

Validation of the macroscopic model
- Validation of CO_2 transport:
  - Pure diffusion ✓
  - Advection with some diffusion ✓
  - Advection–diffusion ✓
- Validation of the carbonation reaction ✓
- Coupled diffusion–carbonation reaction ✗

2. Multi-scale model
- Aims to overcome the limitations of the macroscopic approach (assumes a continuous medium)
- Captures material heterogeneities at the micro-scale (e.g., aggregates and mortar phases)
- Uses a Representative Volume Element (RVE) to establish the link between micro-scale behavior and macro-scale response

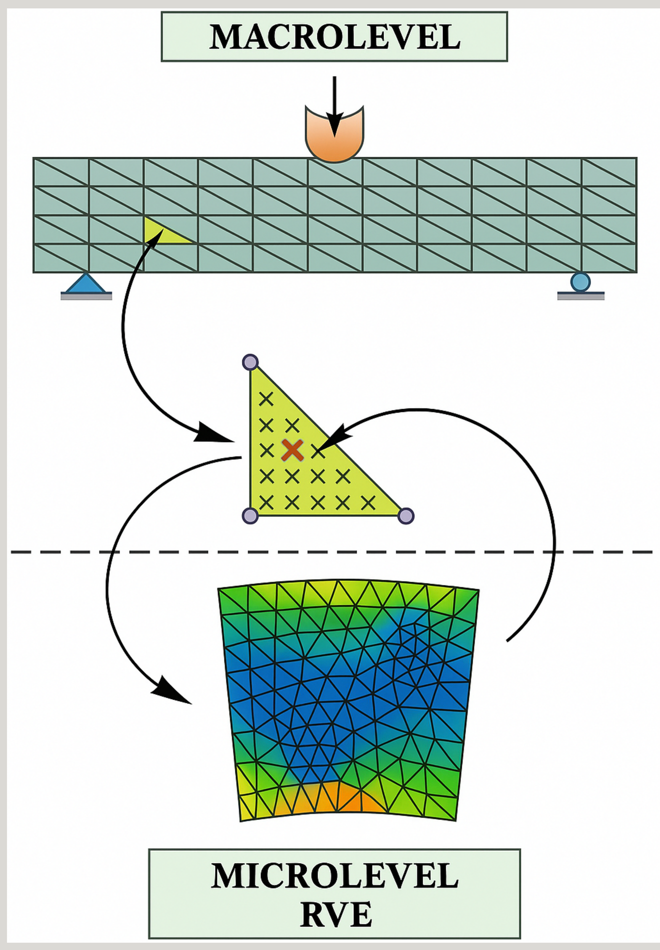


Figure 5: Illustration of a Multi-Scale Model

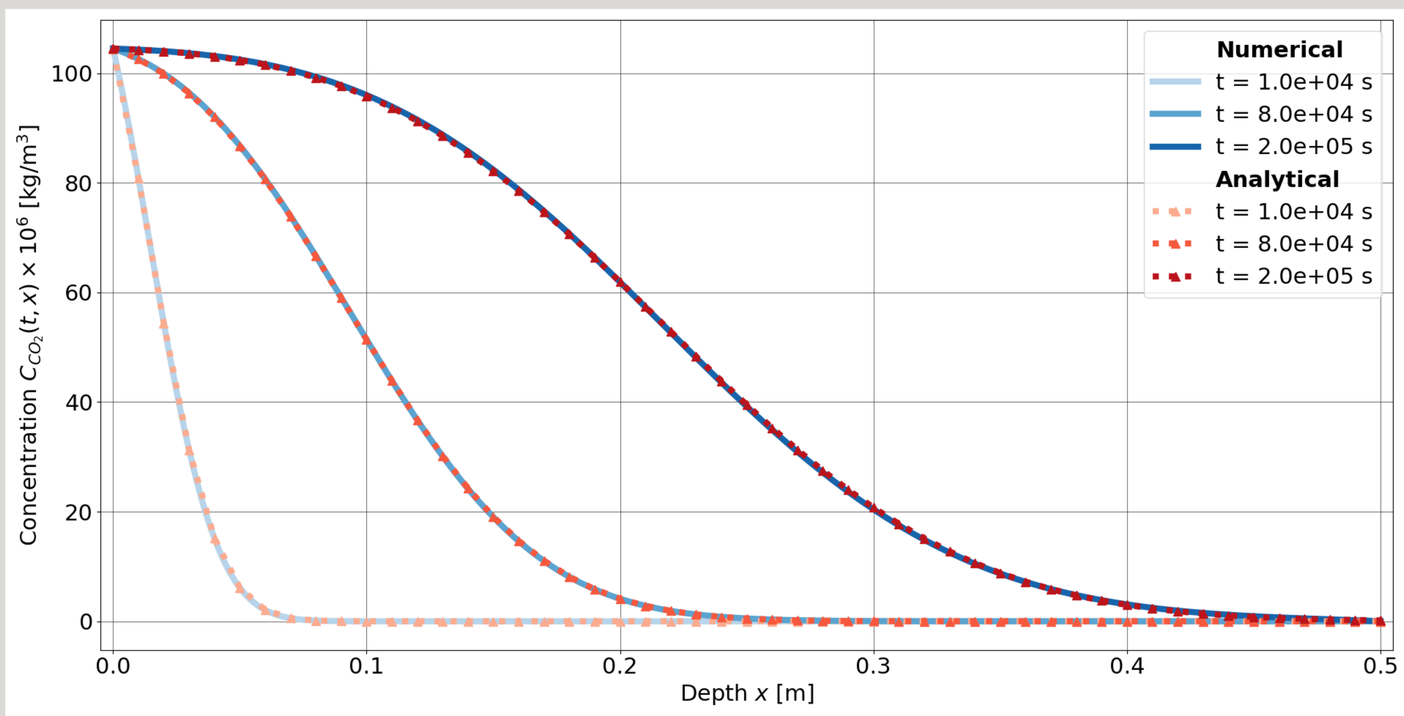


Figure 6: CO_2 profiles in diffusive–advective case

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EsPOIR – **E**co-friendly high **P**erformance c**O**ncrete for sustainable **I**nfrastructu**R**es

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