A MATHEMATICAL MODEL FOR CO_2 CAPTURE VIA MINERAL CARBONATION USING HYDRATED LIME

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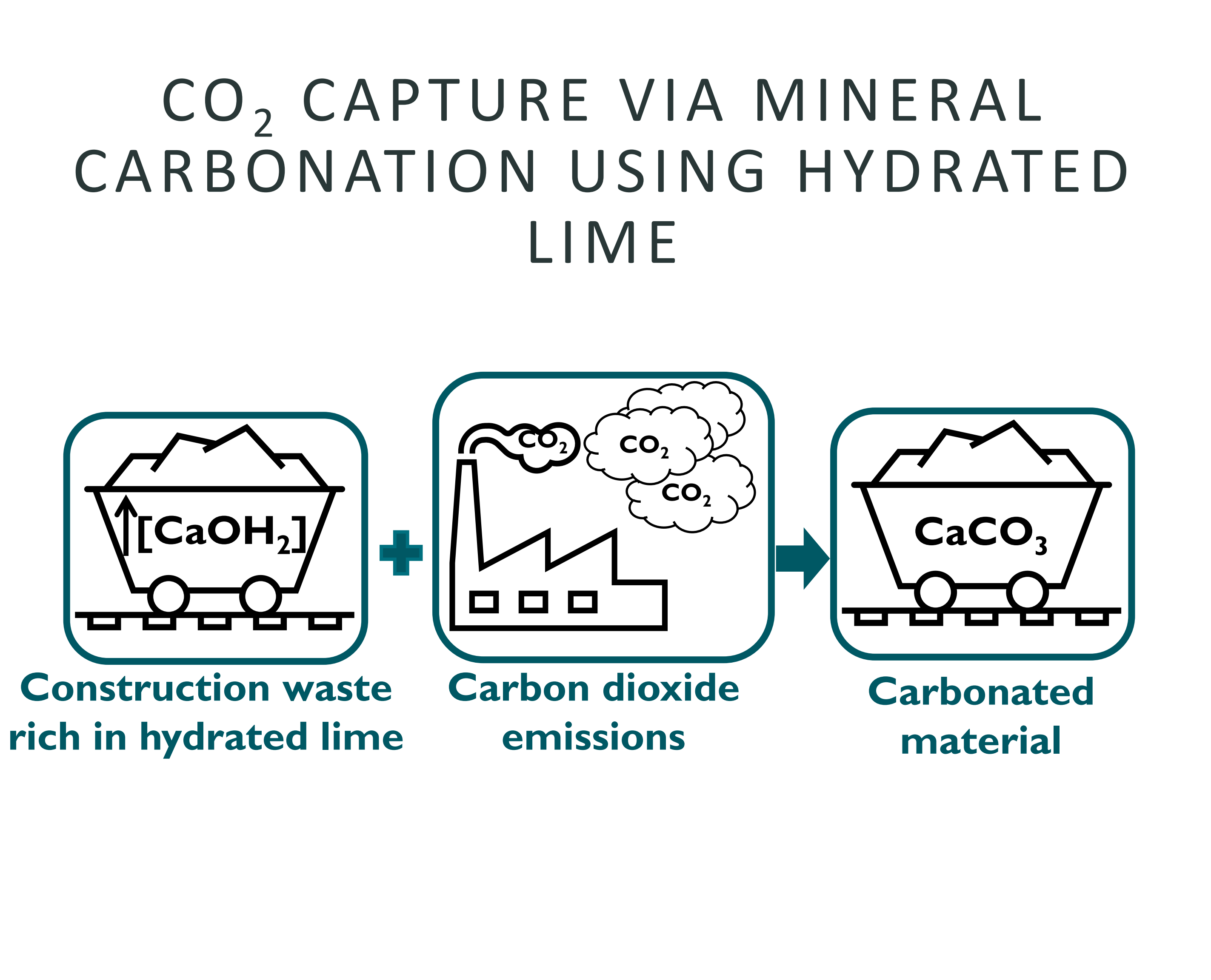
Mineral Loop Project

Work package objectives



Static Carbonation Model

- Explanation and simulation of the static carbonation process
- Characterization of key phenomena: reaction, diffusion, evaporation, heat transfer
- Optimization of operating parameters (e.g., CO_2 flow rate)

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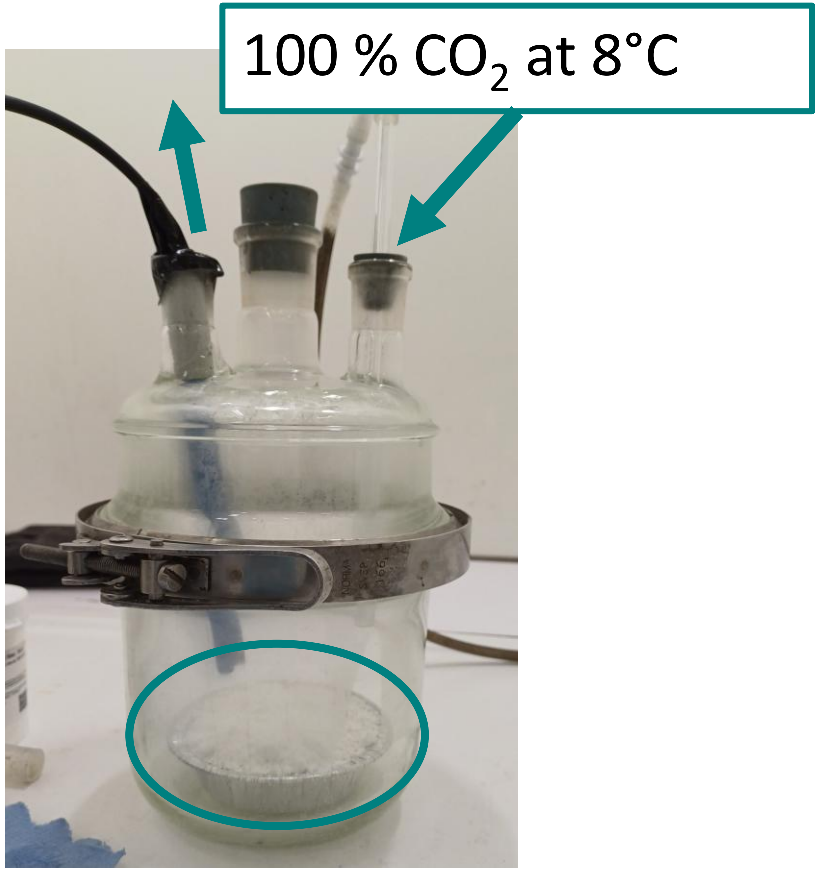
N. Vidal de la Peña, S. Grigolleto, D.Toye, L.Courard, G.Léonard, 2023, CO2 Capture by mineral carbonation of construction and industrial wastes, in Circular Economy Processes for CO2 Capture and Utilization: Strategies and case studies, Editor: Baena-Moreno, F.M. et al. Cambridge, MA: Woodhead Publishing,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

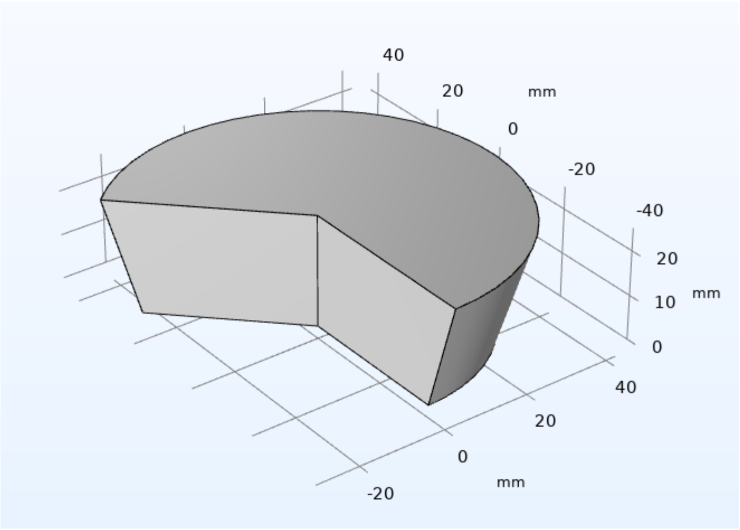
https://www.carmeuse.com/eu-en/mineral-loop

CARBONATION EXPERIMENTAL SETUP & METHODOLOGY

- $Ca(OH)_2(s) + CO_2(g) \Rightarrow CaCO_3(s) + H_2O(l)$
- Humidification of $Ca(OH)_2$
  - Initial water-to-solid ratio:
  - w_0 ($g_{H_2O}/g_{Ca(OH)_2}$)
- Static carbonation:
  - No convection through the material



PRINCIPLES OF THE PROPOSED MATHEMATICAL MODEL



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Reaction kinetics	• Dependent on the **liquid water saturation level** (**S_b**) in the material
Diffusion mechanism	• Governed by **porosity (ϕ)**, **liquid water saturation** and **temperature**
Heat transfer	• **Exothermic** reaction • Heat transfer by **convection**, **conduction** and **radiation** • **Evaporation**

PRINCIPLES OF THE PROPOSED MATHEMATICAL MODEL

- **Diffusion Mechanism:** CO_2 diffusion along the granular bed

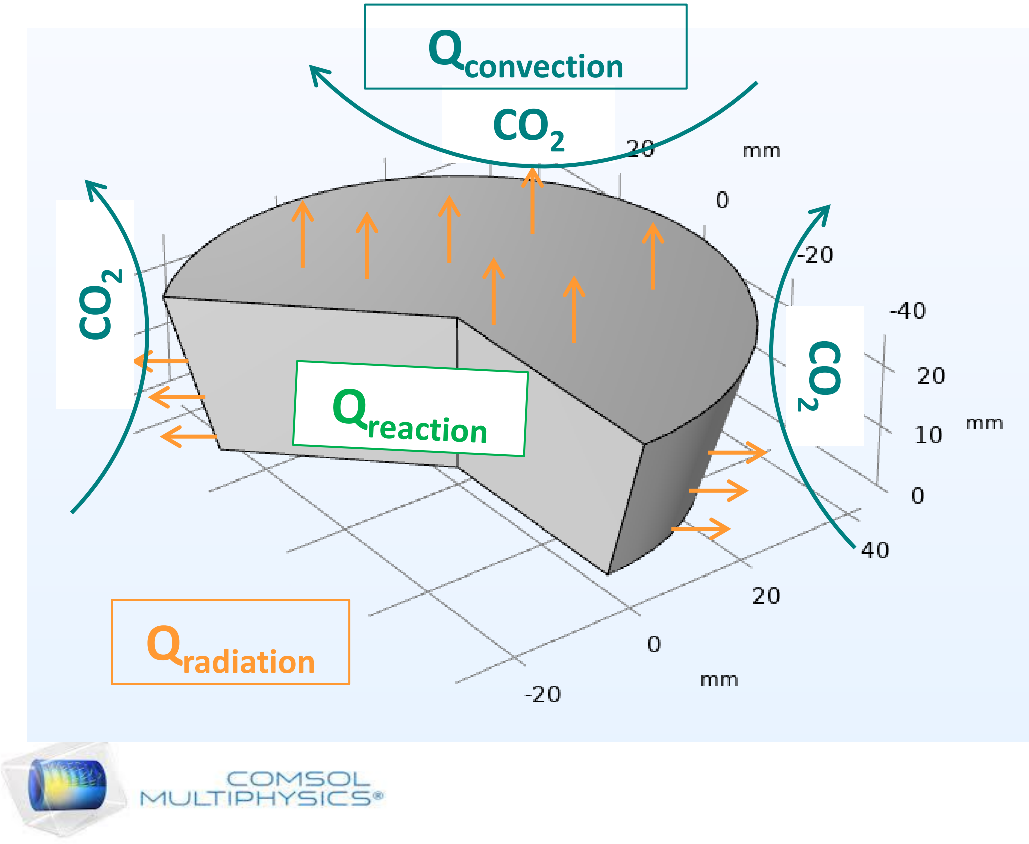
$$\mathbb{D} = D_{CO_2,0} \cdot \phi_{bed}^{4/3} \cdot (1 - S_{bed})^{10/3} \cdot \left(\frac{T}{T_{ref}}\right)^{1.75}$$

↑ Porosity ↑ Diffusion

↑ Liquid water saturation ↓ Diffusion

PRINCIPLES OF THE PROPOSED MATHEMATICAL MODEL

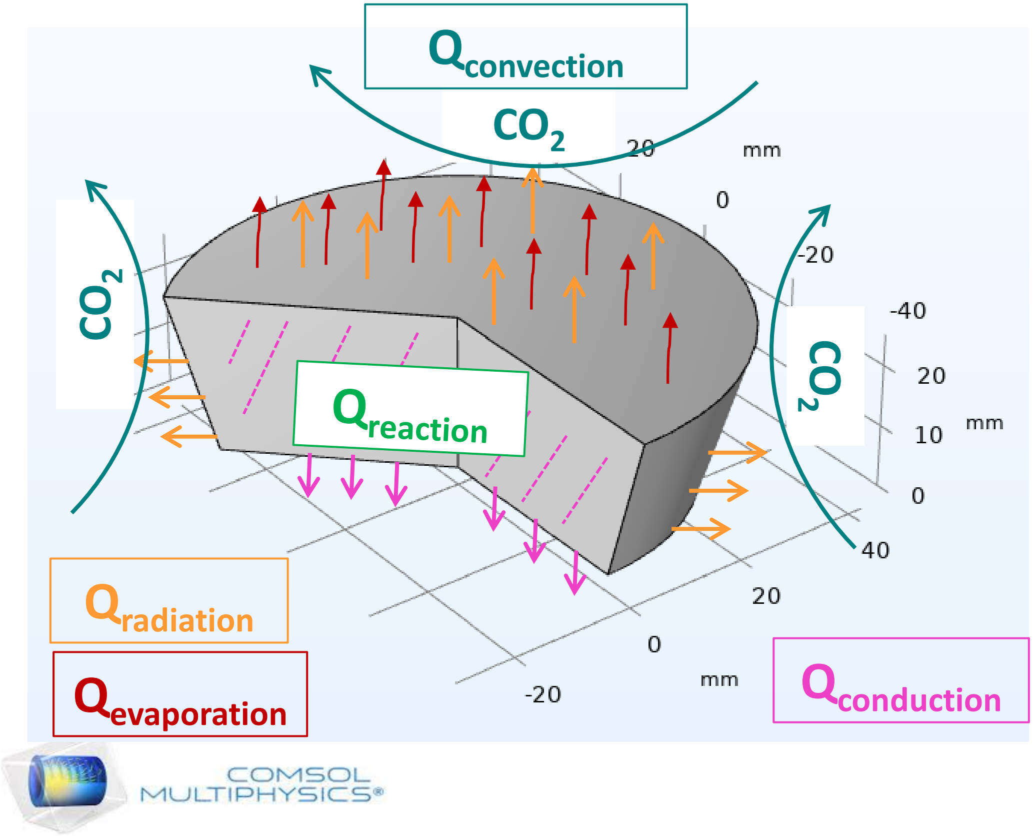
- **Heat Transfer**



- **Exothermic reaction**: ΔH = -107 kJ/mol
- **Convection**:
  - $h_{surface}$ = 3.7 W/(m^{2}K)
  - h_{wallAl} = 5.52 W/(m^2 K)
  - T_{fluid} = 13.5°C
- **Radiation:**
  - **from aluminium walls and solid**

PRINCIPLES OF THE PROPOSED MATHEMATICAL MODEL

- **Heat Transfer**



- **Evaporation:**
  - Saturation conditions at the surface
- **Conduction:**
  - Heat transfer in porous media
    → equivalent thermal conductivity
  - Conduction through two different layers
    - Aluminum
    - Pyrex glass

SIMULATION AND VALIDATION RESULTS

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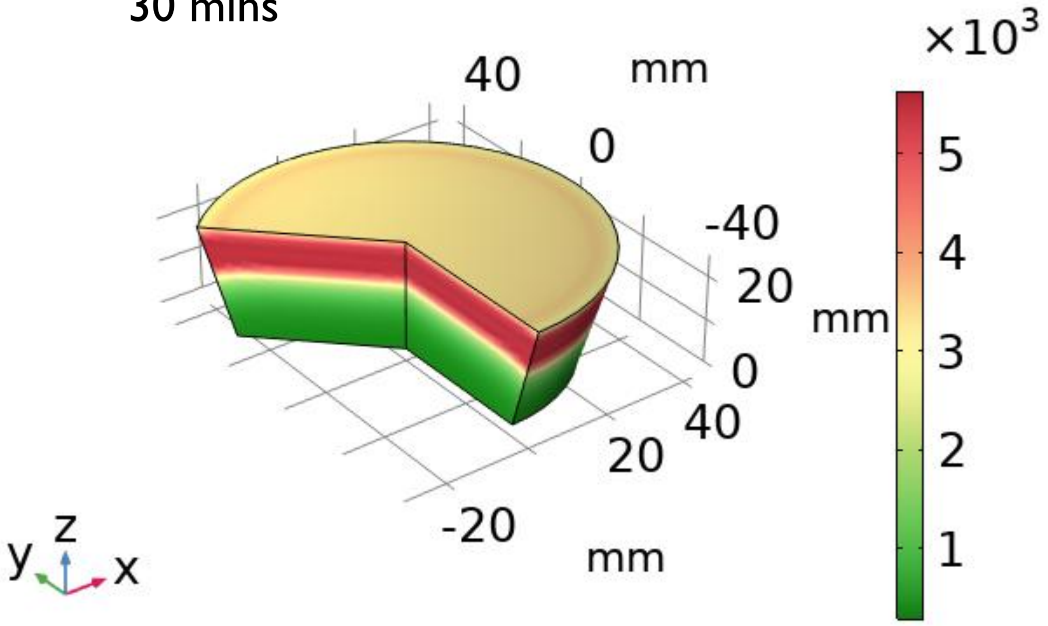
$CaCO_3$ concentration profile (mol/m³)

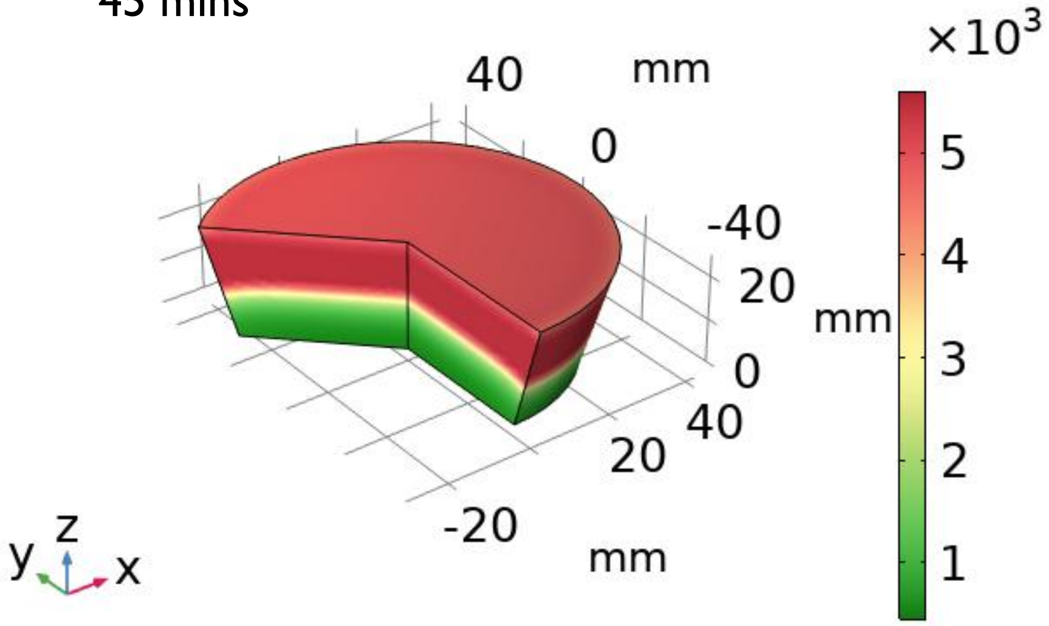
W_0 = 0.3 ($g_{H_2O}/g_{Ca(OH)_2}$)

CO_2 flow rate of 200 ml/min

30 mins



45 mins

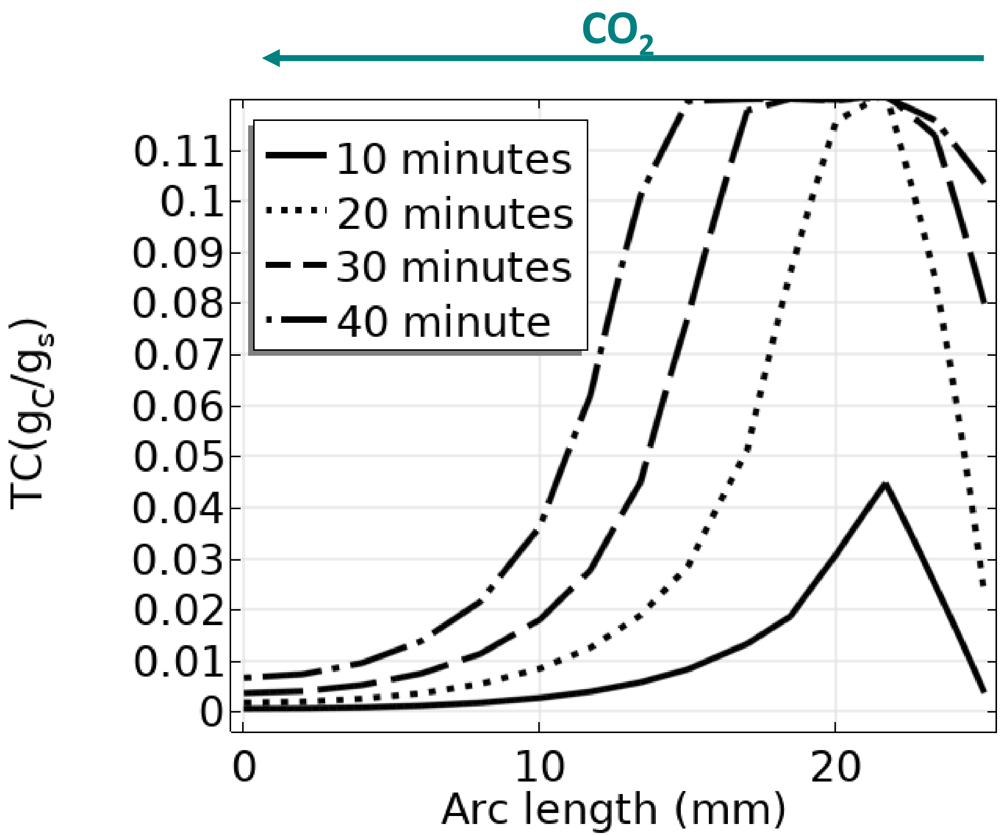


SIMULATION AND VALIDATION RESULTS

Total carbon (TC) at different carbonation times

$W_0 = 0.3\ (g_{H_2O}/g_{Ca(OH)_2})$

CO_2 flow rate of 200 ml/min



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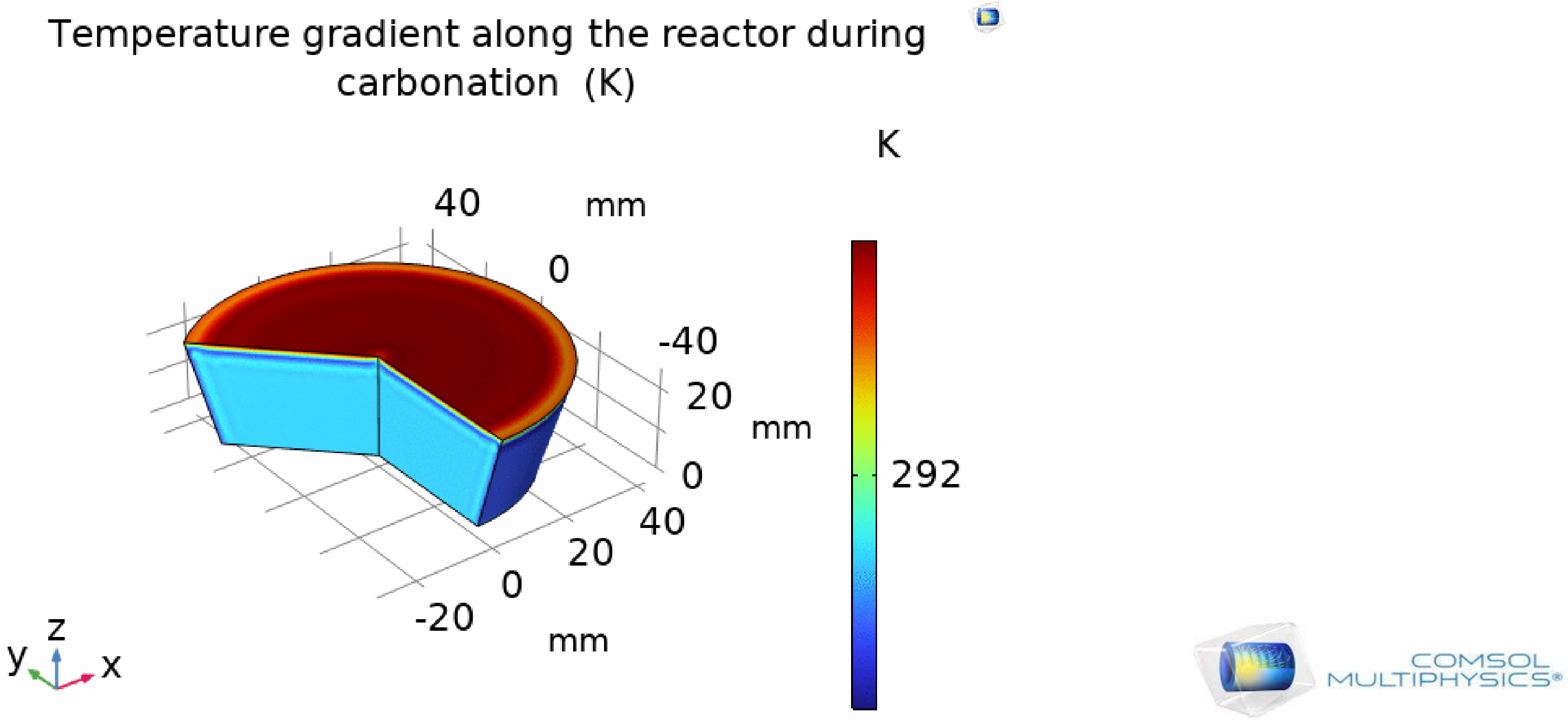
SIMULATION AND VALIDATION RESULTS

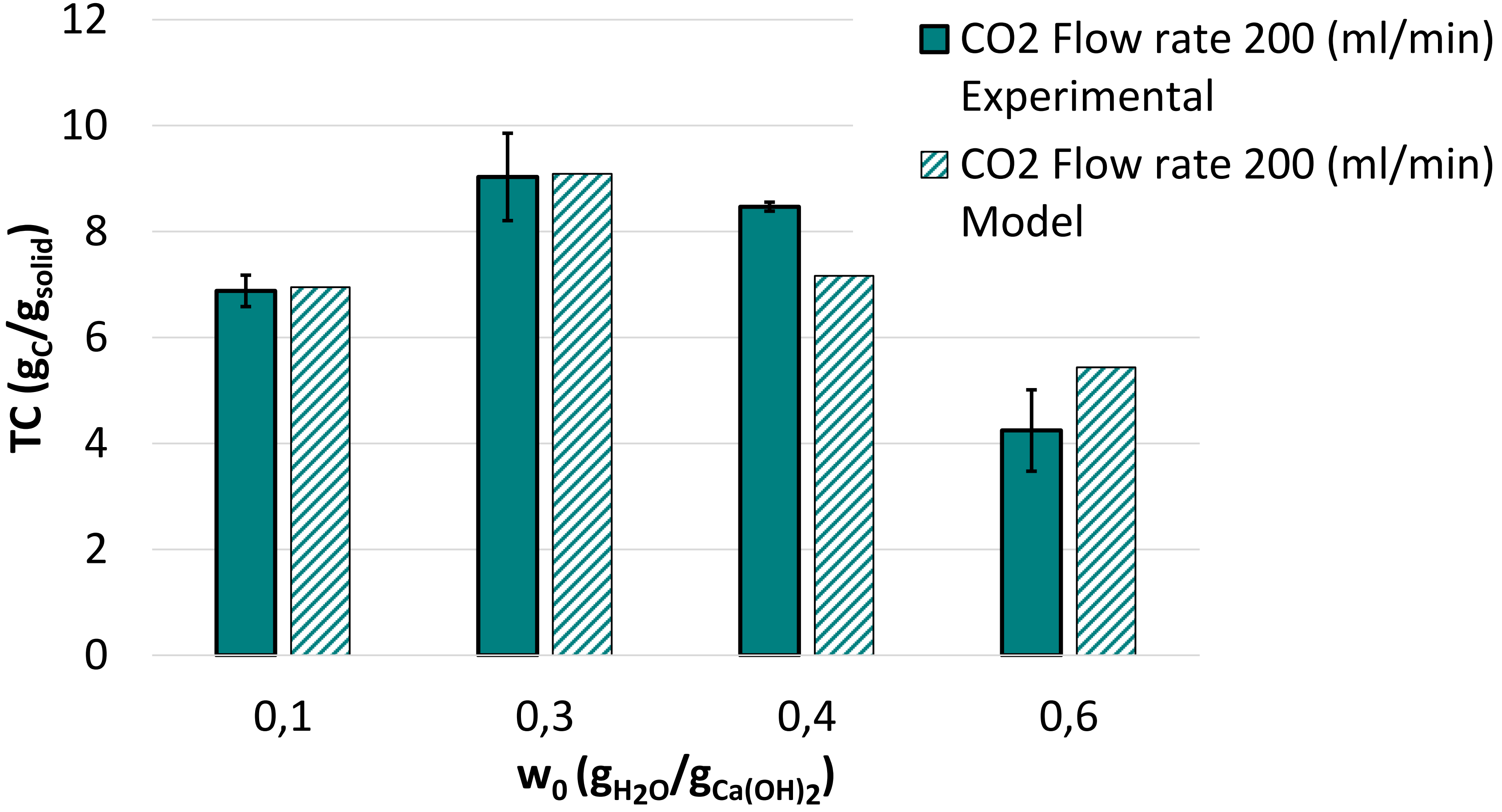
Temperature gradient for 45 minutes (K)

$W_0 = 0.3\ (g_{H_2O}/g_{Ca(OH)_2})$

CO_2 flow rate of 200 ml/min



SIMULATION AND VALIDATION RESULTS



CONCLUSIONS

- **Validated comprehensive multiphysics model** capturing the full complexity of carbonation
  - Reaction kinetics
  - Diffusion
  - Heat balance
- **Key insights** delivered: **carbonation degree** and **carbonation front**
- **Process optimization** through control of **reactor design**, **CO_2 temperature**, and **water-to-solid ratio**
  - Optimization of operational conditions on a larger scale
- **Versatile tool** extendable to other hydrated lime–based materials
  - Over-limed sewage sludge
- Contribution to the **circular economy** of the **construction sector**

THANK YOU SO MUCH

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