MODELLING STUDY OF CO_2 SEQUESTRATION BY MINERAL WASTE CARBONATION

Natalia Vidal de la Peña

PhD student from University of Liège

Promoters: Grégoire Léonard

Dominique Toye

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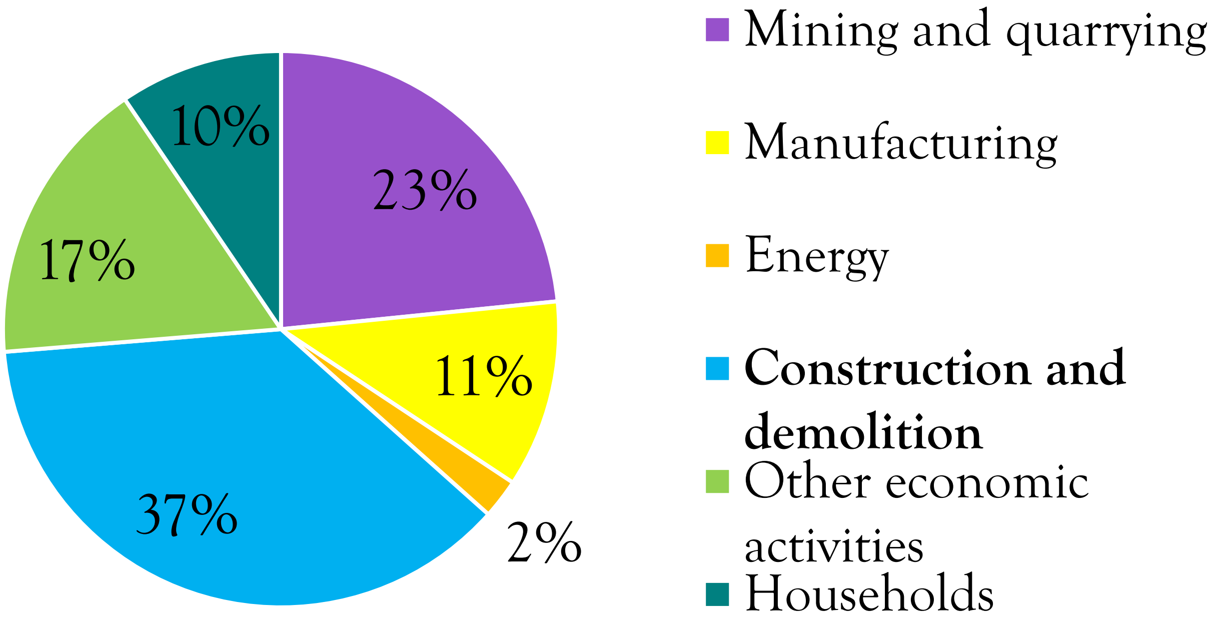
INTRODUCTION

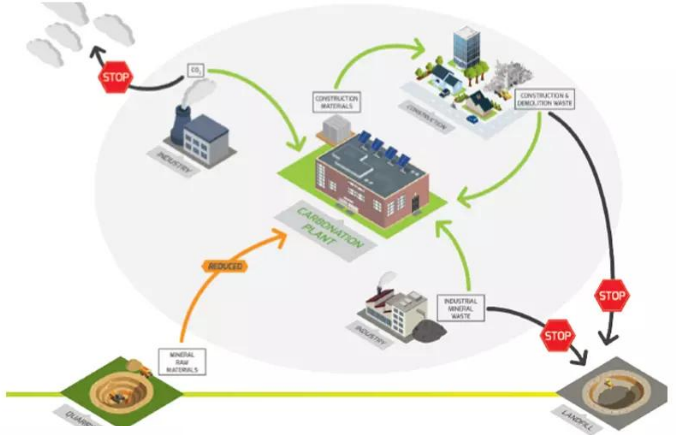
Waste generation by economic activities and households in Europe 2020



N. Vidal de la Peña, S. Grigolleto, D.Toye, L.Courard, G.Léonard, 2023, CO2 Capture by mineral carbonation of construction and industrial wastes, in Circular Economy Processes for CO2 Capture and Utilization: Strategies and case studies, Editor: Baena-Moreno, F.M. et al. Cambridge, MA: Woodhead Publishing, Pages 163-185

Mineral Loop Project

- Transformation of mineral wastes-by-products into higher value-added products
- Circular economy of construction wastes

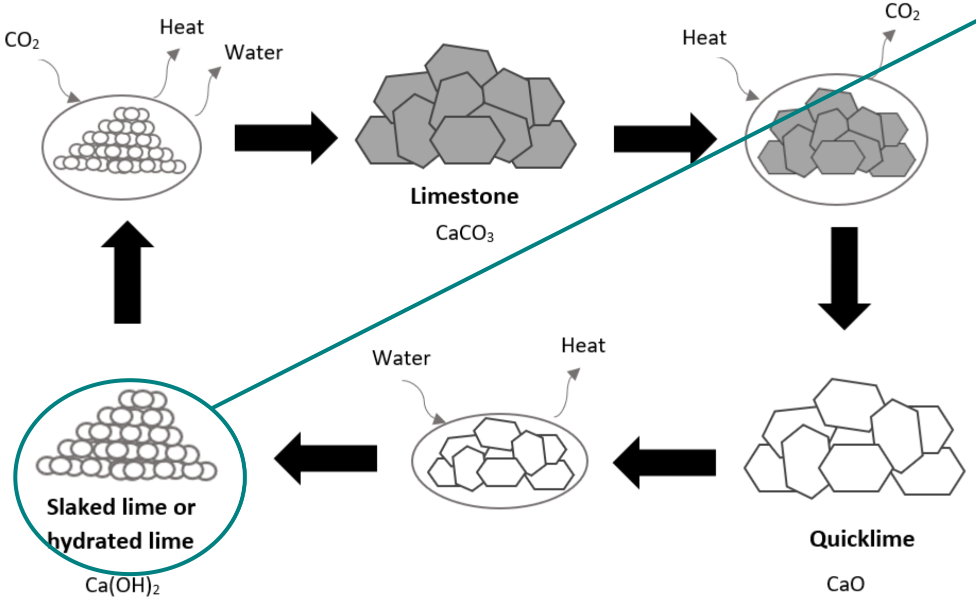


Wallonie
PEPs PRODUCTS, ENVIRONMENT, AND PROCESSES
LESSINE TAILORED BULK TECHNOLOGIES
CTP member of EMRA
CARMEUSE
REVATECH
Tradecowall

https://www.carmeuse.com/eu-en/mineral-loop

CO_2 CAPTURE BY MINERAL CARBONATION BY USING CONSTRUCTION WASTE

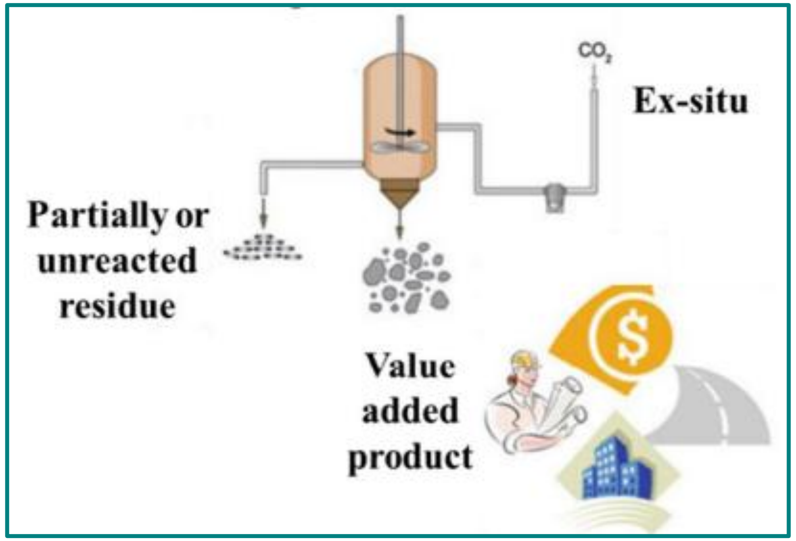
Lime production cycle



Direct carbonation

Gas-solid carbonation of hydrated lime

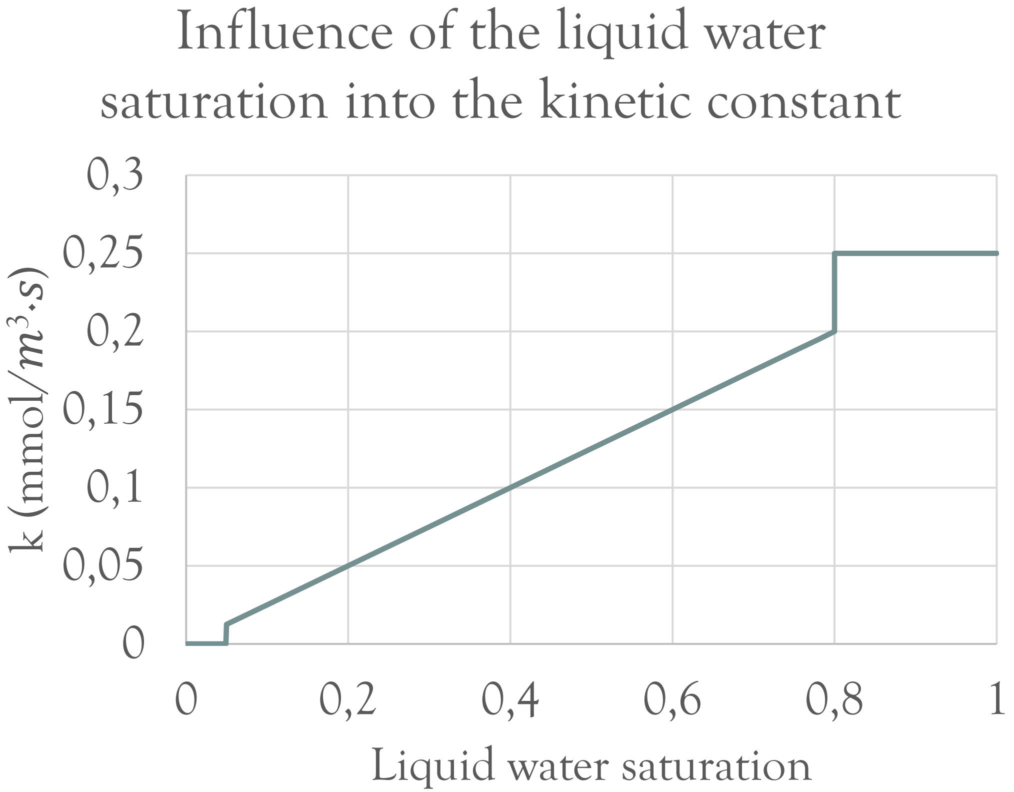
$$Ca(OH)_2 + CO_2 \Rightarrow CaCO_3 + H_2O$$



Puthiya Veetil, Sanoopkumar & Hitch, Michael. (2021). Aqueous mineral carbonation of ultramafic material: a pre-requisite to integrate into mineral extraction and tailings management operation. Environmental Science and Pollution Research. 28. 1-14. 10.1007/s11356-021-12481-0.

COUPLING BETWEEN CHEMICAL REACTIONS AND TRANSFER PHENOMENA

- **Chemical reaction:** $Ca(OH)_2$ carbonation = f(liquid water saturation)



COUPLING BETWEEN CHEMICAL REACTIONS AND TRANSFER PHENOMENA

- **Physical interactions:** CO_2 diffusion between the particles and inside the particles = f(porosity, liquid water saturation)

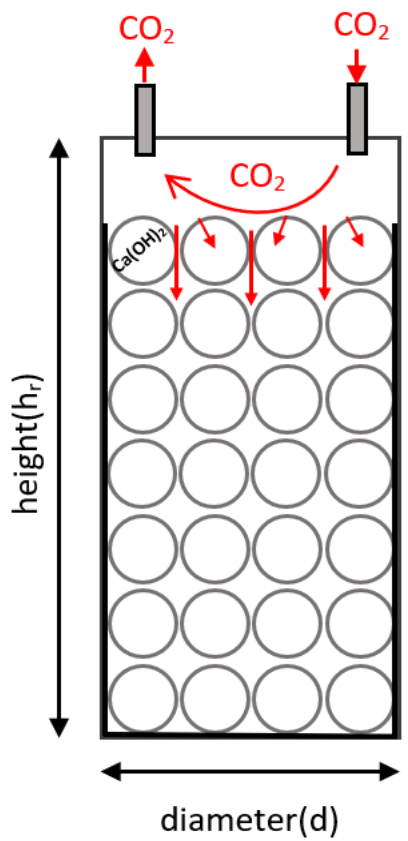
  - **Diffusion between the particles**

    $$\mathbb{D} = D_{CO_2,0} \cdot \varepsilon_{bed}^{4/3} \cdot (1 - sl_{bed})^{10/3}$$

  - **Diffusion inside the particles**

    $$D_{eff} = D_{CO_2,0} \cdot \varepsilon_{pellet}^{2,7} \cdot \left(1 - sl_{pellet}\right)^{4,2}$$

Where: $D_{CO_2,0}$ is the specific diffusion coefficient of CO_2 (1.6E-5m^2/s)



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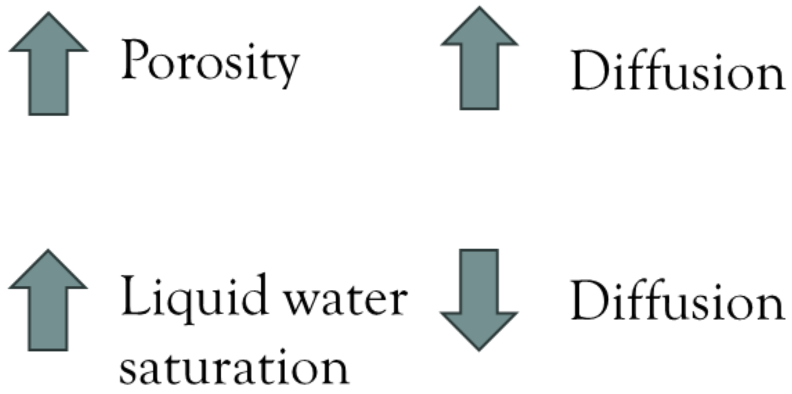

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COUPLING BETWEEN CHEMICAL REACTIONS AND TRANSFER PHENOMENA

- **Variation of the liquid water saturation during the carbonation process**

$Ca(OH)_2 + CO_2 \Rightarrow CaCO_3 + H_2O$ Initial water-to-solid ratio ($w_{CHt,0}$)

- **Variation of pellet porosity during the carbonation process = f(carbonation rate, volume change)**

$$\varepsilon_{pellet}(t) = \varepsilon_0 \cdot \left((1-\eta) + \eta \cdot \frac{\rho_{CaCO_3} \cdot Mm_{Ca(OH)_2}}{\rho_{Ca(OH)_2} \cdot Mm_{CaCO_3}} \right)$$

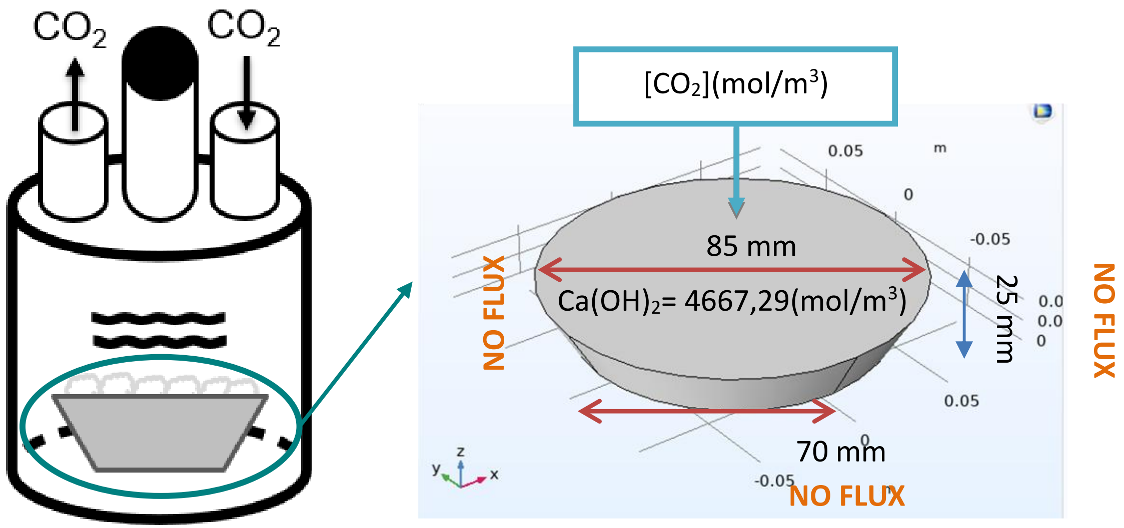
→ Volume change

$$Carbonation\ rate\ (\eta) = \frac{[CaCO_3]}{[Ca(OH)_2]_{t0}}$$

MODEL DESCRIPTION

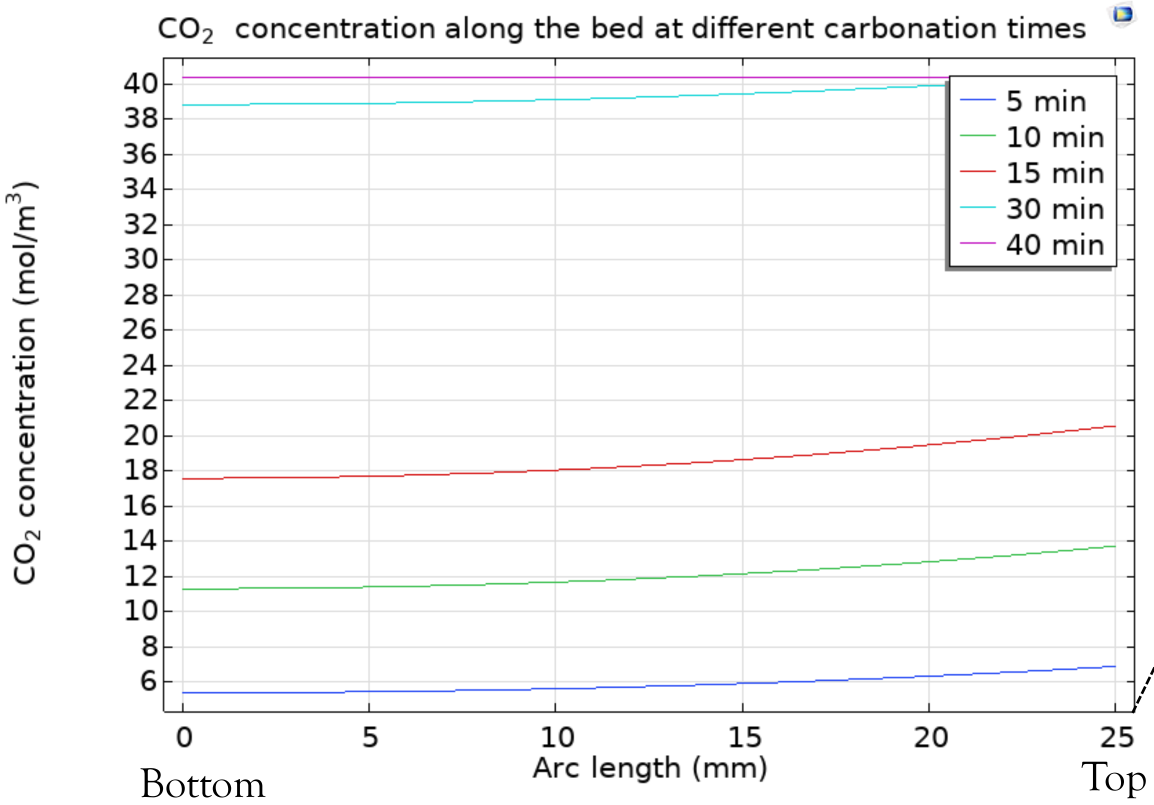
Assumptions

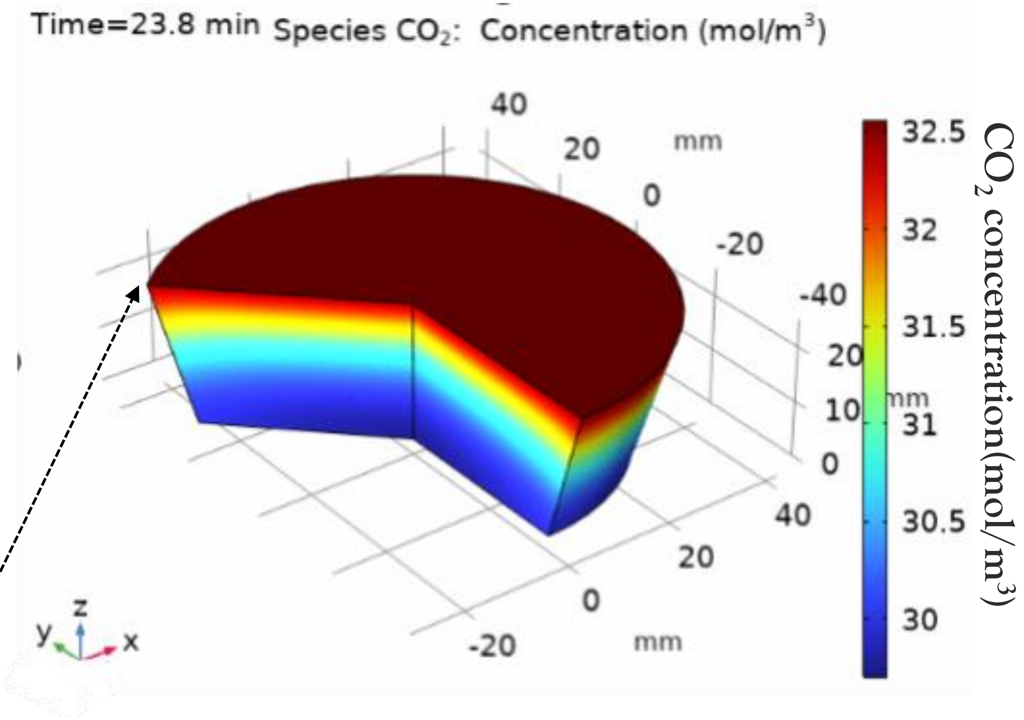
- Bed porosity= 0.69
- Pellet porosity= 0.12
- Temporal evolution of the CO_2 concentration in the enclosure
- CO_2 flow rate= 200 (ml/min)
- Particle radius= 1 mm
- Initial water-to-solid ratio(w_{CH})= 0.2



SIMULATION RESULTS

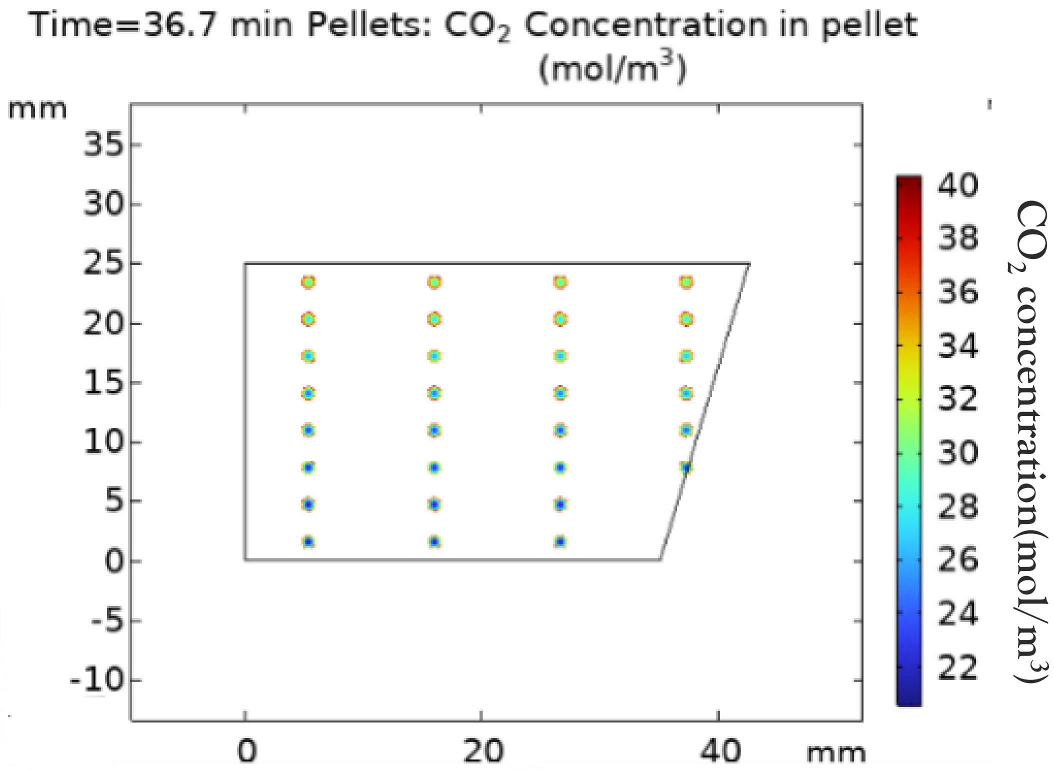
CO_2 concentration profile-Granular bed

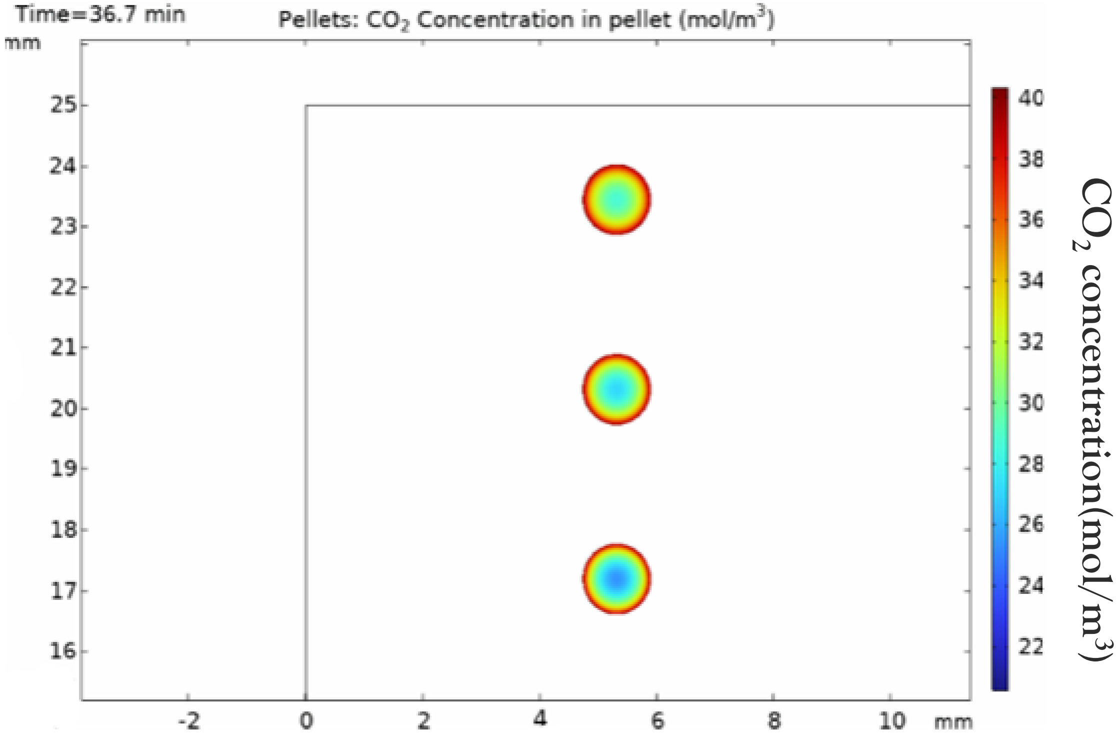




SIMULATION RESULTS

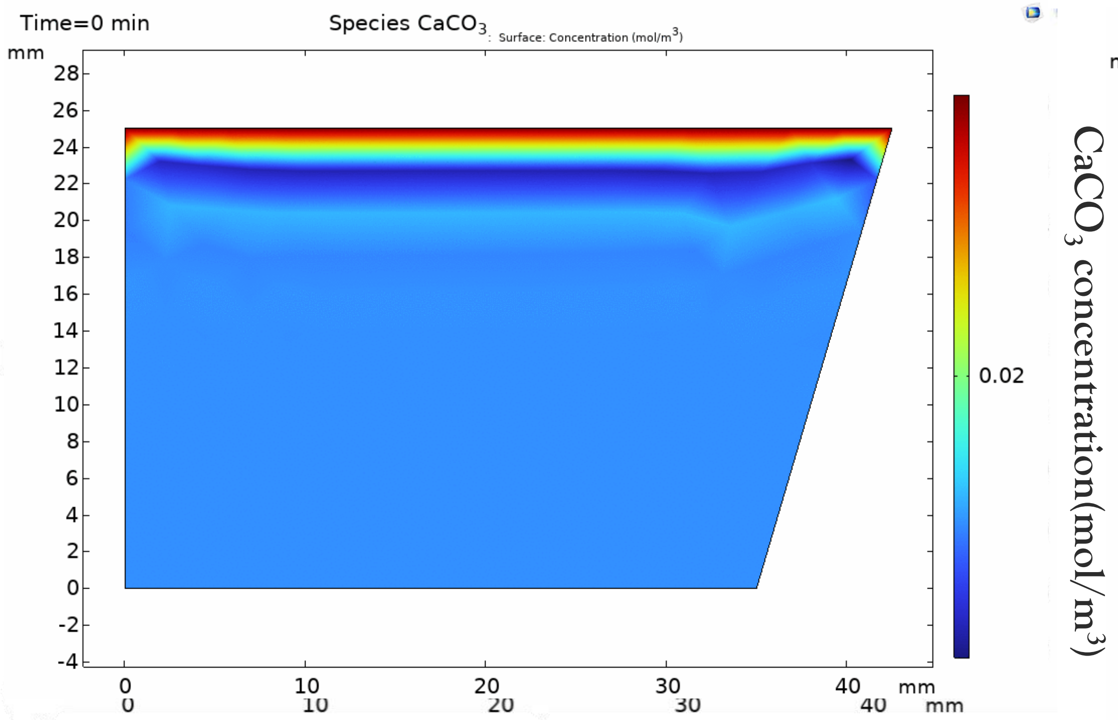
CO_2 concentration profile-Pellets

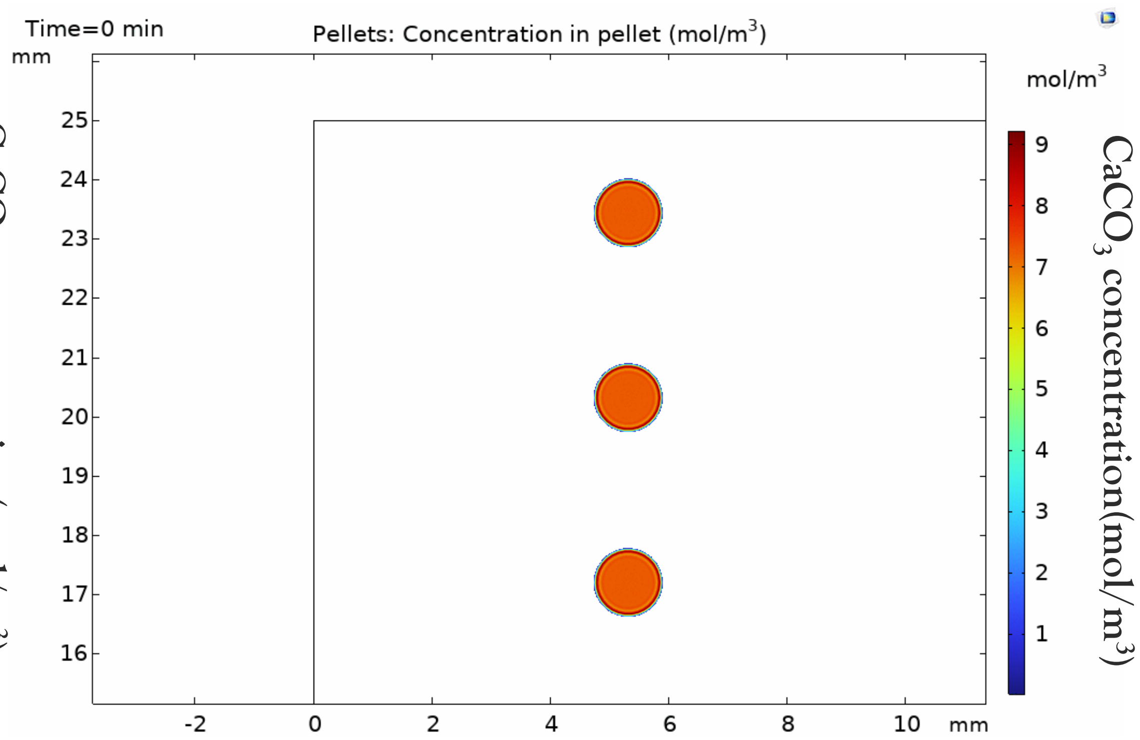




SIMULATION RESULTS

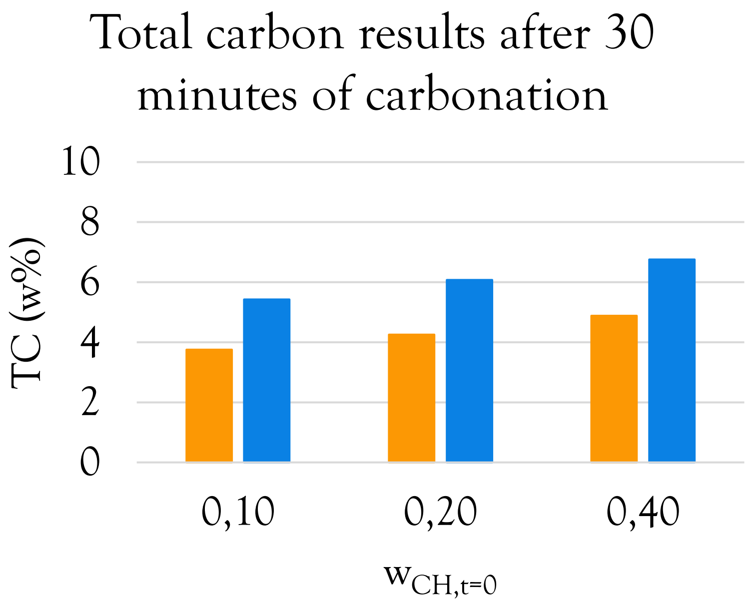
$CaCO_3$ concentration profiles

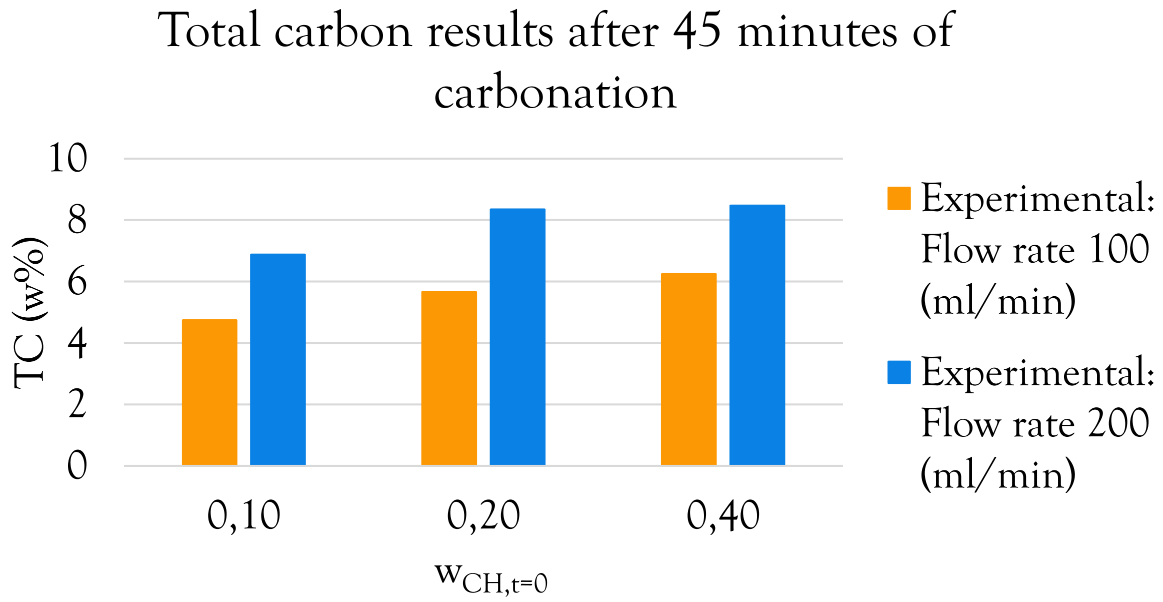




EXPERIMENTAL RESULTS

- Pellet porosity of 10% with a particle diameter of 35.5 µm
- Bed porosity equal to 68%→Reaction mostly between the particles
- Parameter evaluated: total carbon (TC)

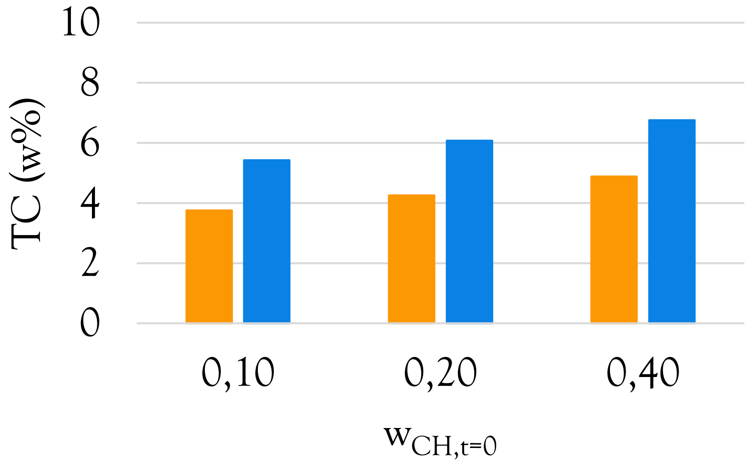




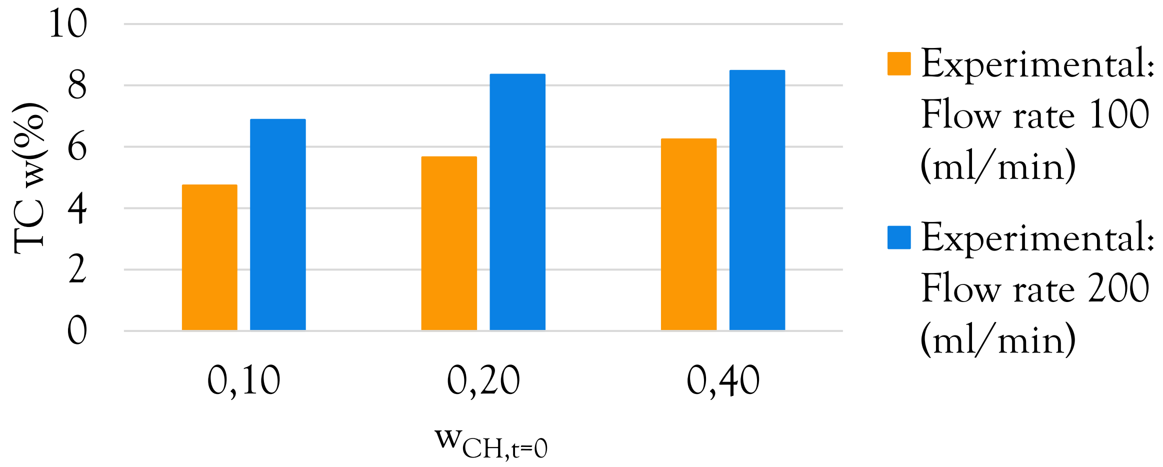
EXPERIMENTAL RESULTS

- Influence of Flow rate: ↑ Flow rate ↑ Total carbon
- Influence of initial water-to-solid ratio: ↑ $w_{CH,t=0}$ ↑ Total carbon → Optimal value between 0,2 and 0,4

Total carbon results after 30 minutes of carbonation



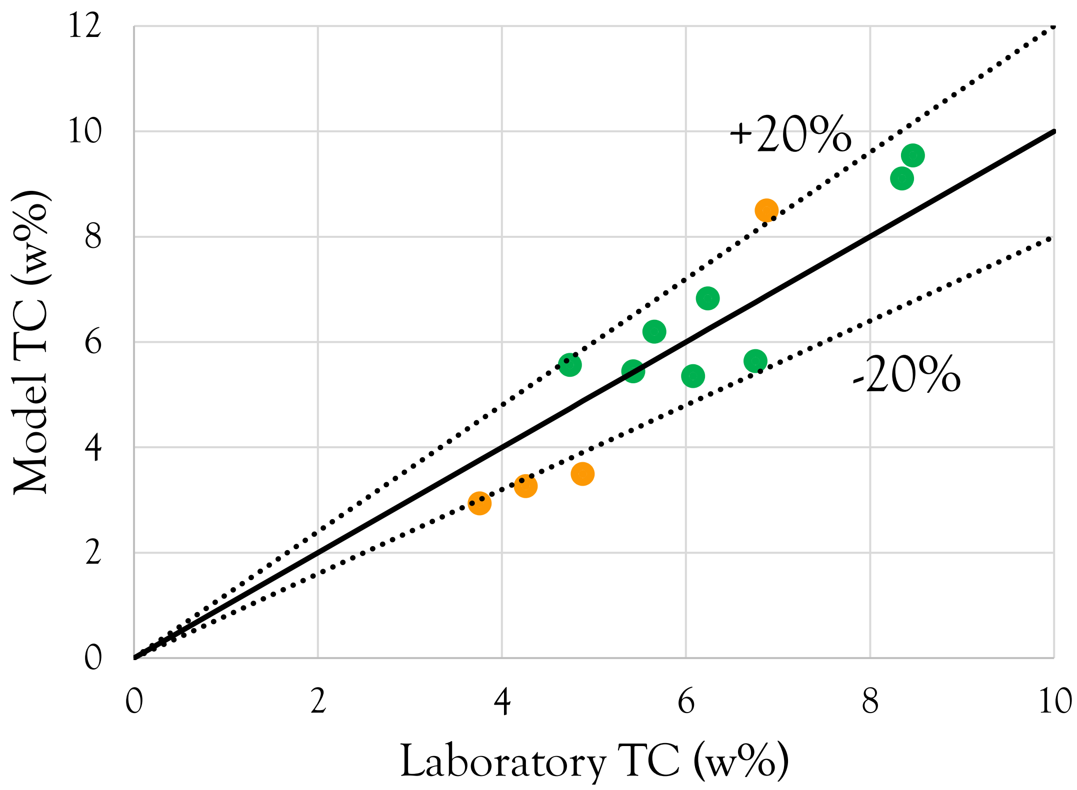
Total carbon results after 45 minutes of carbonation



MODEL VALIDATION

- Pellet porosity of 10%
- Particle diameter of 35.5 µm
- Bed porosity of 68%

=>Successful validation



CONCLUSIONS

- Physical parameters influence the system and evolve with time
  - Porosity →Enhances the diffusion of the gas
  - Liquid water saturation→ Enhances the reaction but slows the diffusion of CO_2
- Process parameters influence the carbonation
  - Carbon dioxide flow rate→ The higher the CO_2 flow rate, the more carbonation
  - Initial water-to-solid ratio→ Optimal value between 0.2 and 0.4
- COMSOL Multiphysics dual-scale model able to represent the carbonation process of hydrated lime

PERSPECTIVES

- Contribution to the circular economy of the construction sector
- Application of the model to predict the behavior of more complex materials, such as recycled concrete aggregates
- Optimization of operational conditions on a larger scale

THANK YOU SO MUCH

COUPLING BETWEEN CHEMICAL REACTIONS AND TRANSFER PHENOMENA

- **Variation of the liquid water saturation during the carbonation process**

$$sl_{bed,pellet} = \frac{[H_2O]\left(\frac{mol}{m^3}\right) \cdot MM_{H_2O}\ \left(\frac{g}{mol}\right)}{\rho_{H_2O} \cdot \varepsilon_{bed,pellet}}$$

- **Variation of pellet porosity during the carbonation process**

$$\varepsilon_{pellet}(t) = \varepsilon_0 \cdot \left((1-\eta) \quad + \frac{\eta \cdot \quad \rho_{CaCO_3} \cdot Mm_{Ca(OH)_2}}{\rho_{Ca(OH)_2} \cdot Mm_{CaCO_3}} \right)$$

$$Carbonation\ rate\ (\eta) = \frac{[CaCO_3]}{[Ca(OH)_2]_{t0}}$$

COUPLING BETWEEN CHEMICAL REACTIONS AND TRANSFER PHENOMENA

- **Variation of bed porosity during the carbonation process**

$$\varepsilon_{bed}(t) = \varepsilon_0 + 4 \cdot 10^{-6}\ (m^3/mol) * ([Ca(OH)_2]_{t,0} - [Ca(OH)_2](t))$$